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FAST ITERATIVE METHODS FOR DISCRETE-ORDINATES PARTICLE TRANSPORT CALCULATIONS

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ABSTRACT

In discrete-ordinates (S_N) simulations of large problems involving linear interactions between radiation and matter, the underlying linear Boltzmann problem is discretized and the resulting system of algebraic equations is solved iteratively. If the physical system contains subregions that are optically thick with small absorption, the simplest iterative process, Source Iteration, is inefficient and costly. During the past 40 years, significant progress has been achieved in the development of *acceleration* methods that speed up the iterative convergence of these problems. This progress consists of (*i*) a theory to derive the acceleration strategies, (*ii*) a theory to predict the convergence properties of the new strategies, and (*iii*) the implementation of these concepts in production computer codes. In this Review we discuss the theoretical foundations of this work, the important results that have been accomplished, and remaining open questions. © 2002 Published by Elsevier Science Ltd.

Keywords: discrete ordinates; transport; iteration; acceleration

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I. INTRODUCTION

I.A. Overview

One of the most challenging tasks in computational physics is to simulate, accurately and efficiently, the interaction of radiation with matter (*particle transport* or *radiation transport* processes). In this Review we discuss computational aspects of transport processes in which the "rarefied" particles (neutrons, photons, electrons, etc.) interact directly with the "dense" atoms of the background material, but not with each other. Such transport processes are usually described by a linear Boltzmann equation [1, 3, 4, 5, 9, 10, 14], but certain nonlinearities can occur – for example, through the temperature-dependence of the material cross sections or opacities [97].

Most numerical algorithms for the linear Boltzmann equation are *stochastic* (Monte Carlo) or *deterministic* in nature. Deterministic algorithms have the following features:

1. The linear Boltzmann equation is discretized into a (typically) large system of linear algebraic equations. (This discretization process should be as accurate and algebraically simple as possible.)
2. The resulting discrete system of equations is solved. (Because of the system's typically large size, direct solution methods are impractical; iterative methods must be used. The best iterative methods are unconditionally and rapidly convergent.)

Each of these two steps is fraught with difficulties. This Review is concerned with step 2: the development of efficient iterative methods for solving deterministic transport problems in which the *angular* (direction-of-flight) variable is discretized using the discrete-ordinates (S_N) approximation. We do not discuss iterative methods for other angular discretizations, such as the spherical harmonics or P_N approximation, which possess different mathematical properties and difficulties.

The development of efficient iteration schemes for S_N problems has been carried out by many researchers since the early 1960's and has led to dramatic theoretical and practical successes. In the present day, it is almost unthinkable to write a large-scale S_N particle transport code that does not employ a reasonably efficient iterative method. Nevertheless, the development of such methods is not easy, and significant difficulties remain. For example, some iterative methods require the solution of differential equations whose discretizations must be carefully matched to that of the transport scheme, and the spatial grid. Also, recent research has led to more sophisticated (sometimes nonlinear) S_N spatial discretizations on more complicated (sometimes unstructured) grids. These new discretizations have

driven the search for new strategies to provide efficient and robust iterative convergence. In this Review we discuss the basic iterative concepts, the mathematical techniques to analyze iteration schemes, and the current overall state of affairs.

First, we describe why the development of accurate and robust transport discretization methods (step 1 above) remains an active area of research:

1. The solution of a general-geometry radiation transport problem is a function of seven independent variables: three spatial variables (x, y, and z), two *angular* or direction-of-flight variables (μ = cosine of the polar angle, γ = azimuthal angle); one energy variable (E), and one time variable (t). To illustrate why this can be problematic, suppose that each variable is discretized on a grid consisting of 10^N points; one obtains a discrete problem with 10^{7N} unknowns! Clearly, the sheer number of algebraic unknowns can be immense, even in problems having a modest grid for each independent variable. This imposes severe demands on computer processors and memory.
2. The solution of the linear Boltzmann equation is typically not a smooth function of its spatial and angular variables. *Shadow singularities* often exist, across which the solution or its derivatives are discontinuous [45]. These singularities degrade the accuracy of deterministic methods, which often require smoothness of the exact solution to provide accurate approximations.
3. In void-like regions of a physical system, the linear Boltzmann equation behaves like a hyperbolic wave equation; in optically thick, highly scattering regions it behaves like an elliptic (steady-state) or parabolic (time-dependent) diffusion equation [172]; and in regions with highly forward-peaked scattering, it can behave like a parabolic equation [17, 16, 219]. It is extremely difficult to find discretization methods that are accurate over this wide range of behavior.

For these reasons, and because of the practical challenge of modeling increasingly complex problems with increasing accuracy, the development of advanced discretization methods for the transport equation has long been an important area of research.

Equally important is the problem of developing efficient iterative strategies to solve the algebraic system of discretized equations – the subject of this Review. To introduce the basic concepts, we consider a steady-state, one-group, isotropically-scattering, fixed-source particle transport problem in planar geometry:

$$\mu\frac{\partial\psi}{\partial x}(x,\mu)+\Sigma_t(x)\psi(x,\mu)=\frac{\Sigma_s(x)}{2}\int_{-1}^{1}\psi(x,\mu')d\mu'+\frac{Q(x)}{2}\ ,\ 0<x<X\ ,\ -1\le\mu\le 1\ , \tag{1.1}$$

$$\psi(0,\mu)=\psi^i(\mu)\ ,\ 0<\mu\le 1\ , \tag{1.2}$$

$$\psi(X,\mu)=\psi(X,-\mu)\ ,\ -1\le\mu<0\ . \tag{1.3}$$

This notation is standard: x = position, $\mu = \cos\theta$ is the cosine of the angle of flight θ relative to the positive x-axis, $\Sigma_t(x)$ is the total cross section, $\Sigma_s(x)$ is the scattering cross section, $Q(x)$ is the interior isotropic source, $\psi^i(\mu)$ is the prescribed incident angular flux on the left edge of the system, specular reflection occurs on the right edge, and $\psi(x,\mu)$ is the to-be-determined angular flux.

The discretization of Eqs. (1.1)-(1.3) introduces significant complications in the development of iterative methods. Therefore, we shall introduce some basic concepts in the simpler setting of the continuum equations. To simplify notation, we write Eq. (1.1) in abstract form by defining:

$$L = \mu\frac{\partial}{\partial x} + \Sigma_t(x) = \text{"leakage plus collision" operator} \quad , \tag{1.4}$$

$$S = \frac{\Sigma_s(x)}{2}\int_{-1}^{1}(\cdot)d\mu' = \text{scattering operator} \quad , \tag{1.5}$$

$$q(x) = \frac{Q(x)}{2} \quad . \tag{1.6}$$

Then Eq. (1.1) may be written

$$L\psi = S\psi + q \quad . \tag{1.7}$$

[Also, for simplicity, we temporarily disregard the boundary conditions (1.2), (1.3).]

I.B. Source Iteration

The most basic transport iteration scheme is *Source Iteration* (SI). This is defined mathematically by

$$L\psi^{(\ell+1)} = S\psi^{(\ell)} + q \quad , \quad \ell \geq 0 \quad , \tag{1.8}$$

where $\psi^{(0)}$ is chosen by the user. Operationally, the SI scheme works in the following way. At the beginning of each iteration, one introduces an "old" estimate of the scalar flux

$$\phi(x) = \int_{-1}^{1}\psi(x,\mu')d\mu' \tag{1.9}$$

in the right side of Eq. (1.1). Using this estimate, Eqs. (1.1)-(1.3) are solved to obtain an estimate for ψ, which is introduced into Eq. (1.9) to obtain the "new" estimate for ϕ. This iterative process is repeated until the difference between successive scalar flux estimates is less than a preassigned convergence criterion.

If the initial SI guess for the scalar flux $\phi^{(0)} = 0$ and the ℓ-th estimate of the angular flux is denoted as $\psi^{(\ell)}$, then for $\ell \geq 1$, it is easy to show that

$$\psi^{(\ell)}(x,\mu) = \text{the angular flux due to particles that have scattered at most } \ell - 1 \text{ times.} \tag{1.10}$$

Thus, for problems in which particles typically undergo few collisions, the SI scheme converges rapidly. Such problems are posed in small, "leaky" systems (in which particles are likely to exit through the outer boundary after a few collisions), or in systems of arbitrary size containing significant amounts of absorption throughout (in which particles are likely to be captured after a few collisions).

However, for systems containing "diffusive" spatial regions that are optically thick (the probability of leakage is small) *and* scattering-dominated (the probability of capture is small), significant numbers of particles undergo many collisions before being captured or leaking out. For such systems, the SI scheme converges slowly, i.e. is inefficient and expensive. These problems are of great practical importance.

I.C. False Convergence

A more subtle difficulty associated with slowly converging iterative schemes is the phenomenon of *false convergence*. To describe this, we define $B = L^{-1}S$ and $\xi = L^{-1}q$ and write Eq. (1.8) in the form

$$\psi^{(\ell)} = B\psi^{(\ell-1)} + \xi \quad , \quad \ell \geq 1 \quad . \tag{1.11}$$

In particle transport (and many other) problems, ξ is a modified source and B is a bounded operator, whose eigenvalues are discrete and less than unity in magnitude. The exact solution ψ satisfies

$$\psi = B\psi + \xi \quad . \tag{1.12}$$

Subtracting Eq. (1.11) from Eq. (1.12), we obtain:

$$\psi - \psi^{(\ell)} = B(\psi - \psi^{(\ell-1)}) \quad . \tag{1.13}$$

Applying this equation recursively, we get

$$\psi - \psi^{(\ell)} = B(\psi - \psi^{(\ell-1)}) = B^2(\psi - \psi^{(\ell-2)}) = \cdots = B^\ell(\psi - \psi^{(0)}) \quad . \tag{1.14}$$

This yields the estimate:

$$||\psi - \psi^{(\ell)}|| \leq ||B^\ell||\,||\psi - \psi^{(0)}|| \approx \sigma^\ell ||\psi - \psi^{(0)}|| \quad , \tag{1.15}$$

where σ is the *spectral radius* of B: the magnitude of the largest eigenvalue of B (by assumption, $\sigma < 1$).

Eq. (1.13) also implies

$$\psi - \psi^{(\ell)} = B(\psi - \psi^{(\ell-1)}) = B(\psi - \psi^{(\ell)}) + B(\psi^{(\ell)} - \psi^{(\ell-1)}) \quad , \tag{1.16}$$

so

$$\psi - \psi^{(\ell)} = (I - B)^{-1}B(\psi^{(\ell)} - \psi^{(\ell-1)}) \quad . \tag{1.17}$$

This yields a second estimate:

$$||\psi - \psi^{(\ell)}|| \leq ||(I-B)^{-1}B||\,||\psi^{(\ell)} - \psi^{(\ell-1)}|| \approx \frac{\sigma}{1-\sigma}||\psi^{(\ell)} - \psi^{(\ell-1)}|| \quad . \tag{1.18}$$

If the largest eigenvalue of B is distinct, then

$$||\psi - \psi^{(\ell)}|| = \frac{\sigma}{1-\sigma}||\psi^{\ell)} - \psi^{(\ell-1)}|| \qquad \text{as} \qquad \ell \to \infty \quad .$$

Because $\sigma < 1$, Eq. (1.15) implies that the iteration converges as $\ell \to \infty$. However, convergence is very slow if $\sigma \approx 1$. If the preassigned convergence criterion is ε, then in most codes the iteration stops when $||\psi^{(\ell)} - \psi^{(\ell-1)}|| < \varepsilon$. For this value of ℓ, Eq. (1.18) implies

$$||\psi - \psi^{(\ell)}|| \leq \frac{\sigma\varepsilon}{1-\sigma} \quad . \tag{1.19}$$

Thus, if $\sigma \approx 1$ (slow convergence) and the convergence test is $||\psi^{(\ell)} - \psi^{(\ell-1)}|| < \varepsilon$, the error in the final iterate can be much greater than the preassigned convergence criterion ε. This is the phenomenon of *false convergence*. For example, if $\sigma = 0.999$, Eq. (1.15) indicates that roughly

$$\ell = \frac{\ln(0.1)}{\ln(0.999)} \approx 2303 \tag{1.20}$$

iterations are required to reduce the iterative error by one order of magnitude, and Eq. (1.19) indicates that when the iteration stops, the iteration error may be three orders of magnitude greater than the convergence criterion.

This discussion shows that slowly converging iteration schemes have two undesirable features: they are inefficient (expensive), and it can be difficult to determine when their iterations are suitably converged. The latter difficulty can be overcome, given a suitably good estimate of σ, by using the convergence criterion $||\psi^{(\ell)} - \psi^{(\ell-1)}|| < \varepsilon(1-\sigma)$. If the largest eigenvalue of B is real and simple, which is usually true in transport problems, it is not difficult to estimate σ; for example, one can use

$$\sigma \approx ||\psi^{(\ell+1)} - \psi^{(\ell)}||/||\psi^{(\ell)} - \psi^{(\ell-1)}|| \quad .$$

In summary, the SI scheme is the most basic iterative scheme for solving particle transport problems. It has a simple physical interpretation, and it is efficient for problems in which particle histories are typically short. However, it becomes inefficient and susceptible to false convergence for problems in which sufficiently many particle histories are long. Since many important problems are of this latter type, it has long been desired to speed up, or *accelerate*, the iterative convergence of SI.

I.D. Early Acceleration Methods (Chebyshev and Rebalance)

The first practical iterative acceleration schemes implemented in production neutron transport codes were (*i*) Chebychev acceleration [8], (*ii*) Fine- and Coarse-Mesh Rebalance [15, 46, 53, 150], and (iii) Asymptotic Source Extrapolation, also known as Lyusternik's method [19]. (These schemes are described in detail later in this Review.) Chebyshev acceleration utilizes standard matrix iteration techniques. Although this does speed up the convergence rate, the performance often remains unacceptably slow in difficult problems with scattering ratios $c = \Sigma_s/\Sigma_t$ close to unity, which have small probabilities of absorption. Rebalance methods normalize the discrete transport solution so that at the conclusion of each iteration, the normalized solution satisfies the angularly-integrated neutron balance equation over individual cells (fine mesh rebalance) or larger clusters of cells (coarse mesh rebalance). Rebalance methods can accelerate effectively if the size of the coarse meshes is chosen properly. However, if this is not done, rebalance can diverge. Also, for difficult problems with high scattering ratios, rebalance often cannot provide acceptable acceleration even when it does converge. Finally, Asymptotic Source Extrapolation can also speed the convergence of problems that are not very difficult, but care must be taken to avoid divergence in problems with high scattering ratios. However, even when care is taken, the method loses effectiveness for such problems.

I.E. Preconditioning ("KP" and "Synthetic") Methods

In an effort to develop more efficient iteration strategies, transport researchers in the 1960's explored two basic paths. One path is often described as *synthetic acceleration.* The other is a class of rapidly convergent methods that are not (necessarily) true acceleration methods, because they do not (necessarily) produce the same discrete solution as does source iteration. We discuss both types of solution strategies in this review.

The concept of a "synthetic" acceleration scheme was introduced by Kopp [26]. (We show below that synthetic acceleration is equivalent to *preconditioning*, which is well-known in the mathematical community.) Independently, and essentially simultaneously, Lebedev [27, 36, 37, 39, 40, 10] developed and tested a family of "KP" acceleration schemes, which can be viewed as synthetic acceleration schemes (or, to use more conventional terminology, as clever prescriptions for good preconditioners). In these schemes, one regards a single source iteration, Eq. (1.8), as the first stage of (at least) a two-stage iteration process. Thus, we define $\psi^{(\ell+1/2)}$ as the result of a single source iteration, or *transport sweep*:

$$L\psi^{(\ell+1/2)} = S\psi^{(\ell)} + q \quad , \quad \ell \geq 0 \quad , \tag{1.21}$$

and it is necessary to formulate an equation for $\psi^{(\ell+1)}$. The goal is for $\psi^{(\ell+1)}$ to be a

significantly more accurate approximation to ψ than is $\psi^{(\ell+1/2)}$.

To accomplish this by the *synthetic* method, we subtract Eq. (1.21) from Eq. (1.7):

$$L(\psi-\psi^{(\ell+1/2)}) = S(\psi-\psi^{(\ell)}) = S(\psi-\psi^{(\ell+1/2)}) + S(\psi^{(\ell+1/2)}-\psi^{(\ell)}) \quad . \tag{1.22}$$

This yields the following exact equation for the *additive correction* $\psi-\psi^{(\ell+1/2)}$:

$$(L-S)(\psi-\psi^{(\ell+1/2)}) = S(\psi^{(\ell+1/2)}-\psi^{(\ell)}) \quad . \tag{1.23}$$

Hence,

$$\psi = \psi^{(\ell+1/2)} + (L-S)^{-1}S(\psi^{(\ell+1/2)}-\psi^{(\ell)}) \quad , \tag{1.24}$$

which defines the exact solution ψ in terms of $\psi^{(\ell+1/2)}$ and $\psi^{(\ell+1/2)}-\psi^{(\ell)} = \Delta\psi$. Unfortunately, Eq. (1.24) requires one to invert the full transport operator $L-S$; but if this could be done efficiently, one could more directly solve Eq. (1.7) for ψ.

The idea of synthetic acceleration [26] is to replace $(L-S)^{-1}$ in Eq. (1.24) by a "low-order" approximation

$$M \approx (L-S)^{-1} \quad , \tag{1.25}$$

for which $MS\Delta\psi$ is easier to evaluate than $(L-S)^{-1}S\Delta\psi$. Eq. (1.24) becomes:

$$\psi^{(\ell+1)} = \psi^{(\ell+1/2)} + MS(\psi^{(\ell+1/2)}-\psi^{(\ell)}) \quad . \tag{1.26}$$

The synthetic scheme is now defined by Eqs. (1.21) and (1.26). Eq. (1.21) is the *high-order* equation; Eq. (1.26) uses a *low-order* approximation to the exact additive correction to $\psi^{(\ell+1/2)}$. If the synthetic scheme converges, the converged solution must satisfy the original transport equation, no matter how M is defined. [To see this, subtract $\psi^{(\ell)}$ from both sides of Eq. (1.26) and rearrange.] Different choices of M yield different synthetic acceleration schemes. If Eq. (1.25) holds, then Eqs. (1.26) and (1.24) are nearly the same, so $\psi^{(\ell+1)} \approx \psi$, and convergence should be rapid. However, a constraint that conflicts with Eq. (1.25) is that $MS\Delta\psi$ should be much less costly to evaluate than $(L-S)^{-1}S\Delta\psi$. Thus, the low-order approximation M should be "close" to the high-order operator $(L-S)^{-1}$, but not *too* close.

To clarify the mathematical structure of the SI and synthetic acceleration schemes, we now show that they can be written as *Richardson* and *Preconditioned Richardson* matrix iteration schemes [8]. That is, the concept of synthetic acceleration is mathematically equivalent to the better-known concept of preconditioning. (This was recognized early on by many researchers in the former Soviet Union, but it received little attention in the West until after the publications by Derstine and Gelbard [100] and Faber and Manteuffel [139].)

We operate on Eqs. (1.7) and (1.8) by L^{-1} and define

$$A \equiv I - L^{-1}S \quad , \quad \hat{q} \equiv L^{-1}q \quad , \tag{1.27}$$

to obtain

$$A\psi = \hat{q} \tag{1.28}$$

and

$$\psi^{(\ell+1)} = (I-A)\psi^{(\ell)} + \hat{q} \quad . \tag{1.29}$$

Eq. (1.29) is a *Richardson Iteration* scheme for Eq. (1.28). This is a special case of a family of iterative methods proposed by Schmidt in 1907 [20].

Next, we write Eq. (1.21) as

$$\psi^{(\ell+1/2)} = (I-A)\psi^{(\ell)} + \hat{q} \quad . \tag{1.30}$$

Using this result, we eliminate $\psi^{(\ell+1/2)}$ from Eq. (1.26) to obtain

$$\psi^{(\ell+1)} = \psi^{(\ell)} + (I+MS)(-A\psi^{(\ell)} + \hat{q}) \quad . \tag{1.31}$$

Defining

$$P \equiv I + MS \quad , \tag{1.32}$$

we may rewrite Eq. (1.31) as

$$\psi^{(\ell+1)} = (I-PA)\psi^{(\ell)} + P\hat{q} \quad . \tag{1.33}$$

Eq. (1.33) is the *Preconditioned Richardson* scheme for Eq. (1.28), with *preconditioner P*. (This is also a special case of Schmidt's family of methods [20].) We have already assumed that $M \approx (L-S)^{-1}$. Then, by Eqs. (1.32) and (1.27),

$$P \approx I + (L-S)^{-1}S = (L-S)^{-1}[(L-S)+S] = (I-L^{-1}S)^{-1} = A^{-1} \quad . \tag{1.34}$$

This implies $PA \approx I$, so the convergence of Eq. (1.33) should be rapid.

Hence, the SI scheme can be interpreted as a Richardson iteration; and the general synthetic scheme can be viewed as a Preconditioned Richardson iteration, in which the preconditioner P [Eq. (1.32)] is a good approximation to A^{-1} if M is a good approximation to $(L-S)^{-1}$. This demonstrates the close connection between the SI and synthetic acceleration schemes for the transport equation, and the regular and preconditioned Richardson iteration schemes that are familiar in numerical analysis [8].

At least part of the preceding information was recognized in the late 1950's by Vorobyov [21]. Vorobyov examined a two-step iteration process whose second step uses an approximate operator – the equivalent of what we have called a "low-order" operator – to obtain an additive correction. He recognized that the resulting iterative method was a particular instance of Schmidt's method; in fact, it is algebraically equivalent to preconditioned Richardson iteration, which is a special case of Schmidt's family of methods [20].

I.F. "KP" Acceleration Methods - Historical Review

Next, we summarize the general history of the development of rapidly convergent methods for S_N iterations, discussing both of the main paths that researchers have taken. We begin with a discussion of the "preconditioning" path, which was first explored independently by Lebedev and Kopp. First we discuss Lebedev's "KP" approach, which spawned an active line of research throughout the 1960's in Russia. We then turn to Kopp's "synthetic" approach, which led to a different but related line of research in the west. Then, we discuss the second distinct path of work, which was initiated by Gol'din's "Quasidiffusion" method.

In the early 1960's, V.I. Lebedev proposed and developed the "KP" family of transport iterative methods. For the next decade, he and co-workers analyzed and tested a variety of methods in this family. KP methods, which are not limited to transport problems, embodied two main new concepts. First, the preconditioning step – which is equivalent to solving for the additive correction to $\psi^{(\ell+1/2)}$ in Eq. (1.26) – should occur in a *subspace* of the solution's function space, thereby reducing the computational cost of obtaining the correction. The use of a subspace allows one to rewrite the preconditioning step shown in Eqs. (1.26). We recall that this step is intended to find an approximation to the exact additive correction (call it $f_{exact}^{(\ell+1/2)}$), which by Eq. (1.23) satisfies

$$(L-S)f_{exact}^{(\ell+1/2)} = S(\psi^{(\ell+1/2)} - \psi^{(\ell)}) \ . \tag{1.35}$$

We suppose that (i) the operator K projects the scattering-source *residual*, $S(\psi^{(\ell+1/2)} - \psi^{(\ell)})$, onto a subspace of the full position-and-angle space, and (ii) the operator D in that subspace is an approximation to $(L-S)$. (This is often called the *low-order* operator.) Then, if we solve the problem

$$DF^{(\ell+1)} = KS(\psi^{(\ell+1/2)} - \psi^{(\ell)}) \ , \tag{1.36}$$

the solution $F^{(\ell+1)}$ (which lives in the subspace) is an approximation to $f_{exact}^{(\ell+1/2)}$. If the operator E *extends* or *prolongs* functions from the subspace to the full space, then $E\hat{f}^{(\ell+1)}$ is the correction applied to $\psi^{(\ell+1/2)}$. The equations that describe one full KP iteration are now:

$$L\psi^{(\ell+1/2)} = S\psi^{(\ell)} + q \ , \tag{1.37}$$

$$DF^{(\ell+1)} = KS(\psi^{(\ell+1/2)} - \psi^{(\ell)}) \ , \tag{1.38}$$

$$\psi^{(\ell+1)} = \psi^{(\ell+1/2)} + EF^{(\ell+1)} \ . \tag{1.39}$$

A comparison with Eqs. (1.21) and (1.26) shows that the operator M, which approximates $(L-S)^{-1}$, is given by

$$M = ED^{-1}K \ . \tag{1.40}$$

This operator is not constructed in practice; it is more efficient to solve Eqs. (1.37)-(1.39) step-by-step than to build M. We note that solving the *low-order problem*, Eq. (1.38), involves essentially all of the computational effort required for the preconditioning step. In KP methods, this solution takes place in a subspace and therefore involves fewer unknowns than Eq. (1.37); thus, there is hope that the preconditioning step will add only a minimal amount of computational effort to each iteration.

The second main new concept introduced by Lebedev is that the preconditioning step can itself be a sequence of steps, each performed in a different subspace. Also, the subspaces are typically nested. (This conceptualizes a very early *multi-level* iterative method, well-known examples of which are *multigrid* methods.) An example of a scheme with two low-order operators in two different subspaces is Eq. (1.37) and

$$D_\alpha F_\alpha^{(\ell+1)} = K_\alpha S(\psi^{(\ell+1/2)} - \psi^{(\ell)}) \ , \tag{1.41}$$

$$\psi^{(\ell+3/4)} = \psi^{(\ell+1/2)} + E_\alpha F_\alpha^{(\ell+1)} \ , \tag{1.42}$$

$$D_\beta F_\beta^{(\ell+1)} = K_\beta S(\psi^{(\ell+3/4)} - \psi^{(\ell)}) \ , \tag{1.43}$$

$$\psi^{(\ell+1)} = \psi^{(\ell+3/4)} + E_\beta F_\beta^{(\ell+1)} \ . \tag{1.44}$$

In this case the operator M of Eq. (1.26) is

$$M = E_\alpha D_\alpha^{-1} K_\alpha + E_\beta D_\beta^{-1} K_\beta [I + E_\alpha D_\alpha^{-1} K_\alpha] \ .$$

Lebedev explored many specific methods in the KP family during the 1960's. In his notation, the "K" part of a KP iteration gives $\psi^{(\ell+1/2)}$ from $\psi^{(\ell)}$, as in Eq. (1.37). The "P" part of the iteration is the *preconditioning*, or low-order part. Lebedev's notation $\mathrm{KP}_1(n_1)\mathrm{P}_2(n_2)$, for example, indicates a method with two low-order levels; in the first level the low-order differential operator is of order $2n_1$, and in the second the low-order differential operator is of order $2n_2$.

A simple but powerful method is $\mathrm{KP}_1(1)$; in this method the low-order subspace contains functions that are linear in the angle variable, and the low-order operator is the diffusion operator. Given isotropic scattering, Lebedev analyzed a model problem (periodic boundary conditions, uniform material properties) and showed that in the absence of discretization, the $\mathrm{KP}_1(1)$ method yields a spectral radius $\sigma < 0.225c$ (see Section XI.11 of [10]). He also determined an optimal factor by which to multiply the diffusion coefficient in the low-order operator; this yielded a spectral radius $\sigma < 0.185c$ (Section XI.10 of [10]). He analyzed many other KP methods; for example, he showed that the $\mathrm{KP}_1(1)\mathrm{P}_2(0)$ method has spectral radius $\sigma < 0.127c$. (This method, discussed later in Section II.D, uses a transport sweep, a diffusion calculation, and a simple algebraic calculation in each full

iteration.) Lebedev also studied generalizations such as two transport sweeps per low-order calculation; these schemes he termed K^2P methods (Section XI.12 of [10]). Further generalizations included the "cyclic" KP schemes, in which a cycle is N consecutive KP iterations, each with different parameters; Lebedev theoretically derived the values of these parameters that provide the fastest overall convergence (Section XI.14 of [10]). He also analyzed the *cost* of various KP schemes and proved that certain schemes minimized cost, given certain constraints and assumptions (Section XI.20 of [10]). Some original references are [27, 36, 37, 39, 40]; others are found in the book by Marchuk and Lebedev [10], the first edition of which was published in Russian in 1971.

I.G. "Synthetic" Acceleration Methods – Historical Review

Related activity in the west began in 1963 with a paper by Kopp [26], which introduced the *synthetic method* for accelerating the iterative convergence of transport problems. (As we have shown, synthetic acceleration is equivalent to preconditioning.) In his paper, Kopp used the diffusion equation as the low-order operator to accelerate transport iterations. The scheme he tested is algebraically equivalent to Lebedev's $\mathrm{KP}_1(1)$ scheme, at least with a certain initial guess, although Kopp cast the equations in a different form. Western researchers followed up on Kopp's work but were generally unaware of (or did not understand) Lebedev's work. Also, whereas Lebedev focused much of his attention on the even-parity form of the transport equation (described below), western researchers focused on the first-order form shown in Eq. (1.1).

Crawford et al. applied Kopp's synthetic method to speed up Monte Carlo transport calculations, with limited success [22, 23]. In 1969, Gelbard and Hageman [32] explored two options for the low-order operator: diffusion and S_2 (discrete-ordinates with order-2 quadrature set), using these to accelerate S_N iterations in 2-D Cartesian geometry. For the analytic equations with a diffusion preconditioner, they derived a spectral radius $< 0.2247c$, but for discretized equations they observed convergence rates this fast only for fine spatial meshes. Reed [51] then showed by testing *and* analysis that while the "diffusion" synthetic method employed by Gelbard and Hageman is rapidly convergent for sufficiently fine spatial grids, it diverges for coarser grids. (Lebedev never observed divergence of his KP methods [280], for reasons discussed later.)

In 1976, Alcouffe [57, 63] proposed a remedy for the divergence described by Reed. Alcouffe considered the diamond-differenced $\mathrm{S_N}$ operator $L-S$, with the discrete transport problem for the correction (1.23) replaced by a discrete diffusion approximation. Most importantly, Alcouffe showed that if the discrete diffusion operator in the low-order problem is derived *consistently* with the high-order diamond-differenced $\mathrm{S_N}$ transport operator, then the resulting synthetic algorithm, which he called *Diffusion Synthetic Acceleration* (DSA),

is rapidly convergent for all spatial mesh thicknesses. This seminal result showed that it is possible to accelerate a discretized SI scheme using DSA in an efficient and robust manner. Discrete transport problems that with SI would require hundreds, thousands, or even millions of iterations to converge, could now be solved with DSA in less than ten iterations.

Alcouffe's work had an immense impact on western work concerning synthetic acceleration methods (i.e., preconditioning) for the first-derivative form of the transport equation. Prior to this work, it was not known whether an unconditionally fast acceleration method even *existed* for the discrete first-order transport equation. After Alcouffe's work, theoretical efforts were made to understand its underlying principles, and to extend these principles to non-diamond differencing schemes.

For example, Miller [64] showed that DSA could be understood as a generalized form of rebalance. Morel [86] showed that DSA applied to problems with highly anisotropic scattering will have a degraded performance, which can be partly remedied by accelerating both the flux and current using the solution of the low-order diffusion calculation, at least in 1-D planar geometry. Larsen and McCoy [83, 85] successfully extended Alcouffe's ideas to a *four-step* procedure, which they applied to several non-diamond differencing schemes in planar geometry. (An equivalent procedure is described later in this Review. This procedure is *very* similar in principle to Lebedev's "multilevel" approach described above, but applied to the discrete rather than the continuous transport equation.) Azmy and Dorning [98] and Khalil [101] successfully applied DSA to the acceleration of multidimensional nodal transport equations; Zmijarevic et al. later extended that methodology to other nodal methods and to multidimensional characteristic methods [301]. Morel, Larsen, and Matzen [103] developed an effective DSA scheme for radiative diffusion calculations; in this scheme a one-group operator is used as the preconditioner for a multigroup problem. Adams and Martin [169] developed a simpler, slightly inconsistent version of four-step DSA that provides rapid convergence for discontinuous finite element (DFE) spatial discretizations, but they did not develop an efficient way to solve the low-order equations. Wareing, Larsen, and Adams [167] proposed an even simpler DSA scheme for bilinear discontinuous (BLD) discretizations on rectangles in XY geometry, although the performance of this scheme degrades for spatial cells with high aspect ratios. Morel, Dendy, and Wareing [189, 190] developed an efficient multigrid technique for solving the Adams-Martin BLD equations, thus creating the first unconditionally efficient DSA method for a 2-D spatial discretization, other than diamond differencing, of the first-order transport equation. Wareing et al. [200] later showed that this procedure also works for the bilinear nodal differencing, and Adams et al. showed the same for the bilinear characteristic differencing [247].Very recently, Warsa et al. have shown that the Adams-Martin method can diverge given the linear discontinuous (LD) method on a distorted tetrahedral grid [300].

In 1986, Lorence, Morel, and Larsen [113] used the low-order S_2 operator rather than the diffusion operator to effectively accelerate the one-dimensional S_N equations with linear discontinuous spatial differencing. Adams and Martin [116] developed a family of boundary projection acceleration (BPA) methods, in which the D of Eq. (1.38) is also not the diffusion operator, but is obtained by projecting onto a different angular subspace. Lawrence [141] independently and simultaneously developed and tested one method in this BPA family. In 1986, Larsen and Miller [110] showed that it is possible to accelerate transport iterations using a low-order transport operator containing no scattering, at least in 1-D planar geometry. Unknown to them, Morozov [28] had proposed the same method in 1962, which Lebedev had analyzed in 1968 [38]. Much later, Ramoné, Adams, and Nowak [243] generalized this idea in the Transport Synthetic Acceleration (TSA) scheme.

Other transport acceleration schemes have been proposed in recent years. For example, in 1991 Manteuffel and Morel [164] presented an angular multigrid method for problems with highly anisotropic scattering. Lebedev's multilevel KP family appears to contain the Manteuffel-Morel method as a special case [40], but Lebedev apparently did not study such a method tailored for problems with highly forward-peaked scattering. Pautz et al. [270] later extended the Morel-Manteuffel method to multiple dimensions. (These angular multigrid methods do not replace DSA or its alternatives; in fact, they depend on them for solving the problem on the coarsest angular grid.) Khattab and Larsen [161, 241] developed an approximate low-order P_N method for similar problems. Faber and Manteuffel recognized that DSA is equivalent to preconditioned Richardson iteration and explored the benefits of using the Conjugate Gradient (CG) method in combination with DSA. Ashby, Brown, Dorr, and Hindmarsh [158, 204] extended this work to problems with anisotropic scattering. B. Adams and Morel [180] devised an efficient scheme for converging the upscattering iteration in multigroup S_N equations. Azmy [194, 259] devised new alternative preconditioners using cell-centered low-order operators. In 1993, Adams and Wareing [181] showed that DSA can become divergent in multidimensional geometries with sufficiently forward-peaked scattering or asymmetric quadrature sets. (Unknown to them, Marchuk and Lebedev had previously shown some of these results in their book [10].) Wareing, Walters, and Morel [231] devised an acceleration method for a new Nonlinear Characteristic spatial differencing scheme. Anistratov, Adams, and Larsen [234] applied the same basic idea to a Nonlinear Corner-Balance spatial differencing scheme. Voloschenko [229] proposed a new acceleration scheme for charged-particle transport problems. This is not an exhaustive list of preconditioner-based methods that have been explored for transport iterations, but we believe that it is representative.

I.H. Quasidiffusion and Related Methods – Historical Review

We turn now to the "second path" taken by researchers in the development of rapidly convergent iterative methods for transport problems. These methods are not preconditioned Richardson schemes, and in fact are not usually true acceleration schemes, for they do not usually obtain the solution $(L-S)^{-1}q$ given by the discrete transport operator. They do obtain a discrete transport solution, but this solution is generally influenced by the discretization of a low-order operator that contains transport corrections. In other words, *the truncation errors in these solutions generally differ from the truncation errors in the discrete transport solution obtained by SI.*

Gol'din initiated this line of research in 1964, with his development of the nonlinear *Quasidiffusion* (QD) method for solving the linear Boltzmann equation [25]. (We describe this and related methods in detail in Chapters II and III.) Later, Troshchiev et al. [42] reported the first QD results using *consistent* discretizations, which makes the QD method a true acceleration scheme, obtaining the same solution as the unaccelerated transport equations. In the early 1970's, Gol'din and Chetverushkin [43] generalized the QD boundary conditions. In the late 1970's, Aksenov and Gol'din [71] reported 2-D QD calculations. Later, Gol'din [82] formulated the QD method abstractly, in terms of nonlinear projection and prolongation operators, and he applied this theory to multigroup neutron transport problems with anisotropic scattering. Later still, Anistratov and Gol'din [105] studied the effects of varying the spatial discretization of the transport equation while using a particular spatial discretization for the low-order equation. Also, Gol'din and Kolpakov [170] reported methods for solving the nonsymmetric QD equations. At about the same time, Miften and Larsen proposed alternative boundary conditions [188] and a way to symmetrize the nonsymmetric 2-D QD diffusion equation [187]. Aristova and Kolpakov [183] presented a method for spatially discretizing the QD equations in two dimensions. Gol'din and his colleagues also reported using the QD method to solve the coupled material-temperature and radiative transfer equations [108, 216]. Gol'din described the application of the method to problems with anisotropic scattering in an early paper [25]; Aristova and Gol'din [235, 239, 278] later implemented and improved it for problems with strongly anisotropic scattering.

Shortly after QD was created, Nikolaishvilli devised a variant that he described as an "Yvon-Mertens" approximation [41]. A distinct nonlinear method was later created, apparently independently, by Germogenova [33, 34] and Gol'din et al. [35]. Germogenova called it the "method of averaged fluxes," and Gol'din referred to it as a "flux version of quasidiffusion." Gol'din et al. extended these methods to electron transport problems in 1976 [60]; in this work the low-order angular domain was divided into more than two subdomains. (Germogenova had suggested this idea but did not implement it [34].) Anis-

tratov and Gol'din studied and compared two members of this family, which they called the *First-Flux* and *Second-Flux* methods [182]. The Second Flux method had been proposed by Surzhikov [131]. Recently, Anistratov and Larsen [217, 288] have developed a one-parameter family of methods that includes the First- and Second-Flux methods; they term this family the nonlinear *Weighted Alpha* (WA) methods. (This method is described in detail in Chapters II and III.)

Adams [178] combined the ideas of nonlinear WA methods and linear boundary projection acceleration (BPA) methods in a 1-D *nonlinear* BPA method (when linearized, this scheme produces a linear BPA method). Later, Hong and Cho [223, 240, 252, 266, 267] developed a related family of 1-D and 2-D nonlinear rebalance methods that also yield BPA methods when linearized. (Adams' nonlinear BPA method is a special 1-D member of this family.) Hong and Cho also implemented modern matrix techniques to solve their low-order 2-D problems.

Lewis and Miller [61] created a scheme that, like DSA, is linear and involves the solution of a diffusion equation each iteration. Like QD, it is not a true acceleration scheme, for it does not generally yield the unaccelerated solution. Larsen [109] studied this and related schemes, clarifying many of their properties and their close relation to synthetic acceleration and QD schemes.

Significant practical differences exist between the preconditioning (synthetic and *KP*) schemes and the other schemes (such as QD) discussed in the previous paragraphs. Preconditioning schemes are conceptually linear; as we have shown, the "low-order" equation in each iteration yields an additive correction to the previously-calculated transport iterate. In practice, preconditioning schemes can be divergent unless the low-order equations are discretized *consistently* with the high-order S_N equations. (We discuss this thoroughly later in this Review.) If a preconditioned iteration converges, it must converge to the discretized solution of the unaccelerated S_N equations. Thus, preconditioning (synthetic) schemes, if they are convergent, do not change the unaccelerated S_N solution – but they usually yield this solution more efficiently. The principal disadvantage of these methods is the "tyranny of consistent low-order discretization": for the most difficult iterative problems (such as those encountered in thermal radiative transfer, discussed in Section VII.C), it is necessary, but often very difficult, to derive discretizations of the low-order equations that are consistent enough with the transport discretization that they render the overall synthetic scheme rapidly convergent, yet are efficient to solve even for optically thick, highly scattering problems. In the language of the numerical analysis literature, it is difficult to find a preconditioner that works effectively for these difficult problems and is not prohibitively expensive to implement.

To illustrate this, let us define the integral operator K_0 such that $\phi = K_0\psi$ and the scat-

tering operator $\hat{S}$ such that for isotropic scattering, $S\psi = \hat{S}K_0\psi = \hat{S}\phi$. Then, a transport sweep can be written as

$$\psi^{(\ell+1/2)} = L^{-1}\hat{S}\phi^{(\ell)} + L^{-1}q \ .$$

Thus,

$$\phi^{(\ell+1/2)} = X_{SI}\phi^{(\ell)} + K_0L^{-1}q \ ,$$

where $X_{SI} = K_0L^{-1}\hat{S}$ is the iteration matrix for source iteration (given isotropic scattering). Writing this last equation in the form of Richardson Iteration [see Eq. (1.29)],

$$\phi^{(\ell+1)} = [I - (I - X_{SI})]\phi^{(\ell)} + K_0L^{-1}q \ ,$$

we find that the Preconditioned Richardson Iteration [see Eq. (1.33)] with preconditioner $P = I + M\hat{S}$ is:

$$\begin{aligned} \phi^{(\ell+1)} &= [I - P(I - X_{SI})]\phi^{(\ell)} + PK_0L^{-1}q \\ &= [X_{SI} - M\hat{S}(I - X_{SI})]\phi^{(\ell)} + (I + M\hat{S})K_0L^{-1}q \ . \end{aligned} \tag{1.45}$$

As noted above, if the iteration converges, the converged solution satisfies the original equation $\phi = (I - X_{SI})^{-1}K_0L^{-1}q$, at least if $I + M\hat{S}$ is invertible. Also, we note that $I - X_{SI}$ has small eigenvalues when X_{SI} has eigenvalues close to unity. Thus, for such error modes, $M\hat{S}$ must have large eigenvalues to keep the iteration matrix $X_{SI} - M\hat{S}(I - X_{SI})$ from approaching the unaccelerated matrix X_{SI}. However, if the eigenvalues of $M\hat{S}$ are too large, then the scheme diverges. Thus, the operator M must be chosen *very carefully* if the synthetic scheme's iteration matrix is to have eigenvalues whose magnitudes are bounded well below unity. This is equivalent to saying that it can be very difficult to find a preconditioner that causes preconditioned Richardson iteration to be rapidly convergent.

Iteration schemes that do not involve preconditioning, such as QD and Lewis-Miller (LM) [61], also consist of a transport sweep followed by a low-order calculation. However, the low-order solution is not an additive correction to the recent transport iterate, but rather is a direct estimate of the scalar flux. The equation for this scalar flux estimate contains either (*i*) nonlinear (multiplicative) functionals that are determined by the transport solution and depend weakly on it, or (*ii*) an additive transport correction term that vanishes when the transport iterate has a certain angular dependence. A key advantage of these methods is that the high-order S_N and low-order diffusion problems can be discretized independently without affecting the rapid convergence. However, this freedom from consistent discretization comes with a price: such schemes yield *two* converged scalar flux solutions – one from the S_N sweep, the other from the low-order calculation. These two solutions differ from each other and from the unaccelerated S_N solution by a truncation error. Thus, the accuracy of the S_N solution can be compromised if the low-order equation is not discretized at least as

accurately as the S_N equations. (On the other hand, a poor S_N solution could be improved if the low-order equation is discretized with high accuracy.)

Hence, non-preconditioning iterative schemes can be rapidly convergent, but they are not simply acceleration schemes – they do not necessarily produce the solution of the unaccelerated S_N discretization. Nevertheless, they do yield legitimate solutions of the transport equation, and as one refines the spatial grid, the high- and low-order scalar fluxes converge to each other and to the (fine-mesh) unaccelerated numerical solution of the S_N equations.

To illustrate this we consider the LM scheme [61], which is developed in Chapter II. In operator form, this scheme can be written:

$$\phi^{(\ell+1)} = 2[(-D+\Sigma_a)^{-1}DK_2L^{-1}\hat{S}]\phi^{(\ell)} + \tilde{q} \quad , \tag{1.46}$$

where

$$D = \text{ discretization of } \frac{d}{dx}\frac{1}{3\Sigma_t(x)}\frac{d}{dx} \quad ,$$

and K_2 is defined such that $\phi_2 = K_2\psi$ [see Eq. (2.78)]. Because the iteration operator does not contain differences of operators, in contrast to the preconditioned method's operator in Eq. (1.45), essentially any discretization for D will produce a rapidly convergent iteration – consistent discretization is not required. (Note that if $\Sigma_a = 0$, D disappears from the iteration operator.) However, upon convergence, nothing forces the discrete solution $\phi^{(\ell)}$ to equal the discrete solution $\phi^{(\ell+1/2)}$, or for either of these solutions to equal the unaccelerated discrete solution, $(I - X_{SI})^{-1}K_0L^{-1}q$. In practice, the discrete solution $\phi^{(\ell)}$ is taken to be "the" solution of the method, for it satisfies the conservation equation whereas $\phi^{(\ell+1/2)}$ does not. This discrete solution can be less accurate than the unaccelerated solution of the discretized S_N equations, $(I - X_{SI})^{-1}K_0L^{-1}q$, but it also can be be more accurate. Whichever happens depends on the details of the discretizations of the S_N and low-order equations. See [178] for a discussion with examples.

I.I. Multigrid Methods

Many of the preconditioning methods discussed above share the property that their low-order operators are obtained by approximating the *angular* variation of the solution. Thus, these methods can be viewed as "angular multigrid" methods, although most have only two grid levels [153]. Some researchers, attracted by the tremendous success that such methods have achieved for elliptic problems, have also explored *spatial* multigrid methods for acceleration of transport iterations. Nowak et al. were among the first to report results, which were encouraging both in 1-D [120] and 2-D [130]. Barnett et al. later achieved success in 1-D with a different approach [137]. Manteuffel and co-authors explored still other approaches to spatial multigrid, developing algorithms that converge exceptionally

fast for the one-dimensional problems that they considered [154, 173, 186, 196, 210, 225]. In Chapter V we discuss some of these spatial multigrid methods in more detail.

I.J. Review Outline

Because of the volume of the literature, it is not possible to discuss in depth all previously developed transport S_N acceleration methods in this Review. Our more limited aim is to describe and illustrate the main concepts that have led to important practical results. We hope that this Review will enable readers to approach the literature on S_N particle transport acceleration methods with greater technical understanding and historical perspective.

The remainder of this Review is organized as follows. Chapter II describes several transport iteration schemes and their theoretical convergence properties for analytic planar-geometry transport problems. Chapter III discusses the same iteration schemes, but applied to discretized S_N equations. (Chapters II and III are tutorial in nature, intended for readers with little background in the subject of transport iterations. The remaining chapters of this Review are less tutorial but cover more material.) Chapter IV briefly describes transport acceleration schemes for more general geometries and spatial differencing schemes. Chapter V discusses rebalance and other iterative methods. Chapter VI describes the role of *algebraic* iterative methods in transport problems, such as Chebyshev and Conjugate Gradient acceleration. Chapter VII deals with special acceleration methods not included in the previous chapters. Chapter VIII treats the iterative acceleration of k-eigenvalue problems. Chapter IX concludes the Review with a summary and discussion of open problems.

II. ITERATION SCHEMES FOR CONTINUOUS TRANSPORT PROBLEMS IN PLANAR GEOMETRY

In this chapter we describe the SI, synthetic (or preconditioning), quasidiffusion, and related iterative methods for solving the continuous transport problem defined by Eqs. (1.1)-(1.3). We also introduce the principal mathematical tool for analyzing the convergence properties of these methods: the infinite-medium Fourier analysis. In the final section of this chapter we introduce forms of the transport equation containing second-order spatial derivatives. These forms present different iterative challenges than do the more commonly used first-order form.

II.A. Source Iteration (SI)

We have already described the Source Iteration (SI) method. For the problem consisting of Eqs. (1.1)-(1.3), this method is defined by:

$$\mu\frac{\partial\psi^{(\ell+1)}}{\partial x}(x,\mu)+\Sigma_t(x)\psi^{(\ell+1)}(x,\mu)=\frac{\Sigma_s(x)}{2}\int_{-1}^{1}\psi^{(\ell)}(x,\mu')d\mu'+\frac{Q(x)}{2}\quad,$$

$$0<x<X\quad,\quad -1\le\mu\le 1\quad, \tag{2.1}$$

$$\psi^{(\ell+1)}(0,\mu)=\psi^{i}(\mu)\quad,\quad 0<\mu\le 1\quad, \tag{2.2}$$

$$\psi^{(\ell+1)}(X,\mu)=\psi^{(\ell+1)}(X,-\mu)\quad,\quad -1\le\mu<0\quad. \tag{2.3}$$

For a given $\psi^{(\ell)}(x,\mu)$, $\psi^{(\ell+1)}(x,\mu)$ is determined by first solving Eqs. (2.1) and (2.2) for $\mu>0$, and then solving Eqs. (2.1) and (2.3) for $\mu<0$. We call this solution process one *source iteration*, or equivalently, one *transport sweep*. The mechanics of this process are described in Chapter III.

We have already noted that if $\psi^{(0)}(x,\mu)=0$, then $\psi^{(\ell)}(x,\mu)$ is the angular flux of all particles that have undergone at most $\ell-1$ collisions. Thus, if the system described by Eqs. (2.1)-(2.3) is nonmultiplying [$\Sigma_s(x)\le\Sigma_t(x)$], then each neutron will undergo a finite number of collisions before it is absorbed or leaks out of the system. In this case, the SI scheme is guaranteed to converge. However, the rate of convergence is directly linked to the mean number of collisions in a neutron lifetime. If this mean number is small (an optically thin, "leaky" system, or one with significant absorption), the SI scheme will converge rapidly. If this number is large (an optically thick system with little absorption), the SI scheme will converge slowly. The larger the mean number of collisions per neutron lifetime, the slower the convergence.

To quantitatively describe the performance of the SI scheme, we consider a model infinite homogeneous medium problem in which the solution and all iterates are assumed to be bounded for $-\infty<x<\infty$. The exact transport equation is

$$\mu\frac{\partial\psi}{\partial x}(x,\mu)+\Sigma_t\psi(x,\mu)=\frac{\Sigma_s}{2}\int_{-1}^{1}\psi(x,\mu')d\mu'+\frac{Q(x)}{2}\quad, \tag{2.4}$$

and the SI scheme is defined by

$$\mu\frac{\partial\psi^{(\ell+1)}}{\partial x}(x,\mu)+\Sigma_t\psi^{(\ell+1)}(x,\mu)=\frac{\Sigma_s}{2}\int_{-1}^{1}\psi^{(\ell)}(x,\mu')d\mu'+\frac{Q(x)}{2}\quad. \tag{2.5}$$

We define *the error in the ℓ-th iterate* to be:

$$f^{(\ell)}(x,\mu)=\psi(x,\mu)-\psi^{(\ell)}(x,\mu)\quad. \tag{2.6}$$

Subtracting Eq. (2.5) from (2.4), we obtain

$$\mu\frac{\partial f^{(\ell+1)}}{\partial x}(x,\mu)+\Sigma_t f^{(\ell+1)}(x,\mu)=\frac{\Sigma_s}{2}\int_{-1}^{1}f^{(\ell)}(x,\mu')d\mu'\quad. \tag{2.7}$$

Eq. (2.7) allows us to determine $f^{(\ell)}(x,\mu)$ recursively. Expanding $f^{(\ell)}(x,\mu)$ as a Fourier integral

$$f^{(\ell)}(x,\mu) = \int_{-\infty}^{\infty} A^{(\ell)}(\lambda,\mu) e^{i\Sigma_t \lambda x} d\lambda \tag{2.8}$$

and introducing Eq. (2.8) into Eq. (2.7), we obtain

$$\int_{-\infty}^{\infty} \left[\Sigma_t (i\lambda\mu + 1) A^{(\ell+1)}(\lambda,\mu) - \frac{\Sigma_s}{2} \int_{-1}^{1} A^{(\ell)}(\lambda,\mu') d\mu' \right] e^{i\Sigma_t \lambda x} d\lambda = 0 \quad . \tag{2.9}$$

The linear independence of the Fourier modes $e^{i\Sigma_t \lambda x}$ implies for each λ

$$A^{(\ell+1)}(\lambda,\mu) = \frac{c}{2} \frac{1}{1+i\lambda\mu} \int_{-1}^{1} A^{(\ell)}(\lambda,\mu') d\mu' \ , \ -\infty < \lambda < \infty \ , \ -1 \le \mu \le 1 \ , \tag{2.10}$$

where $c = \Sigma_s / \Sigma_t$ is the scattering ratio; we assume $c < 1$ so that the infinite medium problem has a solution. Integrating Eq. (2.10) over μ, we find

$$\int_{-1}^{1} A^{(\ell+1)}(\lambda,\mu') d\mu' = \omega(\lambda) \int_{-1}^{1} A^{(\ell)}(\lambda,\mu') d\mu' \quad , \tag{2.11}$$

where

$$\omega(\lambda) \equiv c \int_0^1 \frac{d\mu}{1+\lambda^2\mu^2} = \frac{c}{\lambda} \tan^{-1} \lambda \quad . \tag{2.12}$$

Eq. (2.11) implies for $\ell \ge 0$

$$\int_{-1}^{1} A^{(\ell)}(\lambda,\mu') d\mu' = \omega^{\ell}(\lambda) \int_{-1}^{1} A^{(0)}(\lambda,\mu') d\mu' \quad , \tag{2.13}$$

and we obtain from Eq. (2.10)

$$A^{(\ell+1)}(\lambda,\mu) = \frac{c}{2} \frac{\omega^{\ell}(\lambda)}{1+i\lambda\mu} \left(\int_{-1}^{1} A^{(0)}(\lambda,\mu') d\mu' \right) \quad . \tag{2.14}$$

Thus, Eq. (2.8) yields for $\ell \ge 0$,

$$f^{(\ell+1)}(x,\mu) = \int_{-\infty}^{\infty} \frac{c}{2} \frac{\omega^{\ell}(\lambda)}{1+i\lambda\mu} \left(\int_{-1}^{1} A^{(0)}(\lambda,\mu') d\mu' \right) e^{i\Sigma_t \lambda x} d\lambda \quad . \tag{2.15}$$

This explicitly defines $f^{(\ell+1)}(x,\mu)$ in terms of the Fourier expansion coefficients $A^{(0)}$ of the initial error $f^{(0)}$. For reasonable initial errors, Eq. (2.15) implies

$$\begin{aligned} \left| f^{(\ell+1)}(x,\mu) \right| &\le \frac{c}{2} \int_{-\infty}^{\infty} |\omega(\lambda)|^{\ell} \left| \int_{-1}^{1} A^{(0)}(\lambda,\mu') d\mu' \right| d\lambda \\ &\le \left[\frac{c}{2} \int_{-\infty}^{\infty} \left| \int_{-1}^{1} A^{(0)}(\lambda,\mu') d\mu' \right| d\lambda \right] \sigma_{SI}^{\ell} \\ &= B \sigma_{SI}^{\ell} \ , \end{aligned} \tag{2.16}$$

where B is a constant, and

$$\sigma_{SI} = \max_{-\infty<\lambda<\infty} \omega(\lambda) = \max_{-\infty<\lambda<\infty} \left(\frac{c}{\lambda}\tan^{-1}\lambda\right) = \omega(0) = c \tag{2.17}$$

is the *spectral radius* [the magnitude of the largest iteration eigenvalue = largest value of $|\omega(\lambda)|$] of the iteration scheme. Eq. (2.16) becomes

$$\left|f^{(\ell+1)}(x,\mu)\right| \leq Bc^{\ell} \quad . \tag{2.18}$$

Thus, the error in the ℓ-th iterate decreases as c^{ℓ}. If c is small, the convergence is rapid, but as c approaches unity, the convergence becomes arbitrarily slow. This is consistent with the physical interpretation of the SI scheme.

The above Fourier analysis demonstrates several things. First, Eq. (2.7) for $f^{(\ell)}$ is identical to Eq. (2.5) for $\psi^{(\ell)}$ if we set $Q = 0$. Second, if the error in the starting guess consists of a single Fourier mode:

$$f^{(0)}(x,\mu) = a(\mu)e^{i\Sigma_t\lambda x} \quad , \tag{2.19}$$

then for all $\ell \geq 0$, only this single mode persists and

$$f^{(\ell+1)}(x,\mu) = \omega^{\ell}(\lambda)\left[\frac{c}{2}\frac{1}{1+i\lambda\mu}\left(\int_{-1}^{1} a(\mu')d\mu'\right)\right]e^{i\Sigma_t\lambda x} \quad . \tag{2.20}$$

Hence, the Fourier modes for different λ are independent, and to determine $\omega(\lambda)$, it is only necessary to consider the single Fourier mode defined by Eq. (2.19). Third, the rate of convergence for a general initial guess is the maximum value of $|\omega(\lambda)|$, the spectral radius of the iteration operator. Fourth, the maximum value of ω occurs for $\lambda \approx 0$. The $\lambda \approx 0$ modes correspond to long wavelengths; these are error modes that span large optical distances and have weak spatial gradients. By Eq. (2.20), the angular dependence of these modes is also weak:

$$\frac{1}{1+i\lambda\mu} = 1 - i\lambda\mu + O(\lambda^2) \quad . \tag{2.21}$$

Thus, *in the SI scheme, the most slowly converging component of the iterative solution has weak spatial and angular dependence.* Source Iteration efficiently suppresses the error modes with strong spatial and angular variation ($|\lambda| >> 0$), but not the error modes with weak spatial and angular variation ($\lambda \approx 0$). The acceleration methods discussed below more efficiently suppress the error modes with weak spatial and angular variation. This comes at a price, because each accelerated iteration is more costly than an SI iteration. However, this extra work per iteration usually more than pays for itself by greatly reducing the total number of iterations.

II.B. Diffusion Synthetic Acceleration (DSA)

Next we consider preconditioning schemes, commonly referred to in the transport literature as "synthetic acceleration" schemes. As discussed in Chapter I, each preconditioned iteration begins with one source iteration (i.e., one transport sweep):

$$\mu\frac{\partial\psi^{(\ell+1/2)}}{\partial x}(x,\mu)+\Sigma_t(x)\psi^{(\ell+1/2)}(x,\mu)=\frac{\Sigma_s(x)}{2}\phi^{(\ell)}(x)+\frac{Q(x)}{2} \quad , \tag{2.22}$$

$$\psi^{(\ell+1/2)}(0,\mu)=\psi^{i}(\mu) \quad , \quad 0<\mu\leq 1 \quad , \tag{2.23}$$

$$\psi^{(\ell+1/2)}(X,\mu)=\psi^{(\ell+1/2)}(X,-\mu) \quad , \quad -1\leq\mu<0 \quad . \tag{2.24}$$

We subtract these equations from the original transport equations (1.1)-(1.3) and rearrange to obtain exact equations for the linear correction:

$$f(x,\mu)\equiv\psi(x,\mu)-\psi^{(\ell+1/2)}(x,\mu) \quad . \tag{2.25}$$

Defining

$$\phi^{(\ell+1/2)}(x)=\int_{-1}^{1}\psi^{(\ell+1/2)}(x,\mu)d\mu \quad , \tag{2.26}$$

we obtain:

$$\mu\frac{\partial f}{\partial x}(x,\mu)+\Sigma_t(x)f(x,\mu)-\frac{\Sigma_s(x)}{2}\int_{-1}^{1}f(x,\mu')d\mu'=\frac{\Sigma_s(x)}{2}\left[\phi^{(\ell+1/2)}(x)-\phi^{(\ell)}(x)\right] \quad , \tag{2.27}$$

$$f(0,\mu)=0 \quad , \quad 0<\mu\leq 1 \quad , \tag{2.28}$$

$$f(X,\mu)=f(X,-\mu) \quad , \quad -1\leq\mu<0 \quad . \tag{2.29}$$

As noted earlier, this transport problem for f is just as difficult to solve as the original problem for ψ. Thus, one is motivated to replace this problem by an approximate problem that can be solved more efficiently. We have shown that the first step in this algorithm, Eqs. (2.22)-(2.24), effectively suppresses error modes with strong angular and spatial dependence, but not error modes with weak angular and spatial dependence. To obtain an efficient scheme, the approximation chosen for Eqs. (2.27)-(2.29) should be most accurate when f has weak angular and spatial dependence.

One approximation to Eqs. (2.27)-(2.29) that satisfies this condition is the well-known P_1, or diffusion approximation [4, 1]. This leads to the Diffusion Synthetic Acceleration (DSA) scheme [26, 27, 51, 63, 93], which we sometimes call *Diffusion Preconditioning*:

$$-\frac{d}{dx}\frac{1}{3\Sigma_t(x)}\frac{dF^{(\ell+1)}}{dx}(x)+\Sigma_a(x)F^{(\ell+1)}(x)=\Sigma_s(x)\left(\phi^{(\ell+1/2)}(x)-\phi^{(\ell)}(x)\right) \quad , \tag{2.30}$$

$$F^{(\ell+1)}(0)-\frac{2}{3\Sigma_t(0)}\frac{dF^{(\ell+1)}}{dx}(0)=0 \quad , \tag{2.31}$$

$$\frac{dF^{(\ell+1)}}{dx}(X) = 0 \quad . \tag{2.32}$$

Here, $F^{(\ell+1)}(x)$ is an approximation to the scalar flux component of $f(x,\mu)$:

$$F^{(\ell+1)}(x) \approx \int_{-1}^{1} f(x,\mu)d\mu \quad . \tag{2.33}$$

Thus, using this approximation, integrating Eq. (2.25) over μ, and rearranging, we obtain

$$\phi^{(\ell+1)}(x) = \phi^{(\ell+1/2)}(x) + F^{(\ell+1)}(x) \quad . \tag{2.34}$$

The full DSA scheme is defined as follows. At the beginning of an iteration, one has an estimate of $\phi^{(\ell)}(x)$, known either from the previous iteration or from the initial guess if $\ell = 0$. In the first stage of an iteration, Eqs. (2.22)-(2.24) are solved for $\psi^{(\ell+1/2)}(x,\mu)$ and Eq. (2.26) determines $\phi^{(\ell+1/2)}(x)$. This is a *source iteration*, or a *transport sweep*. In the second stage of an iteration, the low-order diffusion problem (2.30)-(2.32) is solved for the correction $F^{(\ell+1)}(x)$, and $\phi^{(\ell+1)}(x)$ is defined by Eq. (2.34). If the low-order stage of the DSA scheme is suppressed and $F^{(\ell+1)}(x)$ is set to zero, one obtains the basic SI scheme.

The difference between the SI and DSA schemes is the extra low-order diffusion calculation for the additive correction $F^{(\ell+1)}(x)$. Because of this extra step, one DSA iteration is more costly than one source iteration. This extra cost is justified if the number of DSA iterations required for convergence is sufficiently smaller than the required number of source iterations. We will now show that this is the case for the great majority of problems of interest.

To analyze the convergence properties of the DSA scheme, we consider the model infinite-medium problem discussed above. The DSA equations reduce to:

$$\mu\frac{\partial\psi^{(\ell+1/2)}}{\partial x}(x,\mu) + \Sigma_t\psi^{(\ell+1/2)}(x,\mu) = \frac{\Sigma_s}{2}\phi^{(\ell)}(x) + \frac{Q(x)}{2} \quad , \tag{2.35}$$

$$\phi^{(\ell+1/2)}(x) = \int_{-1}^{1} \psi^{(\ell+1/2)}(x,\mu)d\mu \quad , \tag{2.36}$$

$$-\frac{1}{3\Sigma_t}\frac{d^2F^{(\ell+1)}}{dx^2}(x) + \Sigma_a F^{(\ell+1)}(x) = \Sigma_s\left(\phi^{(\ell+1/2)}(x) - \phi^{(\ell)}(x)\right) \quad , \tag{2.37}$$

$$\phi^{(\ell+1)}(x) = \phi^{(\ell+1/2)}(x) + F^{(\ell+1)}(x) \quad . \tag{2.38}$$

By taking $Q(x) = 0$, Eqs. (2.35)-(2.38) become the equations for the iteration error. If we consider a single Fourier error mode with arbitrary $-\infty < \lambda < \infty$ and set

$$\phi^{(\ell)}(x) = \omega^{\ell}(\lambda)e^{i\Sigma_t\lambda x} \quad , \tag{2.39}$$

$$\psi^{(\ell+1/2)}(x,\mu) = \omega^{\ell}(\lambda)\alpha(\lambda,\mu)e^{i\Sigma_t\lambda x} \quad , \tag{2.40}$$

$$\phi^{(\ell+1/2)}(x) = \omega^{\ell}(\lambda)\beta(\lambda)e^{i\Sigma_t\lambda x} \quad , \tag{2.41}$$

$$F^{(\ell+1)}(x) = \omega^{\ell}(\lambda)\gamma(\lambda)e^{i\Sigma_t\lambda x} \quad , \tag{2.42}$$

then Eqs. (2.35)-(2.38) reduce to the following equations for $\alpha(\lambda,\mu)$, $\beta(\lambda)$, $\gamma(\lambda)$ and $\omega(\lambda)$:

$$(i\lambda\mu+1)\alpha(\lambda,\mu) = \frac{c}{2} \quad , \tag{2.43}$$

$$\beta(\lambda) = \int_{-1}^{1} \alpha(\lambda,\mu)d\mu \quad , \tag{2.44}$$

$$\left(\frac{\lambda^2}{3}+1-c\right)\gamma(\lambda) = c[\beta(\lambda)-1] \quad , \tag{2.45}$$

$$\omega(\lambda) = \beta(\lambda)+\gamma(\lambda) \quad . \tag{2.46}$$

These equations readily yield:

$$\alpha(\lambda,\mu) = \frac{c}{2}\frac{1}{1+i\lambda\mu} \quad , \tag{2.47}$$

$$\beta(\lambda) = c\int_0^1 \frac{d\mu}{1+\lambda^2\mu^2} = \frac{c}{\lambda}\tan^{-1}\lambda \quad , \tag{2.48}$$

$$\gamma(\lambda) = \frac{3c}{\lambda^2+3(1-c)}\left(\frac{c}{\lambda}\tan^{-1}\lambda - 1\right) \quad , \tag{2.49}$$

and

$$\begin{aligned}\omega(\lambda) &= c\left[\frac{\lambda^2}{\lambda^2+3(1-c)}\right]\int_0^1 \frac{1-3\mu^2}{1+\lambda^2\mu^2}d\mu \\ &= \frac{3c}{\lambda^2+3(1-c)}\left[\left(\frac{\lambda^2}{3}+1\right)\frac{\tan^{-1}\lambda}{\lambda} - 1\right] \quad .\end{aligned} \tag{2.50}$$

[In Eq. (2.50), ω depends on both λ and c. In the ensuing discussion, if it is necesary to indicate the c-dependence of ω, we write $\omega_c(\lambda)$; otherwise, we simply write $\omega(\lambda)$ as shown.]

The functions $\beta(\lambda)$ (the Fourier eigenvalue for SI) and $\omega(\lambda)$ (the Fourier eigenvalue for DSA) are even functions of λ and are plotted in Figure 1 for $\lambda \geq 0$ and $c = 1$. For $c = 1$, the spectral radius of the SI scheme $\sigma_{SI} = 1$, while the spectral radius of the DSA scheme $\sigma_{DSA} \approx 0.2247$. For all λ, $0 \leq \omega(\lambda) \leq \beta(\lambda)$, and $\omega \to 0$ as $\lambda \to 0$ or $\lambda \to \infty$. Thus, the DSA scheme efficiently suppresses the error modes that have strong spatial and angular dependence *and* those that have weak spatial and angular dependence.

A comparison of the effectiveness of SI and DSA may be obtained from Eq. (2.50) by noting that for any c,

$$\omega_c(\lambda) \leq \omega_1(\lambda)c \leq 0.2247c \quad . \tag{2.51}$$

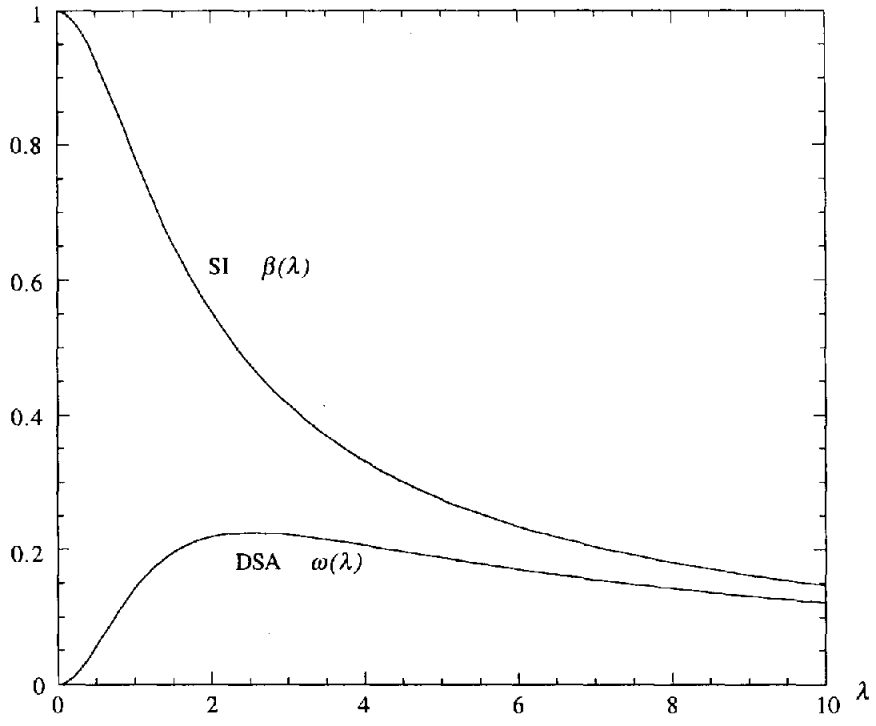

Figure 1: β and ω versus λ for the SI and DSA Schemes ($c = 1$)

The number of iterations ℓ_{DSA} necessary to reduce the DSA iteration error by m orders of magnitude satisfies, approximately,

$$10^{-m} \approx (0.2247c)^{\ell_{\text{DSA}}} \quad . \tag{2.52}$$

Hence, for all $0 \leq c \leq 1$ we have the approximate upper bound

$$\ell_{\text{DSA}} \approx \left(\frac{\ln 10}{\ln \frac{1}{0.2247} + \ln \frac{1}{c}} \right) m \leq 1.54m \quad . \tag{2.53}$$

This shows that the DSA scheme converges very rapidly for all $0 \leq c \leq 1$. (Since Eq. (2.51) is an upper bound to $\omega_c(\lambda)$, sharp only for $c \approx 1$, then Eq. (2.53) is an upper bound on ℓ_{DSA}, which is sharp only for $c \approx 1$.) The number of iterations ℓ_{SI} required for the SI iteration error to reduce by the same amount is

$$\ell_{\text{SI}} \approx \left(\frac{\ln 10}{\ln \frac{1}{c}} \right) m \quad , \tag{2.54}$$

and this number tends to ∞ as $c \to 1$. For example, if $c = 0.999$, Eq. (2.54) yields $\ell_{\text{SI}} = 2301m$.

In 1-D problems, each diffusion calculation is extremely fast and requires only a small fraction of the cost of a transport sweep (one source iteration). In multidimensional problems, each diffusion calculation in the TWODANT code is approximately as costly as one complete S_4 transport sweep (using all S_4 coordinate directions). Assuming that this is the case in general, then one DSA iteration costs roughly twice as much as one SI iteration, and DSA is more computationally efficient than SI if DSA requires less than half as many iterations as SI. Further, assuming that the spectral radius of DSA is less than $0.2247c$ in general problems and using Eqs. (2.53) and (2.54), we may express the condition that DSA be more efficient than SI in general problems as:

$$\left(\frac{\ln 10}{\ln \frac{1}{0.2247} + \ln \frac{1}{c}}\right) \leq \frac{1}{2}\left(\frac{\ln 10}{\ln \frac{1}{c}}\right) \quad . \tag{2.55}$$

This is satisfied for $0.2247 < c \leq 1$. A more careful analysis, using Eq. (2.50) rather than Eq. (2.51) to make the comparisons, shows that DSA is more efficient than SI for roughly $0.1 < c \leq 1$. Therefore, DSA is *much* more efficient than SI for $c \approx 1$ and remains more efficient for c as small as 0.1. For $c < 0.1$, SI is at best twice as efficient as DSA, but here both schemes converge extremely rapidly. This comparison becomes even more favorable to DSA if the quadrature set is finer than S_4.

II.C. S_2 Synthetic Acceleration (S_2SA)

The S_2 preconditioning (S_2SA) scheme differs from DSA in that the problem for the exact transport correction is approximated by an S_2 rather than a diffusion problem [113, 142]. The first (high-order) stage of the S_2SA scheme is given by Eqs. (2.22)-(2.24) and (2.26). The second (low-order) stage is given by the S_2 problem:

$$\pm\frac{1}{\sqrt{3}}\frac{df_{\pm}^{(\ell+1)}}{dx}(x) + \Sigma_t(x) f_{\pm}^{(\ell+1)}(x) - \frac{\Sigma_s(x)}{2}\left(f_{+}^{(\ell+1)}(x) + f_{-}^{(\ell+1)}(x)\right)$$

$$= \frac{\Sigma_s(x)}{2}\left(\phi^{(\ell+1/2)}(x) - \phi^{(\ell)}(x)\right) \quad , \tag{2.56}$$

$$f_{+}^{(\ell+1)}(0) = 0 \quad , \tag{2.57}$$

$$f_{-}^{(\ell+1)}(X) = f_{+}^{(\ell+1)}(X) \quad , \tag{2.58}$$

and the update equation

$$\phi^{(\ell+1)}(x) = \phi^{(\ell+1/2)}(x) + f_{+}^{(\ell+1)}(x) + f_{-}^{(\ell+1)}(x) \quad . \tag{2.59}$$

[In these equations, $f_{\pm}(x)$ is the flux of particles traveling in the $\pm$ direction.]

The infinite medium Fourier analysis for the S_2SA scheme yields the same result as DSA, because in planar geometry, the S_2 and P_1 equations are algebraically equivalent.

Thus, the infinite medium Fourier analysis predicts that the S_2SA and DSA schemes have the same rapid convergence properties in planar geometry. (However, the S_2SA and DSA methods are not equivalent in 2-D and 3-D geometries.)

The main practical advantage of the S_2SA scheme over the DSA scheme is that one can use the same spatial discretization scheme for the low-order S_2 equations and the high-order S_N equations. This eliminates the issue of consistent diffusion differencing present in the DSA scheme. The disadvantage of the S_2SA scheme is that it is generally more costly to solve the discrete S_2 equations (2.56)-(2.58) than the discrete diffusion equations (2.30)-(2.32). Thus, the S_2SA scheme has been used mostly in 1-D geometries, where it is practical to directly solve the discretized equations (2.56)-(2.58). In multidimensional geometries (*i*) it may not be practical to solve these equations directly, and (*ii*) the S_2SA scheme does not have the same small spectral radius as DSA.

II.D. KP Methods

Lebedev's "KP Method" is actually a family of methods. A particular member of this family is denoted $KP_1(n_1)P_2(n_2)...P_\alpha(n_\alpha)$. As discussed earlier, "K" denotes a transport sweep, $P_i(n_i)$ denotes a low-order operation involving a differential operator of order $2n_i$, and α is the number of different low-order operations in one full iteration. A rich variety of methods is obtained by different choices of α and n_i, and there are also variations possible within the low-order operation associated with a given n_i.

Let us consider first a KP method with one low-order level, i.e., a method denoted by $KP_1(n_1)$. If $n_1 = 1$, then the low-order operator is a second-order differential operator. The obvious choice is the diffusion operator, which gives the DSA scheme described above. That is, one variant of $KP_1(1)$ is exactly the DSA method as we have presented it. Lebedev also studied variants in which the diffusion coefficient in Eq. (2.30), $1/(3\Sigma_t)$, is generalized to q/Σ_t, with q a user-defined parameter. For $q = 1/3$ Lebedev obtained the result σ = spectral radius $\leq 0.225c$ (Section XI.10 of [10]), but he also found the optimal value $q = 0.281$ that yields $\sigma \leq 0.186c$. (Much later, Azmy performed an optimization that was similar in spirit, with very similar results [160].) Lebedev studied other variants of $KP_1(1)$ as well (see Section XI.10 of [10]).

The $KP_1(1)P_2(0)$ method, for 1-D planar geometry with isotropic scattering, is:

$$\mu\frac{\partial\psi^{(\ell+1/3)}}{\partial x}(x,\mu)+\Sigma_t(x)\psi^{(\ell+1/3)}(x,\mu)=\frac{\Sigma_s(x)}{2}\phi^{(\ell)}(x)+\frac{Q(x)}{2} \quad , \tag{2.60}$$

$$-\frac{d}{dx}\frac{1}{3\Sigma_t(x)}\frac{dF^{(\ell+2/3)}}{dx}(x)+\Sigma_a(x)F^{(\ell+2/3)}(x)=\Sigma_s(x)\left(\phi^{(\ell+1/3)}(x)-\phi^{(\ell)}(x)\right) \quad , \tag{2.61}$$

$$\phi^{(\ell+2/3)}(x)=\phi^{(\ell+1/3)}(x)+F^{(\ell+2/3)}(x) \quad , \tag{2.62}$$

$$F^{(\ell+1)}(x) = \frac{\beta c}{1-\beta c}\left(\phi^{(\ell+2/3)}(x) - \phi^{(\ell)}(x)\right) \quad , \tag{2.63}$$

$$\phi^{(\ell+1)}(x) = \phi^{(\ell+2/3)}(x) + F^{(\ell+1)}(x) \quad , \tag{2.64}$$

where β is a user-defined parameter. Along with Eqs. (2.60) and (2.61), of course, are suitable boundary conditions such as those shown previously for the DSA method. The second low-order equation, Eq. (2.63), is algebraic and needs no boundary condition. If $\beta = 0$ in this equation, then $F^{(\ell+1)} = 0$ and the method reduces to DSA. For $\beta \neq 0$, an opportunity exists to improve on the performance of DSA by choosing β wisely.

Performing a Fourier Analysis of this $KP_1(1)P_2(0)$ method and leaving β as a parameter, we obtain the following expression for the iteration eigenvalue for the error mode with wave number λ:

$$\begin{aligned}\omega(\lambda) &= \frac{1}{1-\beta c}\left[\omega_{DSA}(\lambda) - \beta c\right] \\ &= \frac{c}{1-\beta c}\left\{\frac{1}{\lambda^2 + 3(1-c)}\left[\left(\frac{\lambda^2}{3}+1\right)\frac{\tan^{-1}\lambda}{\lambda} - 1\right] - \beta\right\} \quad .\end{aligned} \tag{2.65}$$

Using a slightly different approach, Lebedev determined that for this scheme the spectral radius, σ, is minimized by the choice $\beta \approx 1/8.88$ (Section XI.11 of [10]). For this value of β he obtained the bound

$$\sigma \leq 0.127c \quad .$$

In Figure 2 we plot $\omega(\lambda)$ for $KP_1(1)P_2(0)$ using several different values for β; we also show the DSA ($\beta = 0$) result for comparison. Our results agree with Lebedev's, both in the value of β that minimizes σ and in the resulting value for the spectral radius σ.

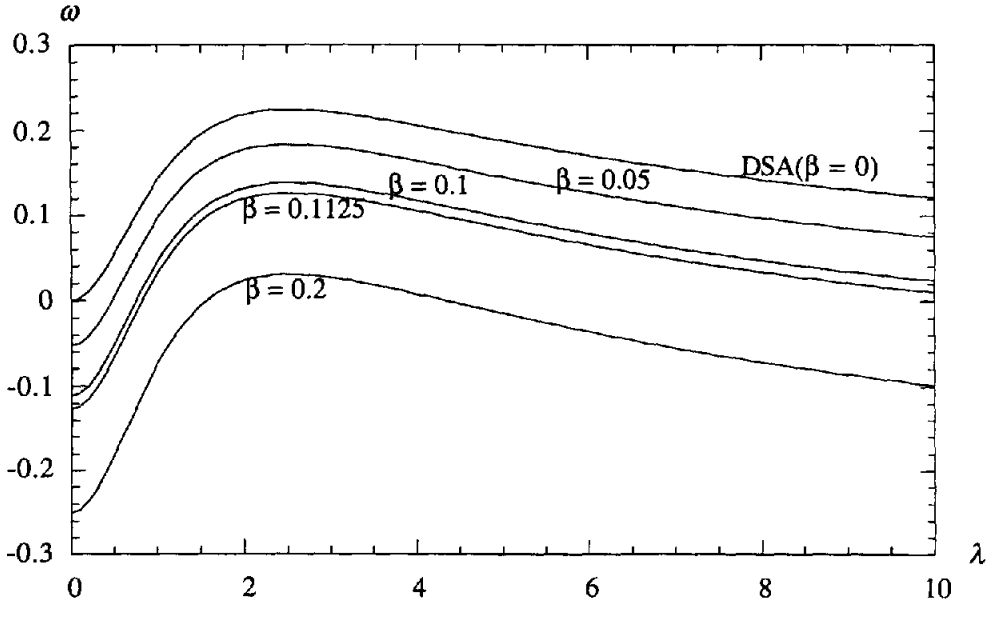

Figure 2: ω versus λ for the $KP_1(1)P_2(0)$ Method ($c = 1$)

Thus, the two extra steps in the $PK_1(1)P_2(0)$ method, Eqs. (2.63) and (2.64), can yield a method with a smaller spectral radius than DSA.

II.E. Transport Synthetic Acceleration (TSA)

The Transport Synthetic Acceleration (TSA) method, developed by Ramoné, Adams, and Nowak [243], is similar to the S_2SA scheme in that a low-order S_N problem is solved for the transport correction. If the low-order quadrature set is chosen to be S_2 (sometimes S_4 is a better choice), then the low-order TSA problem contains Eq. (2.66) as the S_2 approximation to Eq. (2.56):

$$\pm\frac{1}{\sqrt{3}}\frac{df_{\pm}^{(\ell+1)}}{dx}(x)+[\Sigma_t(x)-\beta\Sigma_s(x)]f_{\pm}^{(\ell+1)}(x)-\frac{(1-\beta)\Sigma_s(x)}{2}\left(f_{+}^{(\ell+1)}(x)+f_{-}^{(\ell+1)}(x)\right)$$

$$=\frac{\Sigma_s(x)}{2}\left(\phi^{(\ell+1/2)}(x)-\phi^{(\ell)}(x)\right) \quad . \tag{2.66}$$

Here, the free parameter β satisfies $0 \le \beta \le 1$. If $\beta = 0$, the TSA scheme becomes identical to the S_2SA scheme. For $0 < \beta \le 1$, Eq. (2.66) agrees with Eq. (2.56) if $f^{(\ell+1)}(x,\mu)$ is isotropic, which corresponds to the $\lambda = 0$ error mode. Therefore, for $0 \le \beta \le 1$, the TSA scheme should suppress the most slowly converging ($\lambda \approx 0$) error modes of the unaccelerated SI scheme.

Unlike the S_2SA scheme, the TSA scheme is envisioned for multidimensional problems in which it is impractical to solve the low-order problems directly. Thus, in practice, one solves the low-order TSA equations using Source Iteration and possibly other algebraic acceleration schemes. In the following discussion, we describe these transpowrt sweeps (to converge $f_{\pm}^{(\ell+1)}$) as *inner* iterations. Also, we describe the DSA iterations (to converge ψ as *outer* iterations. (This terminology is intended to be reminiscent of the inner and outer iterations used to converge multigroup transport problems.)

The parameter β plays a crucial role in the TSA scheme. As β increases from 0 to 1, the TSA scheme is affected in the following ways:

1. Assuming only Source Iterations for the *inner iterations* (to converge $f_{\pm}^{(\ell+1)}$) the inner-iteration spectral radius is

$$\hat{c} \equiv \frac{(1-\beta)\Sigma_s}{\Sigma_t - \beta\Sigma_s} = \frac{(1-\beta)c}{1-\beta c} \quad , \tag{2.67}$$

where $c = \Sigma_s/\Sigma_t$ is the scattering ratio. Thus, for $c < 1$, as β increases, $\hat{c}$ decreases. In fact, for $\beta = 1$, the inner iteration spectral radius becomes zero. (In this case, the TSA scheme reduces to the "Two-Step" acceleration scheme proposed independently by Morozov [28] and Larsen and Miller [110].)

2. Unfortunately, as β increases, the spectral radius of the outer iterations (to converge ψ) increases. For planar geometry problems with isotropic scattering, the spectral radius of the outer iterations remains less than c, so the acceleration method is somewhat effective even for $\beta = 1$. For more complicated problems in multidimensional geometries or with anisotropic scattering, the spectral radius can exceed unity for β close to unity. In such problems, β must be kept sufficiently small to maintain convergence of the outer iterations.

3. In practice, one does not fully converge the low-order TSA problem in each iteration; instead, it is iterated only a fixed number of times (M). The overall efficiency of the TSA scheme then depends on the parameters of the original problem, and on the choice of β and M. For optimal choices of β and M, the TSA scheme can dramatically reduce the SI computational cost [243]. However, these optimal values of β and M are problem-dependent, and for optically thick problems with very small absorption, the spectral radius of the TSA scheme (with fixed M) still approaches unity.

If the low-order TSA quadrature set is S_2 and M transport sweeps are employed in this low-order problem per outer iteration, then the TSA scheme for the model infinite homogeneous medium problem is defined by:

$$\mu \frac{\partial \psi^{(\ell+1/2)}}{\partial x}(x,\mu) + \Sigma_t \psi^{(\ell+1/2)}(x,\mu) = \frac{\Sigma_s}{2}\phi^{(\ell)}(x) + \frac{Q(x)}{2} \quad , \tag{2.68}$$

$$\phi^{(\ell+1/2)}(x) = \int_{-1}^{1} \psi^{(\ell+1/2)}(x,\mu')d\mu' \quad , \tag{2.69}$$

$$f_{\pm}^{(\ell+1,0)}(x) = 0 \quad , \tag{2.70}$$

$$\pm \frac{1}{\sqrt{3}} \frac{df_{\pm}^{(\ell+1,m)}}{dx}(x) + (\Sigma_t - \beta\Sigma_s) f_{\pm}^{(\ell+1,m)}(x) = \frac{(1-\beta)\Sigma_s}{2}\left(f_{+}^{(\ell+1,m-1)}(x) + f_{-}^{(\ell+1,m-1)}(x)\right)$$
$$+ \frac{\Sigma_s(x)}{2}\left(\phi^{(\ell+1/2)}(x) - \phi^{(\ell)}(x)\right) \quad , \quad 1 \le m \le M \quad , \tag{2.71}$$

$$\phi^{(\ell+1)}(x) = \phi^{(\ell+1/2)}(x) + f_{+}^{(\ell+1,M)}(x) + f_{-}^{(\ell+1,M)}(x) \quad . \tag{2.72}$$

The Fourier analysis for this problem yields the following expression for $\omega(\lambda)$:

$$\omega = \frac{c}{\lambda}\tan^{-1}\lambda - \left(\frac{3c(1-\beta c)}{\lambda^2 + 3(1-c)(1-\beta c)}\right)\left(1 - \frac{c}{\lambda}\tan^{-1}\lambda\right)$$
$$\times \left[1 - \left(\frac{3c(1-\beta c)(1-\beta)}{\lambda^2 + 3(1-\beta c)^2}\right)^M\right] . \tag{2.73}$$

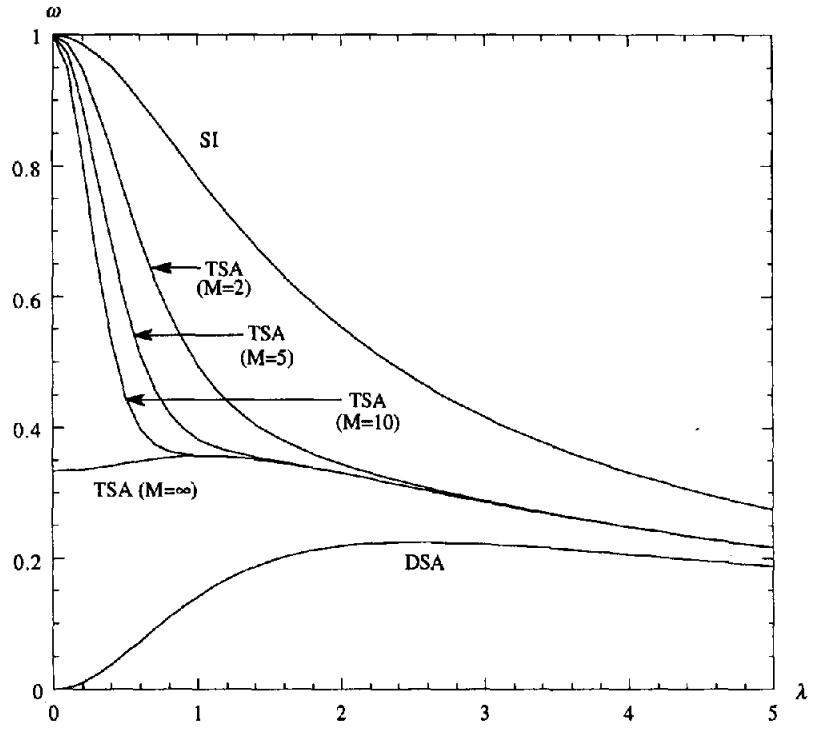

Figure 3: ω versus λ for the SI, TSA and DSA Schemes ($c = 1, \beta = 1/3$)

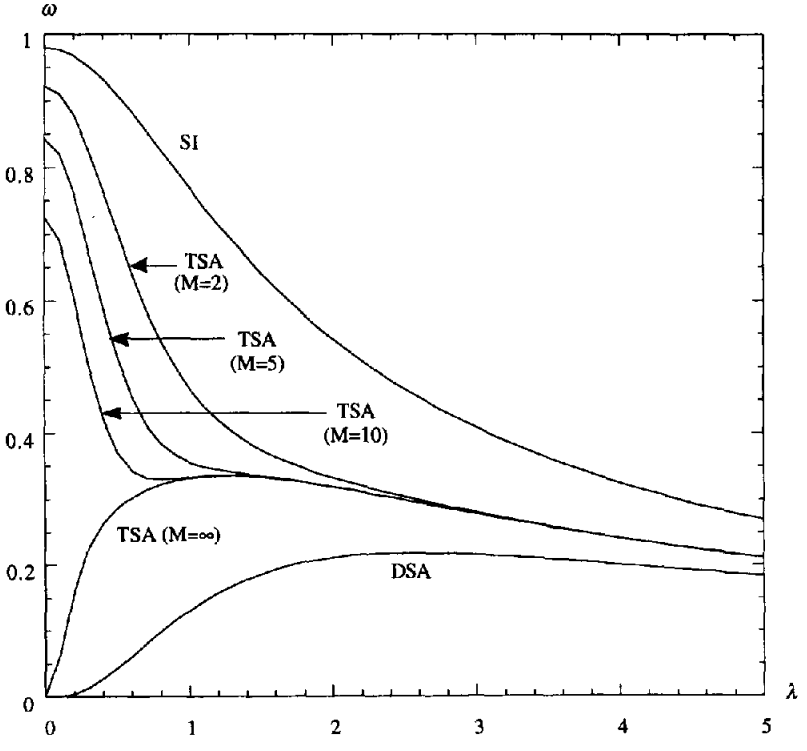

Figure 4: ω versus λ for the SI, TSA and DSA Schemes ($c = 0.98, \beta = 1/3$)

As expected, Eq. (2.73) limits to the DSA result as $\beta \to 0$ and $M \to \infty$. Using Eq. (2.73), we have plotted ω versus λ in Figure 3 for $c = 1.0, \beta = 1/3$, and $M = 5, 10, 20$, and ∞ (fully converged inner iterations). In Figure 4, we plot similar results for $c = 0.98$. It is clear that the (outer iteration) spectral radius of the TSA method is less than that of the SI scheme and larger than that of the DSA (and S_2SA) schemes for all values of M, including $M = \infty$. Also, the TSA spectral radius decreases as one converges more completely the low-order problem (increases M). To achieve maximum overall efficiency in the TSA scheme, an optimal balance must be found between the relative expenses of the high-order and the low-order calculations.

While the development shown here assumes isotropic scattering, TSA can be applied to problems with anisotropic scattering as well. Ramoné et al. did not analyze or test this; they proposed to simply use isotropic scattering in the low-order problem, even when the high-order problem has anisotropic scattering. The logic behind this idea is that the low-order problem already ignores a portion of the scattering; given this, it seems that one might as well choose the simplest possible distribution (isotropic) of the scattered particles.

II.F. The Lewis-Miller (LM) Methods

Next, we discuss the *Second-Moment* scheme proposed by Lewis and Miller [61]. Although this is not a preconditioning (synthetic) method, we show that it is very closely related to both the linear DSA and nonlinear Quasidiffusion schemes.

For the problem described by Eqs. (1.1)-(1.3), one iteration of this scheme begins with a source iteration [Eqs. (2.22)-(2.24)]. Lewis and Miller's concept is to derive a low-order diffusion problem directly for the scalar flux $\phi_0^{(\ell+1)}$, containing linear (additive) transport correction terms that vanish if the angular flux is a linear function of angle. (We show below that the QD strategy is similar, but there the transport correction terms in the low-order equation are *nonlinear*.) To derive the LM equations, we first calculate the zero-th and first angular moments of Eq. (2.22). Defining

$$\phi_n(x) = \int_{-1}^{1} P_n(\mu)\psi(x,\mu)d\mu \quad , \quad 0 \le n \le 2 \quad , \tag{2.74}$$

where $P_n(\mu)$ is the n-th Legendre polynomial, we obtain

$$\frac{d\phi_1^{(\ell+1/2)}}{dx}(x) + \Sigma_t(x)\phi_0^{(\ell+1/2)}(x) = \Sigma_s(x)\phi_0^{(\ell)}(x) + Q(x) \quad , \tag{2.75}$$

$$\frac{d}{dx}\left(\frac{1}{3}\phi_0^{(\ell+1/2)}(x) + \frac{2}{3}\phi_2^{(\ell+1/2)}(x)\right) + \Sigma_t(x)\phi_1^{(\ell+1/2)}(x) = 0 \quad . \tag{2.76}$$

Eq. (2.76) may be solved for $\phi_1^{(\ell+1/2)}$:

$$\phi_1^{(\ell+1/2)}(x) = -\frac{1}{3\Sigma_t(x)}\frac{d}{dx}\left(\phi_0^{(\ell+1/2)}(x) + 2\phi_2^{(\ell+1/2)}(x)\right) \quad . \tag{2.77}$$

Introducing this result into Eq. (2.75), we obtain:

$$-\frac{d}{dx}\frac{1}{3\Sigma_t(x)}\frac{d}{dx}\left(\phi_0^{(\ell+1/2)}(x)+2\phi_2^{(\ell+1/2)}(x)\right)+\Sigma_t(x)\phi_0^{(\ell+1/2)}(x)$$

$$=\Sigma_s(x)\phi_0^{(\ell)}(x)+Q(x) \quad . \tag{2.78}$$

As desired, this equation involves $\phi_0(x)$ and contains a transport correction term $\phi_2(x)$ that vanishes if $\psi(x,\mu)$ is a linear function of μ.

Lewis and Miller did not propose boundary conditions for their method. Here we derive boundary conditions containing additive transport correction terms that – like the additive correction term in the diffusion equation – vanish if $\psi^{(\ell+1)}$ is a linear function of μ.

Multiplying Eq. (2.23) by μ, integrating over the incident directions $0<\mu\leq 1$, and using Eq. (2.74), we obtain

$$\begin{aligned}
\int_0^1 \mu\psi^i(\mu)d\mu &= \int_0^1 \mu\psi^{(\ell+1/2)}(0,\mu)d\mu \\
&= \int_0^1 \mu\left[\frac{1}{2}\phi_0^{(\ell+1/2)}(0)+\frac{3\mu}{2}\phi_1^{(\ell+1/2)}(0)\right]d\mu \\
&\quad +\int_0^1 \mu\left[\psi^{(\ell+1/2)}(0,\mu)-\frac{1}{2}\phi_0^{(\ell+1/2)}(0)-\frac{3\mu}{2}\phi_1^{(\ell+1/2)}(0)\right]d\mu \\
&= \frac{1}{4}\phi_0^{(\ell+1/2)}(0)+\frac{1}{2}\phi_1^{(\ell+1/2)}(0)+\int_0^1 \mu\psi^{(\ell+1/2)}(0,\mu)d\mu \\
&\quad -\frac{1}{4}\int_{-1}^1 \psi^{(\ell+1/2)}(0,\mu)d\mu-\frac{1}{2}\int_{-1}^1 \mu\psi^{(\ell+1/2)}(0,\mu)d\mu \\
&= \frac{1}{4}\phi_0^{(\ell+1/2)}(0)+\frac{1}{2}\phi_1^{(\ell+1/2)}(0) \\
&\quad +\frac{1}{2}\int_{-1}^1 \left(|\mu|-\frac{1}{2}\right)\psi^{(\ell+1/2)}(0,\mu)d\mu \quad .
\end{aligned} \tag{2.79}$$

The final integral on the right side of this equation vanishes if $\psi^{(\ell+1/2)}(0,\mu)$ is a linear function of μ. Using Eq. (2.77), we eliminate $\phi_1^{(\ell+1/2)}$ to obtain:

$$\begin{aligned}
\int_0^1 \mu\psi^i(\mu)d\mu &= \frac{1}{4}\phi_0^{(\ell+1/2)}(0)-\frac{1}{6\Sigma_t(0)}\frac{d}{dx}\left(\phi_0^{(\ell+1/2)}(0)+2\phi_2^{(\ell+1/2)}(0)\right) \\
&+ \frac{1}{2}\int_{-1}^1 \left(|\mu|-\frac{1}{2}\right)\psi^{(\ell+1/2)}(0,\mu)d\mu \quad .
\end{aligned} \tag{2.80}$$

To derive an equation at the right boundary, we multiply Eq. (2.24) by μ and integrate over $-1\leq\mu<0$. Using Eq. (2.77), we obtain

$$0=\phi_1^{(\ell+1/2)}(X)=-\frac{1}{3\Sigma_t(X)}\frac{d}{dx}\left(\phi_0^{(\ell+1/2)}(X)+2\phi_2^{(\ell+1/2)}(X)\right) \quad . \tag{2.81}$$

As desired, Eqs. (2.80) and (2.81) involve $\phi_0^{(\ell+1)}$ on the boundaries and contain transport correction terms that vanish if $\psi^{(\ell+1)}$ is a linear function of μ.

One iteration of the "Second Moment" Lewis-Miller method consists of two stages. The first stage is a transport sweep, Eqs. (2.22)-(2.24), which determines $\psi^{(\ell+1/2)}(x,\mu)$; then $\phi_2^{(\ell+1/2)}$ is determined using Eq. (2.74). The second stage consists of Eqs. (2.78), (2.80), and (2.81), with all scalar flux terms replaced by $\phi_0^{(\ell+1)}$:

$$-\frac{d}{dx}\frac{1}{3\Sigma_t(x)}\frac{d}{dx}\phi_0^{(\ell+1)}(x)+\Sigma_a(x)\phi_0^{(\ell+1)}(x)=Q(x)+\frac{d}{dx}\frac{2}{3\Sigma_t(x)}\frac{d}{dx}\phi_2^{(\ell+1/2)}(x) \quad , \tag{2.82}$$

$$\begin{aligned}\phi_0^{(\ell+1)}(0)-\frac{2}{3\Sigma_t(0)}\frac{d\phi_0^{(\ell+1)}}{dx}(0) &= 4\int_0^1 \mu\psi^i(\mu)d\mu+\frac{4}{3\Sigma_t(0)}\frac{d\phi_2^{(\ell+1/2)}}{dx}(0)\\ &+ \int_{-1}^1 (1-2|\mu|)\,\psi^{(\ell+1/2)}(0,\mu)d\mu \quad ,\end{aligned} \tag{2.83}$$

$$\frac{d\phi_0^{(\ell+1)}}{dx}(X)=-2\frac{d\phi_2^{(\ell+1/2)}}{dx}(X) \quad . \tag{2.84}$$

This low-order problem has the form of a conventional diffusion problem for $\phi_0^{(\ell+1)}$.

If we now define the "correction"

$$F_0^{(\ell+1)}(x)\equiv\phi_0^{(\ell+1)}(x)-\phi_0^{(\ell+1/2)}(x) \tag{2.85}$$

and subtract Eqs. (2.82)-(2.84) from Eqs. (2.78), (2.80), and (2.81), we obtain equations for $F_0^{(\ell+1)}(x)$. These equations are identical to the DSA equations (2.30)-(2.32), and of course Eq. (2.85) is identical to Eq. (2.34). Thus, in the absence of spatial and angular discretizations, the DSA and Lewis-Miller methods are algebraically equivalent, so they have exactly the same convergence properties.

Lewis and Miller [61] also proposed a *First-Moment* scheme, which we will briefly mention here. As with the Second-Moment scheme, the first stage consists of a transport sweep, Eqs. (2.22)-(2.24). Now, using a slightly different approximation, the diffusion equation in Eq. (2.82) is replaced by:

$$-\frac{d}{dx}\frac{1}{3\Sigma_t(x)}\frac{d}{dx}\phi_0^{(\ell+1)}(x)+\Sigma_a(x)\phi_0^{(\ell+1)}(x)=Q(x)-\frac{d}{dx}\left(\phi_1^{(\ell+1/2)}(x)+\frac{1}{3\Sigma_T}\frac{d}{dx}\phi_0^{(\ell+1/2)}(x)\right) . \tag{2.86}$$

Lewis and Miller also did not propose boundary conditions to go with this acceleration equation, but it would be consistent to use Eqs. (2.83) and (2.84). Smith and Rhodes [283] have recently proposed a nonlinear method that is closely-related to the Lewis-Miller First Moment scheme.

II.G. The Quasidiffusion (QD) Method

This early method was formulated by Gol'din [25]. The main concept is similar to that of Lewis and Miller, except that the transport correction terms in Gol'din's low-order problem are formulated nonlinearly (as multiplicative terms), rather than linearly (as additive correction terms).

The Quasidiffusion (QD) method, just like the other acceleration methods discussed here, begins with a transport sweep, Eqs. (2.22)-(2.24). To derive the acceleration equations, we calculate the zero-th and first angular moments of Eq. (1.1):

$$\frac{d\phi_1}{dx}(x) + \Sigma_a(x)\phi_0(x) = Q(x) \quad , \tag{2.87}$$

$$\frac{d}{dx}\int_{-1}^{1} \mu^2 \psi(x,\mu)d\mu + \Sigma_t(x)\phi_1(x) = 0 \quad . \tag{2.88}$$

Next, we define the *Eddington factor:*

$$E(x) \equiv \frac{\int_{-1}^{1} \mu^2 \psi(x,\mu)d\mu}{\int_{-1}^{1} \psi(x,\mu)d\mu} \quad , \tag{2.89}$$

and we rewrite Eq. (2.88) as

$$\phi_1(x) = -\frac{1}{\Sigma_t(x)}\frac{d}{dx}E(x)\phi_0(x) \quad . \tag{2.90}$$

Using this result to eliminate ϕ_1 from Eq. (2.87), we obtain

$$-\frac{d}{dx}\frac{1}{\Sigma_t(x)}\frac{d}{dx}E(x)\phi_0(x) + \Sigma_a(x)\phi_0(x) = Q(x) \quad . \tag{2.91}$$

If $\psi(x,\mu)$ is a linear function of μ, then $E(x) = 1/3$ and Eq. (2.91) reduces to the conventional diffusion equation.

Gol'din's original [25], [42] boundary condition at $x = 0$ is obtained from the identity

$$\phi_1(0) = \int_0^1 \mu\psi^i(\mu)d\mu + \left(\frac{\int_{-1}^{0} \mu\psi(0,\mu)d\mu}{\int_{-1}^{0} \psi(0,\mu)d\mu}\right)\left(\phi_0(0) - \int_0^1 \psi^i(\mu)d\mu\right) \quad . \tag{2.92}$$

Defining the positive nonlinear functional

$$A \equiv \frac{\int_{-1}^{0} |\mu|\psi(0,\mu)d\mu}{\int_{-1}^{0} \psi(0,\mu)d\mu} \tag{2.93}$$

and using Eq. (2.90), we may rewrite Eq. (2.92) as

$$A\phi_0(0) - \frac{1}{\Sigma_t(0)}\frac{dE\phi_0}{dx}(0) = \int_0^1 (A+\mu)\psi^i(\mu)d\mu \quad . \tag{2.94}$$

An alternative equation for $\phi_0(0)$, proposed by Miften and Larsen [188], is also obtained from Eq. (2.92):

$$2\int_0^1 \mu\psi^i(\mu)d\mu = \int_{-1}^1 (|\mu|+\mu)\,\psi(0,\mu)d\mu = \int_{-1}^1 |\mu|\,\psi(0,\mu)d\mu + \phi_1(0) \quad . \tag{2.95}$$

Defining the *boundary Eddington Factor*

$$B \equiv \frac{\int_{-1}^1 |\mu|\,\psi(0,\mu)d\mu}{\int_{-1}^1 \psi(0,\mu)d\mu} \quad , \tag{2.96}$$

and using Eq. (2.90), we rewrite Eq. (2.95) as

$$B\phi_0(0) - \frac{1}{\Sigma_t(0)}\frac{dE\phi_0}{dx}(0) = \int_0^1 2\mu\psi^i(\mu)d\mu \quad . \tag{2.97}$$

If $\psi(0,\mu)$ is any linear function of μ, then $E(0) = 1/3$ and $B = 1/2$ and Eq. (2.97) reduces to the familiar Marshak boundary condition.

The QD boundary condition at the reflecting boundary $x = X$ is obtained by multiplying Eq. (1.3) by μ, integrating over the incoming directions, and using Eq. (2.90). This yields

$$0 = \phi_1(X) = -\frac{1}{\Sigma_t(X)}\frac{dE\phi_0}{dx}(X) \quad . \tag{2.98}$$

One full QD iteration now begins with a transport sweep, Eqs. (2.22)-(2.24). The angular flux $\psi^{(\ell+1/2)}(x,\mu)$ from this calculation is used to compute updated interior and boundary Eddington factors:

$$E^{(\ell+1/2)}(x) \equiv \frac{\int_{-1}^1 \mu^2\psi^{(\ell+1/2)}(x,\mu)d\mu}{\int_{-1}^1 \psi^{(\ell+1/2)}(x,\mu)d\mu} \quad , \quad 0 \le x \le X \quad , \tag{2.99}$$

$$A^{(\ell+1/2)} = \frac{\int_{-1}^0 |\mu|\,\psi^{(\ell+1/2)}(0,\mu)d\mu}{\int_{-1}^0 \psi^{(\ell+1/2)}(0,\mu)d\mu} \tag{2.100}$$

[or

$$B^{(\ell+1/2)} = \frac{\int_{-1}^1 |\mu|\,\psi^{(\ell+1/2)}(0,\mu)d\mu}{\int_{-1}^1 \psi^{(\ell+1/2)}(0,\mu)d\mu} \quad] \quad . \tag{2.101}$$

These quantities are introduced into Eqs. (2.91), (2.94) [or (2.97)], and (2.98) to obtain the following low-order equations for $\phi_0^{(\ell+1)}$:

$$-\frac{d}{dx}\frac{1}{\Sigma_t(x)}\frac{d}{dx}E^{(\ell+1/2)}(x)\phi_0^{(\ell+1)}(x) + \Sigma_a(x)\phi_0^{(\ell+1)}(x) = Q(x) \quad , \tag{2.102}$$

$$A^{(\ell+1/2)}\phi_0^{(\ell+1)}(0) - \frac{1}{\Sigma_t(0)}\frac{dE^{(\ell+1/2)}\phi_0^{(\ell+1)}}{dx}(0) = \int_0^1 \left(A^{(\ell+1/2)}+\mu\right)\psi^i(\mu)d\mu \tag{2.103}$$

[or

$$B^{(\ell+1/2)}\phi_0^{(\ell+1)}(0) - \frac{1}{\Sigma_t(0)}\frac{dE^{(\ell+1/2)}\phi_0^{(\ell+1)}}{dx}(0) = \int_0^1 2\mu\psi^i(\mu)d\mu \ ] \ , \tag{2.104}$$

$$0 = \frac{dE^{(\ell+1/2)}\phi_0^{(\ell+1)}}{dx}(X) \ . \tag{2.105}$$

These 1-D equations can be formulated as a standard diffusion problem for the quantity $E^{(\ell+1/2)}(x)\phi_0^{(\ell+1)}(x)$. [However, in multidimensional problems, the Eddington factor becomes a symmetric positive-definite tensor, and the quasidiffusion equation becomes an asymmetric diffusion problem. Thus, it is more difficult to solve efficiently the discretized 2-D problem than the discretized 1-D problem.]

To establish a connection between the nonlinear QD and other linear methods, we shall *linearize* the QD scheme about the converged solution. We assume that $\psi^{(\ell+1/2)}$ is close to the converged angular flux ψ and that $\phi^{(\ell)}$ is close to the converged scalar flux ϕ:

$$\psi^{(\ell+1/2)}(x,\mu) = \psi(x,\mu) + \varepsilon f^{(\ell+1/2)}(x,\mu) \ , \tag{2.106}$$

$$\phi_0^{(\ell)}(x) = \phi_0(x) + \varepsilon F^{(\ell)}(x) \ , \tag{2.107}$$

with $\varepsilon << 1$. We define the converged interior and boundary Eddington factors $E(x)$, A, and B by Eqs. (2.89), (2.93), and (2.96). Introducing Eqs. (2.106) and (2.107) into the QD equations and expanding in powers of ε, we find that the $O(\varepsilon^0)$ terms are automatically satisfied, while the $O(\varepsilon^1)$ terms yield the following linear high-order problem for $f^{(\ell+1/2)}(x,\mu)$:

$$\mu\frac{\partial f^{(\ell+1/2)}}{\partial x}(x,\mu) + \Sigma_t(x)f^{(\ell+1/2)}(x,\mu) = \frac{\Sigma_s(x)}{2}F^{(\ell)}(x) \ , \ 0 < x < X \ , \tag{2.108}$$

$$f^{(\ell+1/2)}(0,\mu) = 0 \ , \ 0 < \mu \le 1 \ , \tag{2.109}$$

$$f^{(\ell+1/2)}(X,\mu) = f^{(\ell+1/2)}(X,-\mu) \ , \ -1 \le \mu < 0 \ , \tag{2.110}$$

and the linear low-order problem for $F^{(\ell+1)}(x)$:

$$-\frac{d}{dx}\frac{1}{\Sigma_t(x)}\frac{d}{dx}E(x)F^{(\ell+1)}(x) + \Sigma_a(x)F^{(\ell+1)}(x)$$

$$= \frac{d}{dx}\frac{1}{\Sigma_t(x)}\frac{d}{dx}\int_{-1}^1 \left(\mu^2 - E(x)\right) f^{(\ell+1/2)}(x,\mu)d\mu \ , \ 0 < x < X \ , \tag{2.111}$$

$$AF^{(\ell+1)}(0) - \frac{1}{\Sigma_t(0)}\frac{dEF^{(\ell+1)}(0)}{dx}(0) = \int_{-1}^0 (A - |\mu|) f^{(\ell+1/2)}(0,\mu)d\mu$$

$$+\frac{1}{\Sigma_t(0)}\frac{d}{dx}\int_{-1}^0 \left(\mu^2 - E(0)\right) f^{(\ell+1/2)}(0,\mu)d\mu \tag{2.112}$$

[or

$$BF^{(\ell+1)}(0) - \frac{1}{\Sigma_t(0)} \frac{dEF^{(\ell+1)}}{dx}(0) = \int_{-1}^{0} (B - |\mu|) f^{(\ell+1/2)}(0,\mu) d\mu$$

$$+ \frac{1}{\Sigma_t(0)} \frac{d}{dx} \int_{-1}^{0} (\mu^2 - E(0)) f^{(\ell+1/2)}(0,\mu) d\mu \ ] \ , \tag{2.113}$$

$$0 = \frac{dEF^{(\ell+1)}}{dx}(X) \ . \tag{2.114}$$

For any problem in which the exact angular flux is independent of μ [for example, a problem having the infinite medium solution $\psi(x,\mu) = Q/2\Sigma_a$], one has exactly $E(x) = 1/3$, $A = 1/2$, and $B = 1/2$. In this situation, Eqs. (2.108)-(2.114) exactly reduce to the correction equations for the Lewis-Miller method. Thus, for such a problem, the convergence rate of the QD solution [using either $x = 0$ boundary condition (2.103) or (2.104)] is equal to the convergence rate of the Lewis-Miller scheme, which is equal to the convergence rate of the DSA scheme.

For any slightly more general problem in which the exact angular flux is a linear function of μ, one also has $E(x) = 1/3$ and $B = 1/2$, but in general $A \neq 1/2$. In this situation, the QD scheme using Eq. (2.104) at $x = 0$ again has the same convergence rate as the Lewis-Miller and DSA schemes.

This close theoretical connection between the QD, Lewis-Miller (LM), and DSA schemes does not generally hold if the exact solution $\psi(x,\mu)$ is not a linear function of μ. Nevertheless, in practice, the QD and DSA schemes are observed to converge in nearly the same (small) number of iterations, using either of the $x = 0$ boundary conditions [Eq. (2.103) or (2.104)]. Moreover, the properties of the converged QD solution are well-described by those of the LM solution (see the final two paragraphs of Sec. II.F).

II.H. The Weighted Alpha (WA) Methods

We have shown that the QD scheme, when linearized, is closely related to the Lewis-Miller and DSA schemes. Now, we consider a different nonlinear class of *weighted alpha* (WA) acceleration methods, whose linearization is closely related to the S_2SA scheme. The ideas underlying the WA schemes were originally formulated independently by Nikolaishvilli [41], Germogenova [33], and Gol'din et al. [35], and were later generalized by Anistratov and Larsen [217, 288].

These methods begin, like the other methods in this chapter, with a source iteration [Eqs. (2.22)-(2.24)]. To derive the low-order acceleration equations, one chooses a parameter $\alpha > 0$, multiplies Eq. (2.22) by $|\mu|^{\alpha}$, and separately integrates over $-1 \leq \mu < 0$ and $0 < \mu \leq 1$. Defining the nonlinear functionals

$$A_{\pm}^{(\ell+1/2)}(x) \equiv (\alpha+1) \frac{\int_0^{\pm 1} |\mu|^{\alpha+1} \psi^{(\ell+1/2)}(x,\mu) d\mu}{\int_0^{\pm 1} \psi^{(\ell+1/2)}(x,\mu) d\mu} \ , \tag{2.115}$$

$$B_{\pm}^{(\ell+1/2)}(x) \equiv (\alpha+1)\frac{\int_0^{\pm 1}|\mu|^{\alpha}\psi^{(\ell+1/2)}(x,\mu)d\mu}{\int_0^{\pm 1}\psi^{(\ell+1/2)}(x,\mu)d\mu} \quad , \tag{2.116}$$

and the partial scalar fluxes

$$\psi_{+}^{(\ell+1/2)}(x) = \int_0^1 \psi^{(\ell+1/2)}(x,\mu)d\mu \quad , \quad \psi_{-}^{(\ell+1/2)}(x) = \int_{-1}^0 \psi^{(\ell+1/2)}(x,\mu)d\mu \quad , \tag{2.117}$$

we obtain two equations for $\psi_{\pm}^{(\ell+1/2)}(x)$:

$$\pm\frac{d}{dx}A_{\pm}^{(\ell+1/2)}(x)\psi_{\pm}^{(\ell+1/2)}(x) + \Sigma_t(x)B_{\pm}^{(\ell+1/2)}(x)\psi_{\pm}^{(\ell+1/2)}(x) = \frac{\Sigma_s(x)}{2}\phi_0^{(\ell)} + \frac{Q(x)}{2} \quad . \tag{2.118}$$

Boundary conditions are derived from Eqs. (2.23) and (2.24) in a similar manner. At $x = 0$ one obtains either

$$(\alpha+1)\int_0^1 \mu^{\alpha+1}\psi^i(\mu)d\mu = A_{+}^{(\ell+1/2)}(0)\psi_{+}^{(\ell+1/2)}(0) \tag{2.119}$$

or

$$(\alpha+1)\int_0^1 \mu^{\alpha}\psi^i(\mu)d\mu = B_{+}^{(\ell+1/2)}(0)\psi_{+}^{(\ell+1/2)}(0) \quad , \tag{2.120}$$

and at $x = X$,

$$\psi_{+}^{(\ell+1/2)}(X) = \psi_{-}^{(\ell+1/2)}(X) \quad . \tag{2.121}$$

The WA method is defined from the above equations as follows. An iteration begins with a transport sweep, Eqs. (2.22)-(2.24), which determines $\psi^{(\ell+1/2)}(x,\mu)$. Next, the non-linear functionals $A_{\pm}^{(\ell+1/2)}$ and $B_{\pm}^{(\ell+1/2)}$ are defined by Eqs. (2.115) and (2.116). Then the following S_2-like problem is solved for $\psi_{+}^{(\ell+1/2)}(x)$ and $\psi_{-}^{(\ell+1/2)}(x)$:

$$\pm\frac{d}{dx}A_{\pm}^{(\ell+1/2)}(x)\psi_{\pm}^{(\ell+1)}(x) + \Sigma_t(x)B_{\pm}^{(\ell+1/2)}(x)\psi_{\pm}^{(\ell+1)}$$

$$= \frac{\Sigma_s(x)}{2}\left(\psi_{+}^{(\ell+1/2)}(x) + \psi_{-}^{(\ell+1/2)}(x)\right) + \frac{Q(x)}{2} \quad , \tag{2.122}$$

$$(\alpha+1)\int_0^1 \mu^{\alpha+1}\psi^i(\mu)d\mu = A_{+}^{(\ell+1/2)}(0)\psi_{+}^{(\ell+1)}(0) \quad , \tag{2.123}$$

or

$$(\alpha+1)\int_0^1 \mu^{\alpha}\psi^i(\mu)d\mu = B_{+}^{(\ell+1/2)}(0)\psi_{+}^{(\ell+1)}(0) \quad , \tag{2.124}$$

and

$$\psi_{+}^{(\ell+1)}(X) = \psi_{-}^{(\ell+1)}(X) \quad . \tag{2.125}$$

Finally, the update equation

$$\phi^{(\ell+1)} = \psi_{+}^{(\ell+1)}(X) + \psi_{-}^{(\ell+1)}(X) \tag{2.126}$$

determines the next scalar flux iterate.

A linear version of this method, in which the transport correction terms are additive rather than multiplicative, has also been proposed [217]. The WA methods with $\alpha = 0$ or $\alpha = 1$ were termed the *first flux* (FF) and the *second flux* (SF) methods in [182].

For transport problems in which the angular flux is independent of μ on the intervals $0 < \mu \leq 1$ and $-1 \leq \mu < 0$, the functionals $A_\pm$ and $B_\pm$ are independent of x:

$$A_\pm = \frac{1+\alpha}{2+\alpha} \quad , \quad B_\pm = 1 \quad . \tag{2.127}$$

For this case, the WA equations limit to S_2-like equations with constant quadrature values

$$\mu_\pm = \pm \frac{1+\alpha}{2+\alpha} \quad . \tag{2.128}$$

[This quadrature value agrees with the standard S_2 value of $1/\sqrt{3}$ if

$$\alpha = \frac{2-\sqrt{3}}{\sqrt{3}-1} \approx 0.366 \quad . \tag{2.129}$$

For this value of α, the convergence of the WA scheme should be similar to that of the S_2SA scheme, even though the boundary conditions of the two schemes are slightly different.] For general α, a Fourier analysis for the infinite homogeneous medium linearized WA scheme can now be performed, because the coefficients in the WA equations are constant. The spectral radius of this method has been determined for the following values of α:

1. $\alpha = 0$ (the FF method) : $\sigma = 0.3333$,
2. $\alpha = 1$ (the SF method) : $\sigma = 0.3105$,
3. $\alpha \approx 0.366$ (S_2-like) : $\sigma = 0.2247$,
4. $\alpha \approx 0.128$ (optimal) : $\sigma = 0.1865$.

Thus, the WA scheme converges rapidly for these values of α. As expected, the WA scheme for $\alpha \approx 0.366$ has the same theoretical spectral radius as the S_2SA and DSA schemes.

II.I Second-Order Forms of the Transport Equation

We turn next to different forms of the transport equation, namely those with second-order spatial derivatives, which we now derive. We write Eq. (1.1) for μ and for $-\mu$:

$$\mu \frac{\partial \psi}{\partial x}(x,\mu) + \Sigma_t(x)\psi(x,\mu) = \frac{\Sigma_s(x)}{2}\phi(x) + \frac{Q(x)}{2} \quad , \tag{2.130}$$

$$-\mu \frac{\partial \psi}{\partial x}(x,-\mu) + \Sigma_t(x)\psi(x,-\mu) = \frac{\Sigma_s(x)}{2}\phi(x) + \frac{Q(x)}{2} \quad , \tag{2.131}$$

and we define the *even-parity* and *odd-parity* angular fluxes, ψ^+ and ψ^-:

$$\psi^+(x,\mu) \equiv \frac{1}{2}\left[\psi(x,\mu) + \psi(x,-\mu)\right] \ ,$$

$$\psi^-(x,\mu) \equiv \frac{1}{2}\left[\psi(x,\mu) - \psi(x,-\mu)\right] \ .$$

The angular flux is the sum of the even- and odd-parity angular fluxes: $\psi = \psi^+ + \psi^-$. The sum and difference of Eqs. (2.130)-(2.131) yield:

$$\mu\frac{\partial\psi^-}{\partial x}(x,\mu) + \Sigma_t(x)\psi^+(x,\mu) = \frac{\Sigma_s(x)}{2}\phi(x) + \frac{Q(x)}{2} \ , \tag{2.132}$$

$$\mu\frac{\partial\psi^+}{\partial x}(x,\mu) + \Sigma_t(x)\psi^-(x,\mu) = 0 \ . \tag{2.133}$$

Using the second equation to eliminate ψ^- from the first, we obtain the *even-parity* transport equation:

$$-\frac{\partial}{\partial x}\frac{\mu^2}{\Sigma_t(x)}\frac{\partial\psi^+}{\partial x}(x,\mu) + \Sigma_t(x)\psi^+(x,\mu) = \frac{\Sigma_s(x)}{2}\phi(x) + \frac{Q(x)}{2} \ . \tag{2.134}$$

This is a second-order integro-differential equation for the even-parity angular flux $\psi^+(x,\mu)$. It was derived by Kuznetsov in 1940 [18] and rederived in the early 1960's independently by Vladimirov [30], Pomraning and Clark [29], and Feautrier [24]. It has been used widely in the astrophysical community [52, 68, 12].

The scalar flux is obtained by integrating the angular flux over all directions:

$$\phi(x) = \int_{-1}^{1}\psi(x,\mu)d\mu = 2\int_0^1\psi^+(x,\mu)d\mu \ . \tag{2.135}$$

This follows from the fact that the angular flux, ψ, is the sum of the even- and odd-parity angular fluxes (and the odd-parity flux integrates to zero).

If instead of eliminating ψ^- we eliminate ψ^+ from Eq. (2.133) using Eq. (2.132), we obtain:

$$-\frac{\partial}{\partial x}\frac{\mu^2}{\Sigma_t(x)}\frac{\partial\psi^-}{\partial x}(x,\mu) + \Sigma_t(x)\psi^-(x,\mu) = -\mu\frac{\partial}{\partial x}\left[\frac{\Sigma_s(x)}{2}\phi(x) + \frac{Q(x)}{2}\right] \ . \tag{2.136}$$

This *odd-parity transport* equation is a second-order integro-differential equation for the odd-parity angular flux $\psi^-(x,\mu)$.

Adding the even- and odd-parity equations, we obtain a second-order differential equation for the full-range angular flux:

$$-\frac{\partial}{\partial x}\frac{\mu^2}{\Sigma_t(x)}\frac{\partial\psi}{\partial x}(x,\mu) + \Sigma_t(x)\psi(x,\mu) = \frac{\Sigma_s(x)}{2}\phi(x) + \frac{Q(x)}{2} - \mu\frac{\partial}{\partial x}\left[\frac{\Sigma_s(x)}{2}\phi(x) + \frac{Q(x)}{2}\right] \ . \tag{2.137}$$

This has recently been termed the "self-adjoint equation for the angular flux," or the SAAF equation. [268]

Of the three second-order forms shown above, the even-parity form has received the most attention. We shall now define and analyze the SI and $KP_1(1)P_2(0)$ schemes for the even-parity equation. The SI equations are:

$$-\frac{\partial}{\partial x}\frac{\mu^2}{\Sigma_t(x)}\frac{\partial \psi^{+(\ell+1/3)}}{\partial x}(x,\mu)+\Sigma_t(x)\psi^{+(\ell+1/3)}(x,\mu)=\frac{\Sigma_s(x)}{2}\phi^{(\ell)}(x)+\frac{Q(x)}{2} \quad , \tag{2.138}$$

$$\phi^{(\ell+1/3)}(x)=2\int_0^1 \psi^{+(\ell+1/3)}(x,\mu)d\mu \ . \tag{2.139}$$

$$\phi^{(\ell+1)}(x)=\phi^{(\ell+1/3)}(x) \ . \tag{2.140}$$

Fourier-analyzing this iteration for the infinite-medium model problem, we obtain:

$$\omega(\lambda)=c\int_0^1 \frac{d\mu}{1+\lambda^2\mu^2}=\frac{c}{\lambda}\tan^{-1}\lambda \ . \tag{2.141}$$

This is the same result [see Eq. (2.12)] that we obtained for the SI method with the first-order form of the transport equation. However, this is to be expected, for the first-order and second-order forms are just different expressions of the same "transport sweep" physics. We would obtain the same result if we analyzed SI with the odd-parity or SAAF equations as well.

The $KP_1(1)P_2(0)$ method applied to the even-parity equations is given by Eqs. (2.138-2.140) and Eqs. (2.61-2.64), which we repeat here for convenience.

$$-\frac{d}{dx}\frac{1}{3\Sigma_t(x)}\frac{dF^{(\ell+2/3)}}{dx}(x)+\Sigma_a(x)F^{(\ell+2/3)}(x)=\Sigma_s(x)\left(\phi^{(\ell+1/3)}(x)-\phi^{(\ell)}(x)\right) \quad , \tag{2.142}$$

$$\phi^{(\ell+2/3)}(x)=\phi^{(\ell+1/3)}(x)+F^{(\ell+2/3)}(x) \quad , \tag{2.143}$$

$$F^{(\ell+1)}(x)=\frac{\beta c}{1-\beta c}\left(\phi^{(\ell+2/3)}(x)-\phi^{(\ell)}(x)\right) \quad , \tag{2.144}$$

$$\phi^{(\ell+1)}(x)=\phi^{(\ell+2/3)}(x)+F^{(\ell+1)}(x) \ . \tag{2.145}$$

A Fourier analysis of this method produces the following expression for the iteration eigenvalue, $\omega(\lambda)$:

$$\omega(\lambda)=\frac{c}{1-\beta c}\left(\frac{1}{\lambda^2+3(1-c)}\left[\left(\frac{\lambda^2}{3}+1\right)\frac{\tan^{-1}\lambda}{\lambda}-1\right]-\beta\right) \ . \tag{2.146}$$

Not surprisingly, this is identical to Eq. (2.65), the result for $KP_1(1)P_2(0)$ applied to the first-order form of the equation.

In the next chapter, we shall see that for the first-order transport equation, spatial discretization introduces significant complications in the low-order equations (preconditioners). In the terminology of the literature, it is difficult to obtain a diffusion discretization that is *consistent* with a given discretization of the first-order transport equation; further, when such a discretization is obtained, it is often non-standard and algebraically complicated. Second-order forms of the transport equation do not have this difficulty. Because the second-order transport equations are already in diffusion-like form, it is straightforward to discretize the diffusion equation *consistently* with them. For example, it is a simple matter to discretize Eqs. (2.138) and (2.142) with the same technique. Thus, the use of a second-order transport equation avoids one of the difficulties associated with rapidly convergent iterative methods for transport problems. Unfortunately, the second-order form has disadvantages of its own. Because of the structure of the second-order equations, they cannot be solved by simple transport sweeps. Hence, the high-order equations in the second-order form are more costly to solve than in the first-order form. Also, the second-order form is problematic in problems with void regions, where $\Sigma_t = 0$ and the diffusion coefficient in Eq. (2.134) is infinite.

III. THE EFFECT OF SPATIAL AND ANGULAR DISCRETIZATIONS IN PLANAR GEOMETRY

In Chapter II, we introduced basic iterative acceleration schemes for the continuous transport equation, with no spatial or angular discretization. Now we discuss the same iterative schemes, but applied to the diamond-differenced discrete-ordinates (S_N) equations [9]. We show that the angular discretization generally has a benign effect on the convergence properties. However, unless special care is taken, the spatial discretizations have a significant effect on either (*i*) the rate of iterative convergence, or (*ii*) the nature of the converged discrete solution.

III.A. Source Iteration (SI)

The Diamond-Differenced (DD) S_N equations corresponding to Eqs. (1.1)-(1.3) are:

$$\frac{\mu_n}{h_j}\left(\psi_{n,j+1/2}-\psi_{n,j-1/2}\right)+\Sigma_{t,j}\psi_{n,j}=\frac{\Sigma_{s,j}}{2}\left(\sum_{n'=1}^{N}\psi_{n',j}w_{n'}\right)+\frac{Q_j}{2}\ ,\ 1\le n\le N\ ,\ 1\le j\le J\ , \tag{3.1}$$

$$\psi_{n,j}=\frac{1}{2}\left(\psi_{n,j+1/2}+\psi_{n,j-1/2}\right)\ ,\ 1\le n\le N\ ,\ 1\le j\le J\ , \tag{3.2}$$

$$\psi_{n,1/2}=\psi_n^i\ ,\ \mu_n>0\ , \tag{3.3}$$

$$\psi_{n,J+1/2}=\psi_{m,J+1/2}\ ,\ \mu_n=-\mu_m<0\ . \tag{3.4}$$

Our notation is standard: $x_{j\pm1/2}$ are the edges of the j-th spatial cell ($1 \le j \le J$), $h_j = x_{j+1/2} - x_{j-1/2}$ = width of the j-th spatial cell, and $\{(\mu_n, w_n) | 1 \le n \le N\}$ is an even-order Gauss-Legendre quadrature set. Also,

$$\Sigma_{t,j} = \text{total cross section for the } j^{\text{th}} \text{ cell} \quad , \tag{3.5}$$

$$\Sigma_{s,j} = \text{scattering cross section for the } j^{\text{th}} \text{ cell} \quad , \tag{3.6}$$

$$Q_j = \text{cell} - \text{average interior source for the } j^{\text{th}} \text{ cell} \quad , \tag{3.7}$$

$$\psi_{n,j+1/2} \approx \psi(x_{j+1/2}, \mu_n) = \text{cell} - \text{edge angular flux} \quad , \tag{3.8}$$

$$\psi_{n,j} \approx \frac{1}{h_j} \int_{x_{j-1/2}}^{x_{j+1/2}} \psi(x, \mu_n) dx = \text{cell} - \text{average angular flux} \quad . \tag{3.9}$$

Eq. (3.1) above is the *balance* equation, which is obtained by integrating the S_N equation over the j-th spatial cell. Eq. (3.2) is the diamond-difference *auxiliary* equation. (Most spatial discretization schemes for the S_N equations include the balance equation as one of the relations that the cell-edge and cell-average fluxes must satisfy; the various schemes differ in their choice of auxiliary equations.)

The SI method applied to Eqs. (3.1)-(3.4) is defined by:

$$\frac{\mu_n}{h_j}\left(\psi_{n,j+1/2}^{(\ell+1/2)} - \psi_{n,j-1/2}^{(\ell+1/2)}\right) + \Sigma_{t,j}\psi_{n,j}^{(\ell+1/2)} = \frac{\Sigma_{s,j}}{2}\phi_j^{(\ell)} + \frac{Q_j}{2} \quad , \quad 1 \le n \le N \quad , \quad 1 \le j \le J \quad , \tag{3.10}$$

$$\psi_{n,j}^{(\ell+1/2)} = \frac{1}{2}\left(\psi_{n,j+1/2}^{(\ell+1/2)} + \psi_{n,j-1/2}^{(\ell+1/2)}\right) \quad , \quad 1 \le n \le N \quad , \quad 1 \le j \le J \quad , \tag{3.11}$$

$$\psi_{n,1/2}^{(\ell+1/2)} = \psi_n^i \quad , \quad \mu_n > 0 \quad , \tag{3.12}$$

$$\psi_{n,J+1/2}^{(\ell+1/2)} = \psi_{m,J+1/2}^{(\ell+1/2)} \quad , \quad \mu_n = -\mu_m < 0 \quad , \tag{3.13}$$

$$\phi_j^{(\ell+1/2)} = \sum_{n=1}^{N} \psi_{n,j}^{(\ell+1/2)} w_n \quad , \quad 1 \le j \le J \quad , \tag{3.14}$$

with the *update* equation

$$\phi_j^{(\ell+1)} = \phi_j^{(\ell+1/2)} \quad , \quad 1 \le j \le J \quad . \tag{3.15}$$

These equations can be solved non-iteratively for $\psi_{n,j}^{(\ell+1/2)}$ and $\psi_{n,j\pm1/2}^{(\ell+1/2)}$ in the following way. First, one introduces Eq. (3.11) into the left side of Eq. (3.10) to eliminate $\psi_{n,j}^{(\ell+1/2)}$. Then, one solves the resulting equation for the *exiting* flux from cell j:

$$\psi_{n,j+1/2}^{(\ell+1/2)} = \frac{(2\mu_n - \Sigma_{t,j}h_j)\psi_{n,j-1/2}^{(\ell+1/2)} + h_j(\Sigma_{s,j}\phi_j^{(\ell)} + Q_j)}{2\mu_n + \Sigma_{t,j}h_j} \quad , \quad \mu_n > 0 \quad , \tag{3.16}$$

$$\psi_{n,j-1/2}^{(\ell+1/2)} = \frac{(2|\mu_n| - \Sigma_{t,j}h_j)\psi_{n,j+1/2}^{(\ell+1/2)} + h_j(\Sigma_{s,j}\phi_j^{(\ell)} + Q_j)}{2|\mu_n| + \Sigma_{t,j}h_j} \quad , \quad \mu_n < 0 \quad . \tag{3.17}$$

Eq. (3.16) with $j = 1$ yields $\psi_{n,3/2}^{(\ell+1/2)}$ because the fluxes incident on the $j = 1$ cell, $\psi_{n,1/2}^{(\ell+1/2)}$, are specified by the boundary condition (3.12). One then uses Eq. (3.16) with $j = 2$ to determine $\psi_{n,5/2}^{(\ell+1/2)}$; and then $j = 3$, and so on to $j = J$. Eq. (3.13) then determines the fluxes incident on the right side of the J-th cell, for $\mu_n < 0$. Eq. (3.17) then recursively yields $\psi_{n,j-1/2}^{(\ell+1/2)}$; first for $j = J$, then $j = J - 1$; and so on.

This process of "marching" through the cells, from left to right for $\mu_n > 0$ and then from right to left for $\mu_n < 0$, is a *transport sweep*. At the conclusion of a transport sweep, new cell-average scalar flux estimates $\phi_j^{(\ell+1/2)}$ are defined by Eq. (3.14), and using the update equation (3.15), one can begin a new transport sweep. In practice, this iteration process is terminated when $|\phi_j^{(\ell+1)} - \phi_j^{(\ell)}|$ is sufficiently small for $1 \leq j \leq J$.

This discrete SI scheme can be Fourier-analyzed in the same basic manner as the continuous SI scheme. We assume a model infinite ($-\infty < j < \infty$) homogeneous-medium ($\Sigma_{t,j} = \Sigma_t, \Sigma_{s,j} = \Sigma_s$), uniform mesh ($h_j = h$) problem in which the source Q_j and the solution $\psi_{m,j}$ and $\psi_{m,j\pm1/2}$ are bounded as $j \to \infty$. As in Chapter II, we consider a single Fourier mode defined by:

$$Q_j = 0 \quad , \tag{3.18}$$

$$\phi_j^{(\ell)} = \omega^\ell e^{i\Sigma_t\lambda x_j} \quad , \tag{3.19}$$

$$\psi_{n,j}^{(\ell+1/2)} = \omega^\ell a_n e^{i\Sigma_t\lambda x_j} \quad , \tag{3.20}$$

$$\psi_{n,j+1/2}^{(\ell+1/2)} = \omega^\ell b_n e^{i\Sigma_t\lambda x_{j+1/2}} \quad , \tag{3.21}$$

$$\phi_j^{(\ell+1/2)} = \omega^\ell \alpha e^{i\Sigma_t\lambda x_j} \quad . \tag{3.22}$$

Introducing Eqs. (3.18)-(3.22) into Eqs. (3.10), (3.11), (3.14), and (3.15) for the model problem, we obtain the following equations, which are independent of j:

$$2i\frac{\mu_n}{h}\left(\sin\frac{\Sigma_t h\lambda}{2}\right)b_n + \Sigma_t a_n = \frac{\Sigma_s}{2} \quad , \tag{3.23}$$

$$a_n = b_n\left(\cos\frac{\Sigma_t h\lambda}{2}\right) \quad , \tag{3.24}$$

$$\alpha = \sum_{n=1}^{N} a_n w_n \quad , \tag{3.25}$$

$$\omega = \alpha \quad . \tag{3.26}$$

Eqs. (3.23) and (3.24) yield:

$$a_n = \frac{c}{2}\frac{1}{1 + i\mu_n\Lambda} \quad , \tag{3.27}$$

where

$$\Lambda \equiv \frac{2}{\Sigma_t h} \tan\left(\frac{\Sigma_t h}{2}\lambda\right) \quad . \tag{3.28}$$

Then Eqs. (3.25) - (3.28) give:

$$\omega_{SI}(\Lambda) = \alpha(\Lambda) = \frac{c}{2} \sum_{n=1}^{N} \frac{w_n}{1+\mu_n^2\Lambda^2} \quad . \tag{3.29}$$

It is evident from Eq. (3.29) that

$$\sigma_{SI} = \sup_{\Lambda} |\omega_{SI}(\Lambda)| = \omega_{SI}(0) = c \quad . \tag{3.30}$$

This result holds for any even quadrature set order (N) and any spatial cell-size (h). Also, this result agrees with Eq. (2.17), the spectral radius for the SI scheme applied to the continuous transport equation.

In practice, when the SI scheme is applied to finite-medium problems with homogeneous cross sections and a uniform spatial mesh, the observed spectral radius is somewhat less than c. This is because of neutron leakage: neutron lifetimes can end not only by capture, but also by leakage from the system. The inclusion of leakage shortens neutron lifetimes and hastens the convergence of the SI scheme. However, this effect diminishes as the physical system becomes increasingly optically thick, because it becomes increasingly improbable that any single neutron will leak out.

When the problems in the above paragraph are solved on a nonuniform spatial grid, one observes almost no change in the observed SI spectral radius, and in all cases the spectral radius is bounded from above by c.

Generalizing these homogeneous-medium problems to spatially-periodic medium problems [257], the observed spectral radius is bounded from above by the largest value of $c(x)$ for $0 \leq x \leq X$, where $c(x) = c(x+X)$. Also, if the system is optically thick, so that the effect of leakage is negligible, the observed spectral radius is bounded from below by the smallest value of $c(x)$. Thus, in this (optically thick) case, one observes:

$$\min_{0\leq x\leq X} c(x) \leq \sigma_{SI} \leq \max_{0\leq x\leq X} c(x) \quad . \tag{3.31}$$

These results are observed experimentally for more general finite heterogeneous media without a spatially periodic structure. They are also observed for other commonly-used S_N spatial differencing schemes.

Thus, in general, the SI scheme applied to the spatially-discretized S_N equations converges rapidly for optically-thin, leaky systems, or optically-thick systems that are not dominated by scattering. However, the SI scheme converges slowly for systems that are optically-thick and scattering-dominated.

III.B. Diffusion Synthetic Acceleration (DSA)

The DSA scheme for the continuous transport equation is defined by the high-order transport equations (2.22)-(2.24) and (2.26), the low-order diffusion equations (2.30)-(2.32), and the update equation (2.34). We discretize these equations using the Diamond-Differenced S_N approximation for the high-order equations (2.22)-(2.24) and a conventional cell-edge discretization for the low-order diffusion equations (2.30)-(2.32). (Henceforth, we refer to this diffusion discretization as *inconsistent*, for reasons that will soon be explained.) The high-order equations are defined by Eqs. (3.10)-(3.14); the low-order equations are defined by:

$$-\frac{1}{3\Sigma_{t,j+1}h_{j+1}}\left(F_{j+3/2}^{(\ell+1)}-F_{j+1/2}^{(\ell+1)}\right)+\frac{1}{3\Sigma_{t,j}h_j}\left(F_{j+1/2}^{(\ell+1)}-F_{j-1/2}^{(\ell+1)}\right)+\left(\Sigma_{a,j+1/2}h_{j+1/2}\right)F_{j+1/2}^{(\ell+1)}$$

$$=\frac{\Sigma_{s,j+1}h_{j+1}}{2}\left(\phi_{j+1}^{(\ell+1/2)}-\phi_{j+1}^{(\ell)}\right)+\frac{\Sigma_{s,j}h_j}{2}\left(\phi_j^{(\ell+1/2)}-\phi_j^{(\ell)}\right)\quad,\quad 1\le j\le J\quad, \tag{3.32}$$

$$\frac{1}{2}F_{1/2}^{(\ell+1)}-\frac{1}{3\Sigma_{t,1}h_1}\left(F_{3/2}^{(\ell+1)}-F_{1/2}^{(\ell+1)}\right)+\frac{1}{2}\left(\Sigma_{a,1}h_1\right)F_{1/2}^{(\ell+1)}=\frac{\Sigma_{s,1}h_1}{2}\left(\phi_1^{(\ell+1/2)}-\phi_1^{(\ell)}\right)\quad, \tag{3.33}$$

$$\frac{1}{3\Sigma_{t,J}h_J}\left(F_{J+1/2}^{(\ell+1)}-F_{J-1/2}^{(\ell+1)}\right)+\frac{1}{2}\left(\Sigma_{a,J}h_J\right)F_{J+1/2}^{(\ell+1)}=\frac{\Sigma_{s,J}h_J}{2}\left(\phi_J^{(\ell+1/2)}-\phi_J^{(\ell)}\right)\quad, \tag{3.34}$$

and the *update* equation is defined by:

$$\phi_j^{(\ell+1)}=\phi_j^{(\ell+1/2)}+\frac{1}{2}\left(F_{j+1/2}^{(\ell+1)}+F_{j-1/2}^{(\ell+1)}\right)\quad. \tag{3.35}$$

In Eq. (3.32) we have introduced

$$\Sigma_{a,j+1/2}\equiv\frac{\Sigma_{a,j+1}h_{j+1}+\Sigma_{a,j}h_j}{h_{j+1}+h_j}\quad,\quad 1\le j\le J-1\quad, \tag{3.36}$$

$$h_{j+1/2}\equiv\frac{1}{2}\left(h_{j+1}+h_j\right)\quad,\quad 1\le j\le J-1\quad. \tag{3.37}$$

(Other discretizations of the low-order diffusion equation are certainly possible but will not be considered here.)

The resulting discrete DSA equations can be Fourier-analyzed in the same way as the discrete SI equations. We again assume a model infinite ($-\infty<j<\infty$), homogeneous-medium ($\Sigma_{t,j}=\Sigma_t,\Sigma_{s,j}=\Sigma_s$), uniform mesh ($h_j=h$) problem in which the source Q_j and the solution $\psi_{m,j}$ and $\psi_{m,j\pm1/2}$ are bounded as $j\to\infty$. We consider a single Fourier mode defined by Eqs. (3.18)-(3.22) and

$$F_{j+1/2}^{(\ell+1)}=\omega^\ell\beta e^{i\lambda\Sigma_t x_{j+1/2}}\quad. \tag{3.38}$$

We find that β and ω are defined by

$$\beta = -\frac{c(1-\omega_{SI})\left(\cos\frac{\lambda\Sigma_t h}{2}\right)}{1-c+\frac{1}{3}\left(\frac{2}{\Sigma_t h}\sin\frac{\lambda\Sigma_t h}{2}\right)^2} \quad , \tag{3.39}$$

and

$$\omega = \omega_{SI} - \frac{c(1-\omega_{SI})\left(\cos\frac{\lambda\Sigma_t h}{2}\right)^2}{1-c+\frac{1}{3}\left(\frac{2}{\Sigma_t h}\sin\frac{\lambda\Sigma_t h}{2}\right)^2} \quad , \tag{3.40}$$

where ω_{SI} is defined by Eq. (3.29).

Using Eq. (3.28) and a trigonometric identity, we may rewrite Eq. (3.40) as

$$\omega = \omega_{SI} - \frac{c(1-\omega_{SI})}{(1-c)\left[1+\left(\frac{\Sigma_t h}{2}\right)^2\Lambda^2\right]+\frac{1}{3}\Lambda^2} \quad , \tag{3.41}$$

where Λ is defined by Eq. (3.28). Thus, if we fix Λ, i.e. if we choose λ to satisfy

$$\lambda = \frac{2}{\Sigma_t h}\tan^{-1}\left(\Lambda\frac{\Sigma_t h}{2}\right) \quad , \tag{3.42}$$

then Eq. (3.41) implies that ω is a monotonically increasing function of $\Sigma_t h$, taking its minimum value at $\Sigma_t h = 0$:

$$\omega_{min}(\Lambda) = \omega_{SI} - \frac{c(1-\omega_{SI})}{1-c+\frac{1}{3}\Lambda^2} \quad , \tag{3.43}$$

and its maximum value at $\Sigma_t h = \infty$:

$$\omega_{max}(\Lambda) = \omega_{SI} \quad . \tag{3.44}$$

As $\Sigma_t h \to \infty$, Eq. (3.44) holds and the performance of the DSA scheme reduces to that of SI. In this case, the discrete DSA scheme is convergent but ineffective – it performs like Source Iteration. As $\Sigma_t h \to 0$, Eq. (3.43) holds, and σ_{DSA} is obtained by maximizing this expression over Λ.

In Figure 5 we plot σ_{DSA} as a function of $\Sigma_t h$ for various quadrature set orders, and for $c = 0.98$. For all finite values of $\Sigma_t h$ and all quadrature orders N, the discrete DSA scheme is seen to be convergent, with a smaller spectral radius than SI. For small $\Sigma_t h$, the discrete DSA scheme is rapidly convergent, but as $\Sigma_t h$ increases, the scheme degrades in performance, eventually (for $\Sigma_t h >> 1$) converging only marginally faster than the SI scheme.

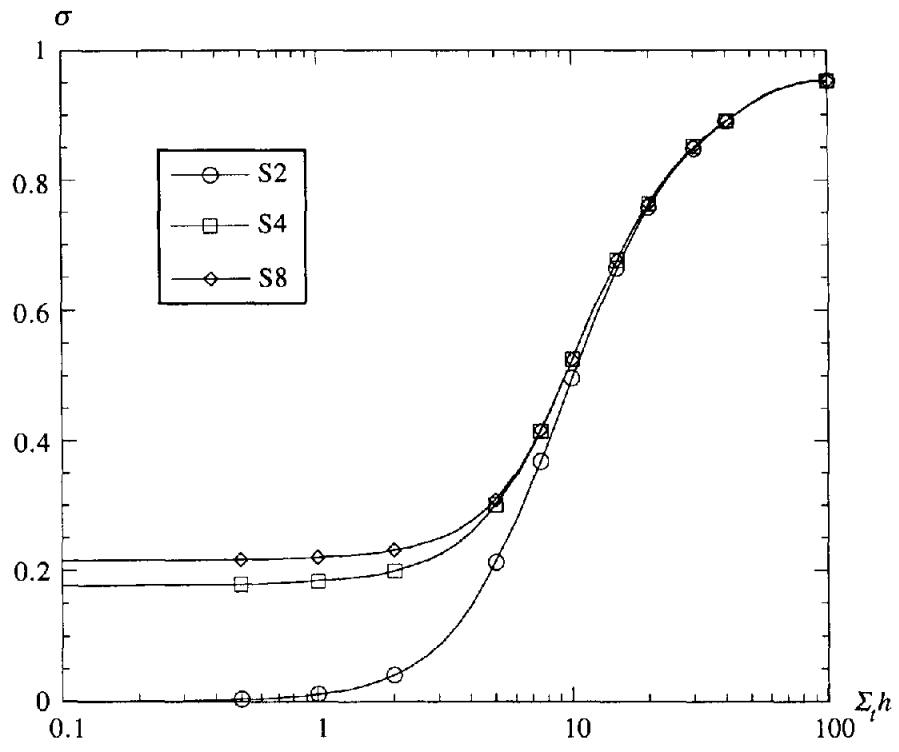

Figure 5: σ_{DSA} versus $\Sigma_t h$
(c=0.98, "Inconsistent" DSA Diffusion Discretizations)

This result is marginally acceptable, but much worse results hold for many other common discretizations of the low-order DSA diffusion problem: the resulting DSA scheme is rapidly convergent for small $\Sigma_t h$, but it degrades as $\Sigma_t h$ increases and then becomes *divergent* or *unstable* ($\sigma_{DSA} > 1$) for $\Sigma_t h$ sufficiently large. This instability occurs, for example, with common cell-centered diffusion discretizations [51].

The problem of discretizing the low-order DSA equations in a way that renders the scheme rapidly convergent for all $\Sigma_t h$ was solved by Alcouffe [57], [63] for the S_N equations employing the Diamond-Differencing scheme. Alcouffe's *source-correction* method is algebraically equivalent to the following *four-step* procedure:

1. After a transport sweep that yields $\psi_{n,j}^{(\ell+1/2)}$, formulate the exact S_N problem for the (discretized) linear cell-edge and cell-average angular corrections $f_{n,j}$ and $f_{n,j+1/2}$. If these corrections are defined as:

$$f_{n,j(\pm 1/2)} \equiv \psi_{n,j(\pm 1/2)} - \psi_{n,j(\pm 1/2)}^{(\ell+1/2)} \quad , \tag{3.45}$$

then Eqs. (3.10)-(3.13) yield

$$\frac{\mu_n}{h_j}\left(f_{n,j+1/2} - f_{n,j-1/2}\right) + \Sigma_{t,j} f_{n,j} - \frac{\Sigma_s}{2}\sum_{n=1}^{N} f_{n,j} w_n = \frac{\Sigma_{s,j}}{2}\left(\phi_j^{(\ell+1/2)} - \phi_j^{(\ell)}\right) \quad , \tag{3.46}$$

$$f_{n,j} = \frac{1}{2}\left(f_{n,j+1/2} + f_{n,j-1/2}\right) \quad , \tag{3.47}$$

$$f_{n,j} = 0 \quad , \quad \mu_n > 0 \quad , \tag{3.48}$$

$$f_{n,J+1/2} = f_{m,J+1/2} \quad , \quad \mu_n = -\mu_m < 0 \quad . \tag{3.49}$$

(As discussed above, this problem for the corrections f is just as difficult to solve as the original S_N problem for ψ.)

2. Next, operate on Eqs. (3.46)-(3.49) by the *discrete P_1 approximation*: multiply by w_n (or $\mu_n w_n$), sum over n, and introduce the approximations

$$f_{n,j(\pm 1/2)} \approx \frac{1}{2}\left(F_{j(\pm 1/2)} + 3\mu_n G_{j(\pm 1/2)}\right) \quad . \tag{3.50}$$

This yields:

$$\frac{1}{h_j}\left(G^{(\ell+1)}_{j+1/2} - G^{(\ell+1)}_{j-1/2}\right) + \Sigma_{a,j} F^{(\ell+1)}_j = \Sigma_{s,j}\left(\phi^{(\ell+1/2)}_j - \phi^{(\ell)}_j\right) \quad , \tag{3.51}$$

$$\frac{1}{3h_j}\left(F^{(\ell+1)}_{j+1/2} - F^{(\ell+1)}_{j-1/2}\right) + \Sigma_{t,j} G^{(\ell+1)}_j = 0 \quad , \tag{3.52}$$

$$F^{(\ell+1)}_j = \frac{1}{2}\left(F^{(\ell+1)}_{j+1/2} + F^{(\ell+1)}_{j-1/2}\right) \quad , \quad G^{(\ell+1)}_j = \frac{1}{2}\left(G^{(\ell+1)}_{j+1/2} + G^{(\ell+1)}_{j-1/2}\right) \quad , \tag{3.53}$$

$$0 = \sum_{\mu_n>0} (2\mu_n) f_{n,1/2} w_n \approx \sum_{\mu_n>0} \mu_n \left(F^{(\ell+1)}_{1/2} + 3\mu_n G^{(\ell+1)}_{1/2}\right) w_n = \gamma F^{(\ell+1)}_{1/2} + G^{(\ell+1)}_{1/2} \quad , \tag{3.54}$$

$$0 = G^{(\ell+1)}_{J+1/2} \quad , \tag{3.55}$$

where, in Eq. (3.54),

$$\gamma = \gamma_N \equiv \sum_{\mu_n>0} \mu_n w_n \approx \frac{1}{2} \quad . \tag{3.56}$$

3. Next, algebraically eliminate all of the unknowns in Eqs. (3.51)-(3.55) except the cell-edge scalar flux corrections $F^{(\ell+1)}_{j\pm 1/2}$. We begin by using Eqs. (3.53) to eliminate $F^{(\ell+1)}_j$ and $G^{(\ell+1)}_j$ from Eqs. (3.51) and (3.52). After minor algebraic operations, we obtain

$$G^{(\ell+1)}_{j+1/2} - G^{(\ell+1)}_{j-1/2} + \frac{\Sigma_{a,j} h_j}{2}\left(F^{(\ell+1)}_{j+1/2} + F^{(\ell+1)}_{j-1/2}\right) = \Sigma_{s,j} h_j \left(\phi^{(\ell+1/2)}_j - \phi^{(\ell)}_j\right) \quad , \tag{3.57}$$

and

$$G^{(\ell+1)}_{j+1/2} + G^{(\ell+1)}_{j-1/2} + \frac{2}{3\Sigma_{t,j} h_j}\left(F^{(\ell+1)}_{j+1/2} - F^{(\ell+1)}_{j-1/2}\right) = 0 \quad . \tag{3.58}$$

Adding these two equations, we obtain

$$G_{j+1/2}^{(\ell+1)} = -\frac{1}{3\Sigma_{t,j}h_j}\left(F_{j+1/2}^{(\ell+1)} - F_{j-1/2}^{(\ell+1)}\right) - \frac{\Sigma_{a,j}h_j}{4}\left(F_{j+1/2}^{(\ell+1)} + F_{j-1/2}^{(\ell+1)}\right)$$

$$+\frac{\Sigma_{s,j}h_j}{2}\left(\phi_j^{(\ell+1/2)} - \phi_j^{(\ell)}\right) \quad , \quad 1 \le j \le J \quad . \tag{3.59}$$

Subtracting Eq. (3.57) from Eq. (3.58) and then replacing j by $j+1$, we obtain:

$$G_{j+1/2}^{(\ell+1)} = -\frac{1}{3\Sigma_{t,j+1}h_{j+1}}\left(F_{j+3/2}^{(\ell+1)} - F_{j+1/2}^{(\ell+1)}\right) + \frac{\Sigma_{a,j+1}h_{j+1}}{4}\left(F_{j+3/2}^{(\ell+1)} + F_{j+1/2}^{(\ell+1)}\right)$$

$$-\frac{\Sigma_{s,j+1}h_{j+1}}{2}\left(\phi_{j+1}^{(\ell+1/2)} - \phi_{j+1}^{(\ell)}\right) \quad , \quad 0 \le j \le J-1 \quad . \tag{3.60}$$

For $1 \le j \le J-1$, we equate the right sides of Eqs. (3.59) and (3.60) to obtain

$$-\frac{1}{3\Sigma_{t,j+1}h_{j+1}}\left(F_{j+3/2}^{(\ell+1)} - F_{j+1/2}^{(\ell+1)}\right) + \frac{1}{3\Sigma_{t,j}h_j}\left(F_{j+1/2}^{(\ell+1)} - F_{j-1/2}^{(\ell+1)}\right)$$

$$+\frac{\Sigma_{a,j+1}h_{j+1}}{4}\left(F_{j+3/2}^{(\ell+1)} + F_{j+1/2}^{(\ell+1)}\right) + \frac{\Sigma_{a,j}h_j}{4}\left(F_{j+1/2}^{(\ell+1)} + F_{j-1/2}^{(\ell+1)}\right)$$

$$= \frac{\Sigma_{s,j+1}h_{j+1}}{2}\left(\phi_{j+1}^{(\ell+1/2)} - \phi_{j+1}^{(\ell)}\right) + \frac{\Sigma_{s,j}h_j}{2}\left(\phi_j^{(\ell+1/2)} - \phi_j^{(\ell)}\right) \quad . \tag{3.61}$$

Also, Eqs. (3.54) and (3.60) yield the left boundary condition

$$\gamma F_{1/2}^{(\ell+1)} - \frac{1}{3\Sigma_{t,1}h_1}\left(F_{3/2}^{(\ell+1)} - F_{1/2}^{(\ell+1)}\right) + \frac{\Sigma_{a,1}h_1}{4}\left(F_{3/2}^{(\ell+1)} + F_{1/2}^{(\ell+1)}\right)$$

$$= \frac{\Sigma_{s,1}h_1}{2}\left(\phi_1^{(\ell+1/2)} - \phi_1^{(\ell)}\right) \quad , \tag{3.62}$$

and Eqs. (3.55) and (3.59) yield the right boundary condition

$$\frac{1}{3\Sigma_{t,J}h_J}\left(F_{J+/2}^{(\ell+1)} - F_{J-1/2}^{(\ell+1)}\right) + \frac{\Sigma_{a,J}h_J}{4}\left(F_{J+/2}^{(\ell+1)} + F_{J-1/2}^{(\ell+1)}\right)$$

$$= \frac{\Sigma_{s,J}h_J}{2}\left(\phi_J^{(\ell+1/2)} - \phi_J^{(\ell)}\right) \quad . \tag{3.63}$$

4. Solve the low-order diffusion Eqs. (3.61)-(3.63) for $F_{j+1/2}^{(\ell+1)}$ and update $\phi_j^{(\ell+1/2)}$ by:

$$\phi_j^{(\ell+1)} = \phi_j^{(\ell+1/2)} + \frac{1}{2}\left(F_{j+1/2}^{(\ell+1)} + F_{j-1/2}^{(\ell+1)}\right) \quad , \quad 1 \le j \le J \quad . \tag{3.64}$$

This "consistent" diffusion discretization [Eqs. (3.61)-(3.63)] is similar, but not identical to the earlier "inconsistent" cell-edge diffusion discretization [Eqs. (3.32)-(3.34)]. The differences are:

1. The "removal" (Σ_a) terms in Eqs. (3.61)-(3.63) are based on a three-point, rather than a one-point cell-edge discretization.

2. Eq. (3.62) contains the parameter γ, which by Eq. (3.56) limits to the Eq. (3.33) value of $1/2$ only as $N \to \infty$.

The Fourier analysis for the discrete DSA scheme using the consistent low-order equations (3.61)-(3.63) yields the following result: as before, a single Fourier mode is defined by Eqs. (3.18)-(3.22) and (3.38), with $\alpha(\Lambda)$ and Λ defined by Eqs. (3.29) and (3.28). Now, however, ω is defined for all $\Sigma_t h$ by

$$\omega = \omega_{SI} - \frac{c(1-\omega_{SI})}{1-c+\frac{1}{3}\Lambda^2} \quad . \tag{3.65}$$

This result is identical to Eq. (3.43), which we have shown represents a rapidly-convergent scheme! In Figure 6 we plot the DSA spectral radii for the "inconsistently" and the "consistently" discretized low-order diffusion equation (3.61). The "consistent" spectral radii [marked by filled-in circles, squares, and triangles] are independent of $\Sigma_t h$, and for all quadrature orders N and all $0 \leq c \leq 1.0$ satisfy $\sigma_{DSA} < 0.2247$. [This upper bound also holds for the DSA scheme applied to the continuous transport equation; see Eq. (2.41).]

This analysis shows that a way to obtain a low-order DSA diffusion discretization that accelerates effectively for any $\Sigma_t h$ is to derive this discretization from the discrete S_N equations, using the discrete P_1 approximation. This was first suggested by Alcouffe [57, 63]

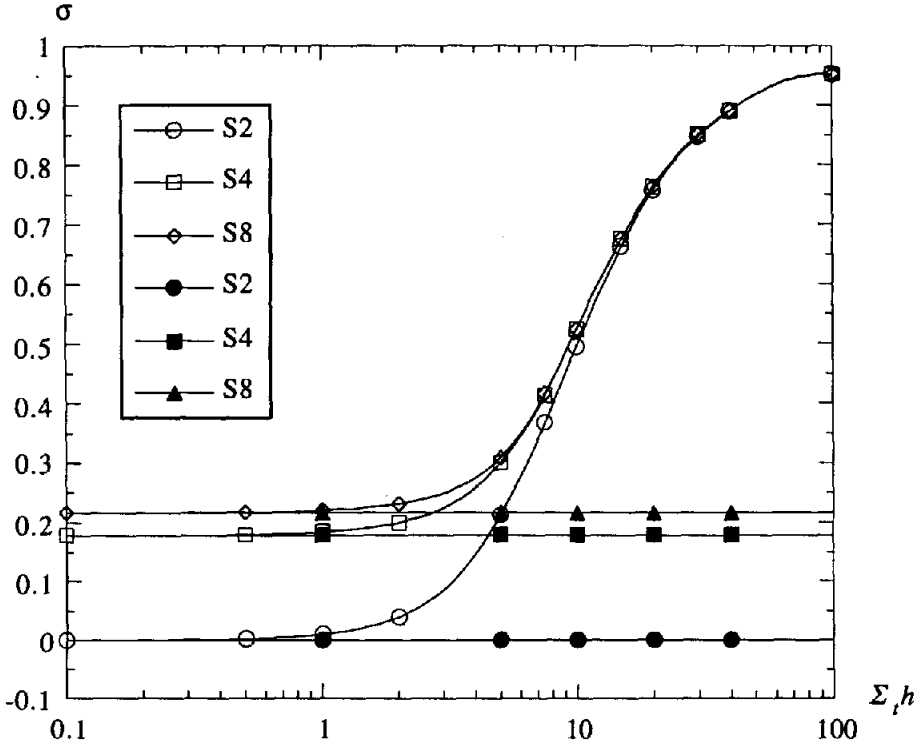

Figure 6: σ_{DSA} versus $\Sigma_t h$
(c=0.98, "Inconsistent" and "Consistent" DSA Diffusion Discretizations)

for the Diamond-Differenced S_N equations in 1-D and 2-D geometries. (In this paper, Alcouffe also proposes other schemes in which the "consistent" method is approximated to make it easier to solve, or to make it more useful for eigenvalue problems.) This same "consistency" principle has been applied to other 1-D spatial differencing schemes by Larsen and McCoy [83, 85], whose method is sometimes called "Larsen's Four-Step" method. The method described in Eqs. (3.45)-(3.64) is a simple generalization, which we describe here as (simply) the "Four-Step" method. The Four-Step method can be viewed as a direct application of Lebedev's $KP_1(1)$ method to the fully-discrete transport problem. [In Eqs. (1.37)-(1.39), $L-S$ is the fully discrete transport operator, K is the (P_1) projection onto the subspace spanned by linear functions of μ_n, and D is the specific discrete operator obtained when K is applied to $L-S$.] Unfortunately, practical algebraic difficulties with the Four-Step method occur with many non-diamond differencing schemes in multidimensional geometries; we discuss this later in detail.

In practical (finite, heterogeneous-media, nonuniform mesh) diamond-differenced S_N calculations using the consistently-differenced diffusion discretization [Eqs. (3.61)-(3.64)], iterative convergence is extremely rapid: the iterative error reduces at least two orders of magnitude for every three DSA iterations. Also, in 1-D, the cost of each DSA iteration is only slightly greater than that of a single source iteration because the low-order diffusion problem is tridiagonal and can be solved directly by Gaussian elimination. Thus, most practical 1-D problems can be solved with a computational cost less than that of about 12 source iterations.

If the underlying transport problem is highly scattering and optically thick, the unaccelerated SI scheme can require hundreds or even thousands of iterations to converge. In these cases, the DSA scheme can enable transport calculations to be performed in a very small fraction of the time required for unaccelerated calculations. Sometimes, DSA enables problems to be solved that would otherwise be viewed as "unsolvable," due to the forbiddingly excessive computational effort required.

In DSA, the importance of a consistently-discretized low-order diffusion equation cannot be overstated. Generally, DSA with a conventionally-discretized low-order diffusion equation becomes inefficient or even divergent as $\Sigma_t h$ increases. To maintain rapid convergence for all $\Sigma_t h$, careful attention must be paid to the low-order diffusion discretization.

III.C. S_2 Synthetic Acceleration (S_2SA)

In the S_2SA and other iterative schemes described below, the problem of consistently discretizing a low-order problem is finessed by choosing a low-order equation that is a transport equation – just like the high-order equation – and employing the same spatial discretization scheme in the high-order and low-order transport equations. In S_2 synthetic

acceleration (S_2 preconditioning), the "low-order" problem (preconditioning step) employs the S_2 quadrature set, while the "high-order" equation employs a higher-order S_N quadrature set.

For the diamond-differenced S_N equations in planar geometry, one can show easily that the S_2SA scheme and consistently-differenced DSA scheme are almost algebraically equivalent. This is because the continuous S_2 and P_1 equations are equivalent (assuming a Gauss-Legendre quadrature set), and the diamond-difference approximation does not alter this fact for the discrete equations. In planar geometry, the only difference between S_2SA and DSA is that the boundary conditions have slightly different extrapolation distances. This has no effect on the infinite medium Fourier analysis and no consistently measurable effect in practical applications. The result is that the S_2SA scheme converges with the same iterative speed as the DSA scheme with a consistently-discretized low-order diffusion equation.

In multidimensional geometries, the continuous S_2 and diffusion equations are algebraically distinct. Hence, the S_2SA and DSA schemes are not algebraically equivalent. We discuss the implications of this fact later.

For many 1-D non-diamond differencing schemes, the S_2SA and DSA methods are not algebraically equivalent. Nevertheless, in practice, both iteration schemes yield very rapid convergence for 1-D problems, provided (in DSA) the low-order diffusion equation is discretized "consistently" with the high-order S_N equation and (in S_2SA) the low-order S_2 equations are discretized using the same discretization scheme as the high-order S_N equations.

Thus, the use of a low-order transport (S_2) equation, rather than a diffusion equation, is a way to circumvent the DSA problem of obtaining a consistently-discretized low-order diffusion equation. However, the price of this success is that it is more costly to solve a discrete S_2 equation than to solve a discrete diffusion equation. Therefore, the cost of the low-order S_2SA calculations is greater than in DSA. In 1-D geometries, this cost is sufficiently low that the S_2 equations can be solved directly (i.e. non-iteratively) with minor penalty. However, the relative cost of directly solving the S_2 equations in multidimensional geometries is greater, in part because multidimensional S_2 quadrature sets contains more angles, so the S_2 equations contain more unknowns per cell. Also, the convergence properties of the S_2SA scheme in multidimensional geometries are not as favorable as in 1-D geometries. (We discuss this point later.)

III.D. KP Methods

Now we illustrate the application of a KP method to a discretized transport problem. We continue to use the DD transport discretization, and we apply the $KP_1(1)P_2(0)$ method

to this discretization using two different discretizations of the diffusion equation that arises in the $P_1(1)$ step. This step is identical to the low-order solution in the DSA method (Section III.B), and the two discretizations that we choose are the edge-centered discretizations shown in that section.

In the absence of discretization, a $KP_1(1)P_2(0)$ iteration is given by Eqs. (2.60)-(2.64). With DD, the "K" step [Eq. (2.60)] in this iteration becomes:

$$\frac{\mu_n}{h_j}\left(\psi_{n,j+1/2}^{(\ell+1/3)}-\psi_{n,j-1/2}^{(\ell+1/3)}\right)+\Sigma_{t,j}\psi_{n,j}^{(\ell+1/3)}=\frac{\Sigma_{s,j}}{2}\phi_j^{(\ell)}+\frac{Q_j}{2}\ , \tag{3.66}$$

$$\psi_{n,j}^{(\ell+1/3)}=\frac{1}{2}\left(\psi_{n,j+1/2}^{(\ell+1/3)}+\psi_{n,j-1/2}^{(\ell+1/3)}\right)\ , \tag{3.67}$$

together with boundary conditions. If we apply the conventional edge-centered discretization to the $P_1(1)$ step [Eq. (2.61)], we obtain

$$\begin{aligned}&-\frac{1}{3\Sigma_{t,j+1}h_{j+1}}\left(F_{j+3/2}^{(\ell+2/3)}-F_{j+1/2}^{(\ell+2/3)}\right)+\frac{1}{3\Sigma_{t,j}h_j}\left(F_{j+1/2}^{(\ell+2/3)}-F_{j-1/2}^{(\ell+2/3)}\right)\\&\qquad+\left(\Sigma_{a,j+1/2}h_{j+1/2}\right)F_{j+1/2}^{(\ell+2/3)}\\&=\frac{\Sigma_{s,j+1}h_{j+1}}{2}\left(\phi_{j+1}^{(\ell+1/2)}-\phi_{j+1}^{(\ell)}\right)+\frac{\Sigma_{s,j}h_j}{2}\left(\phi_j^{(\ell+1/2)}-\phi_j^{(\ell)}\right)\ ,\quad 1\le j\le J\ ,\end{aligned} \tag{3.68}$$

$$\phi_j^{(\ell+2/3)}(x)=\phi_j^{(\ell+1/3)}(x)+F_j^{(\ell+2/3)}(x)\ . \tag{3.69}$$

The $P_2(0)$ step [see Eq. (2.63)] is:

$$F_j^{(\ell+1)}=\frac{\beta c}{1-\beta c}\left(\phi_j^{(\ell+2/3)}-\phi_j^{(\ell)}\right)\ . \tag{3.70}$$

The final step is a simple addition to produce the next iterate:

$$\phi_j^{(\ell+1)}(x)=\phi_j^{(\ell+2/3)}(x)+F^{(\ell+1)}(x)\ . \tag{3.71}$$

Fourier-analyzing this scheme, we obtain:

$$\omega=\frac{\omega_{\mathrm{DSA}}-\beta c}{1-\beta c}\ , \tag{3.72}$$

where β is the adjustable parameter in Eq. (3.70), and where ω_{DSA} was shown in Section III.B to be:

$$\omega_{\mathrm{DSA}}=\omega_{\mathrm{SI}}-\frac{c(1-\omega_{\mathrm{SI}})}{(1-c)\left[1+\left(\frac{\Sigma_t h}{2}\right)^2\Lambda^2\right]+\frac{1}{3}\Lambda^2}\ , \tag{3.73}$$

$$\omega_{\mathrm{SI}}=\frac{c}{2}\sum_{n=1}^{N}\frac{w_n}{1+\mu_n^2\Lambda^2}\ , \tag{3.74}$$

$$\Lambda \equiv \frac{2}{\Sigma_t h} \tan\left(\frac{\Sigma_t h}{2}\lambda\right) \quad . \tag{3.75}$$

As we discussed in Section III.B, $\omega_{\mathrm{DSA}} \rightarrow 1$ as the mesh spacing becomes large and $c \rightarrow 1$. We see from Eq. (3.72) that the $KP_1(1)P_2(0)$ spectral radius approaches unity when $\omega_{\mathrm{DSA}} \rightarrow 1$. Thus, with the standard edge differencing of the diffusion equation, the $KP_1(1)P_2(0)$ loses effectiveness for optically thick cells when $c \rightarrow 1$. If we replace the standard edge-differenced diffusion equation, Eq. (3.68), with the *consistent* differencing developed in Section III.B, we obtain a different result. The consistent differencing is like Eq. (3.68) above except that the absorption and source terms have a three-point discretization:

$$\begin{aligned} &-\frac{1}{3\Sigma_{t,j+1}h_{j+1}}\left(F_{j+3/2}^{(\ell+2/3)} - F_{j+1/2}^{(\ell+2/3)}\right) + \frac{1}{3\Sigma_{t,j}h_j}\left(F_{j+1/2}^{(\ell+2/3)} - F_{j-1/2}^{(\ell+2/3)}\right) \\ &\quad + \frac{\Sigma_{a,j+1}h_{j+1}}{4}\left(F_{j+3/2}^{(\ell+2/3)} + F_{j+1/2}^{(\ell+2/3)}\right) + \frac{\Sigma_{a,j}h_j}{4}\left(F_{j+1/2}^{(\ell+2/3)} + F_{j-1/2}^{(\ell+2/3)}\right) \\ &\quad = \frac{\Sigma_{s,j+1}h_{j+1}}{2}\left(\phi_{j+1}^{(\ell+1/3)} - \phi_{j+1}^{(\ell)}\right) + \frac{\Sigma_{s,j}h_j}{2}\left(\phi_j^{(\ell+1/3)} - \phi_j^{(\ell)}\right) \quad . \end{aligned} \tag{3.76}$$

A Fourier analysis yields the same equation, Eq. (3.72), except that now ω_{DSA} satisfies:

$$\omega_{\mathrm{DSA}} = \omega_{\mathrm{SI}} - \frac{c(1-\omega_{\mathrm{SI}})}{1-c+\frac{1}{3}\Lambda^2} \quad . \tag{3.77}$$

As we discussed in Section III.B, this expression is bounded below $0.2247c$, the same value as the DSA method with no discretization. Thus, given a *consistent* discretization of the diffusion equation, the $KP_1(1)P_2(0)$ scheme applied to the DD equation performs exactly as it does with no discretization. As we showed in Section II.D, if we choose the optimum value $\beta \approx 1/8.88$, we obtain the bound

$$\sigma \leq 0.127c \tag{3.78}$$

on the spectral radius of $KP_1(1)P_2(0)$ scheme applied to DD, independent of the mesh spacing.

Thus, we see once more that the discretization of the low-order operator is extremely important to the performance of a preconditioner. *If an inconsistent discretization is employed, the preconditioner can lose effectiveness or even produce a divergent iteration for sufficiently coarse meshes. However, if a consistent discretization is used, then the preconditioned iteration can retain its un-discretized performance for all mesh spacings.*

III.E. Transport Synthetic Acceleration (TSA)

The TSA method has been developed and applied to spatially discretized S_N equations by Ramoné, Adams, and Nowak [243] and by Zika and Adams [284, 285]. As with the S_2SA scheme on which it is partly based, the TSA method has no loss of iterative convergence as $\Sigma_t h$ increases, assuming that the low-order problem is fully converged for each iteration. Figure 7a shows the TSA spectral radius as a function of $\Sigma_t h$ for the DD spatial

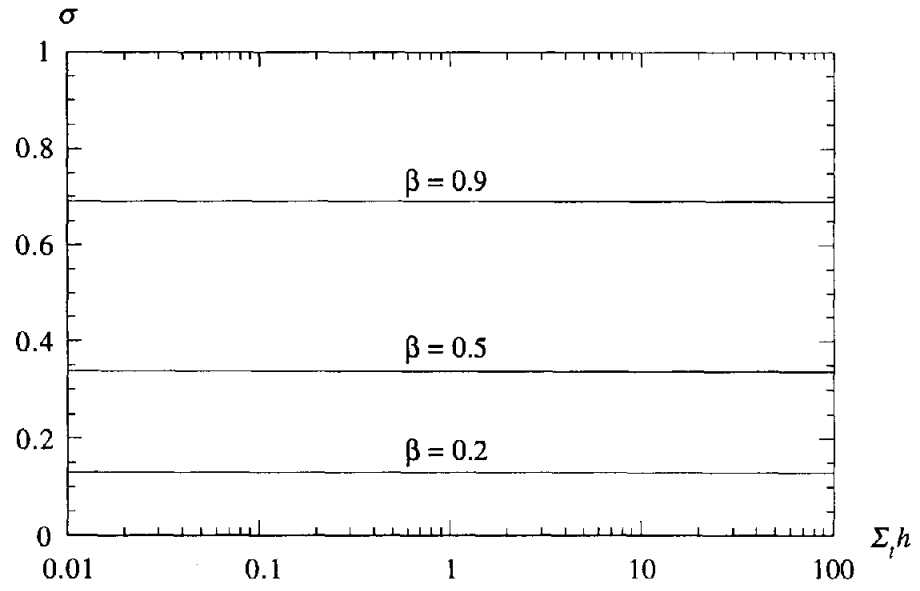

Figure 7a: σ_{TSA} versus $\Sigma_t h$
(c=0.98, Diamond Differencing in Slab Geometry, S_4 high- and low-order.)

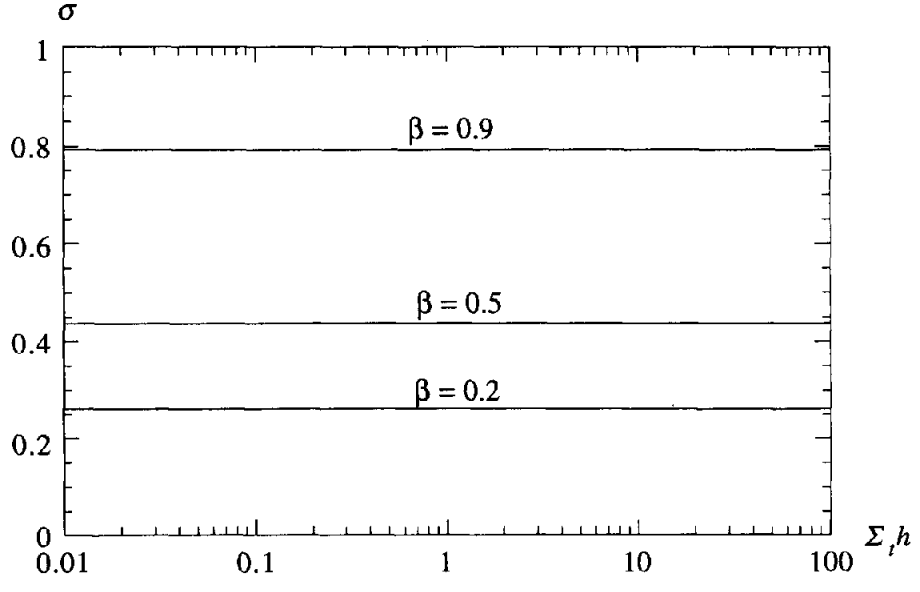

Figure 7b: σ_{TSA} versus $\Sigma_t h$
(c=0.98, Diamond Differencing in Slab Geometry, S_4 high-order, S_2 low-order.)

discretization in slab geometry. We note that there is no dependence of σ on $\Sigma_t h$. (This is true only for DD; for more complicated spatial discretizations, there tends to be some variation, but usually the greatest spectral radius occurs for $\Sigma_t h \approx 0$.) For this figure we used the S_4 quadrature set for both the high-order and low-order problems; the figure displays the effects of various choices of the parameter β (the fraction of the scattering cross section that is neglected in the low-order problem). Figure 7b is identical, except that the S_2 quadrature set is used for the low-order problem. This increases the spectral radius somewhat, but not significantly.

As $c \rightarrow 1$ in the high-order problem, the TSA spectral radius approaches β, provided that the low-order quadrature set is the same as the high-order set [243]. If the low-order quadrature set is S_2, this is true as well if $\beta > 1/2$; otherwise, the spectral radius can be slightly higher than β.

III.F. The Lewis-Miller (LM) Methods

The LM Second-Moment scheme for the continuous transport equation is defined by (*i*) the high-order transport equations (2.22)-(2.24) for $\psi^{(\ell+1/2)}(x,\mu)$, then (*ii*) the calculation of $\phi_2^{(\ell+1/2)}(x)$:

$$\phi_2^{(\ell+1/2)}(x) = \int_{-1}^{1} \left(\frac{3\mu^2 - 1}{2} \right) \psi^{(\ell+1/2)}(x,\mu) d\mu \quad , \tag{3.79}$$

and finally (*iii*) the diffusion equations (2.82)-(2.84) for $\phi^{(\ell+1)}(x)$. Here we consider the same S_N and diffusion discretizations as considered in the "inconsistently"-discretized DSA equations in Sec. III.B. Then the high-order S_N equations are defined by Eqs. (3.10)-(3.13), $\phi_{2,j+1/2}^{(\ell+1/2)}$ is defined by:

$$\phi_{2,j+1/2}^{(\ell+1/2)} = \sum_{n=1}^{N} \frac{3\mu_n^2 - 1}{2} \psi_{n,j+1/2}^{(\ell+1/2)} w_n \quad , \quad 0 \le j \le J \quad , \tag{3.80}$$

$\phi_{j+1/2}^{(\ell+1)}$ is defined by the discrete diffusion equation:

$$\begin{aligned} -\frac{1}{3\Sigma_{t,j+1} h_{j+1}} \left(\phi_{j+3/2}^{(\ell+1)} - \phi_{j+1/2}^{(\ell+1)} \right) + \frac{1}{3\Sigma_{t,j} h_j} \left(\phi_{j+1/2}^{(\ell+1)} - \phi_{j-1/2}^{(\ell+1)} \right) + \left(\Sigma_{a,j+1/2} h_{j+1/2} \right) \phi_{j+1/2}^{(\ell+1)} \\ = \frac{2}{3\Sigma_{t,j+1} h_{j+1}} \left(\phi_{2,j+3/2}^{(\ell+1/2)} - \phi_{2,j+1/2}^{(\ell+1/2)} \right) - \frac{2}{3\Sigma_{t,j} h_j} \left(\phi_{2,j+1/2}^{(\ell+1/2)} - \phi_{2,j-1/2}^{(\ell+1/2)} \right) \quad , \\ + \frac{1}{2} \left(h_{j+1} Q_{j+1} + h_j Q_j \right) \quad , \quad 1 \le j \le J-1 \quad , \end{aligned} \tag{3.81}$$

with boundary conditions

$$\frac{1}{2}\phi_{1/2}^{(\ell+1)} - \frac{1}{3\Sigma_{t,1}h_1}\left(\phi_{3/2}^{(\ell+1)} - \phi_{1/2}^{(\ell+1)}\right) + \frac{1}{2}(\Sigma_{a,1}h_1)\phi_{1/2}^{(\ell+1)} = \frac{h_1}{2}Q_1$$

$$+\frac{2}{3\Sigma_{t,1}h_1}\left(\phi_{2,3/2}^{(\ell+1/2)} - \phi_{2,1/2}^{(\ell+1/2)}\right) + \sum_{n=1}^{N}\left(\frac{1}{2}+\mu_n\right)\psi_{n,1/2}^{(\ell+1/2)}w_n \tag{3.82}$$

and

$$\frac{1}{3\Sigma_{t,J}h_J}\left(\phi_{J+1/2}^{(\ell+1)} - \phi_{J-1/2}^{(\ell+1)}\right) + \frac{1}{2}(\Sigma_{a,J}h_J)\phi_{J+1/2}^{(\ell+1)} = \frac{h_J}{2}Q_J$$

$$-\frac{2}{3\Sigma_{t,J}h_J}\left(\phi_{2,J+1/2}^{(\ell+1/2)} - \phi_{2,J-1/2}^{(\ell+1/2)}\right) \quad , \tag{3.83}$$

and $\phi_j^{(\ell+1)}$ is defined by:

$$\phi_j^{(\ell+1)} = \frac{1}{2}\left(\phi_{j+1/2}^{(\ell)} + \phi_{j-1/2}^{(\ell)}\right) \quad , \quad 1 \le j \le J \quad . \tag{3.84}$$

The Fourier analysis of this discrete LM scheme can be carried out just as described in Secs. III.A and III.B. Omitting the details of this analysis, we shall just state the result. Defining a single Fourier mode for the iterative error by

$$f_j^{(\ell)} = \phi_j - \phi_j^{(\ell)} = \omega_{\mathrm{LM}}^{\ell} e^{i\Sigma_t \lambda x_j} \quad , \tag{3.85}$$

and defining Λ by Eq. (3.28), we obtain

$$\omega_{LM}(h,\Lambda) = \frac{c}{2}\left[\sum_{n=1}^{N}\frac{3\mu_n^2-1}{1+\mu_n^2\Lambda^2}\right]\frac{\Lambda^2}{\Lambda^2+3(1-c)\left[1+\left(\frac{\Sigma_t h}{2}\Lambda\right)^2\right]} \quad . \tag{3.86}$$

Thus, we have the upper bound

$$|\omega_{LM}(h,\Lambda)| \le \frac{c}{2}\left|\sum_{n=1}^{N}\frac{3\mu_n^2-1}{1+\mu_n^2\Lambda^2}\right|\frac{\Lambda^2}{\Lambda^2+3(1-c)} \quad , \tag{3.87}$$

which is attained for $\Sigma_t h \to 0$. This result is a discrete version of Eq. (2.50), which has the same upper bound:

$$|\omega_{LM}(h,\Lambda)| \le 0.2247c \quad . \tag{3.88}$$

Hence, this discretization of the LM scheme converges rapidly for all $0 < \Sigma_t h < \infty$ and $0 \le c \le 1$. This result – rapid convergence with inconsistent discretizations – is very general; it holds for many, and perhaps all, reasonable discretizations of the LM diffusion problem for $\phi^{(\ell+1)}$. Thus, the LM method provides another way to circumvent the problem of obtaining a consistent low-order diffusion discretization for DSA; consistency is not needed.

However, as with the S_2SA method, which also overcomes this difficulty, there is a price to be paid. In the S_2SA method, the price is that the low-order equation is a discrete

S_2 equation, which is more costly to solve than a discrete diffusion equation. The price associated with the LM scheme is that *two* numerical estimates for the scalar flux ϕ_j are obtained: one from the high-order S_N sweep, and one from the low-order diffusion calculation. Upon convergence, these two estimates are identical only if the spatial discretizations of the S_N and diffusion equations are "consistent" in the following sense: when the exact transport expressions for $\phi_{2,j}$ are used in the right side of the low-order diffusion equations, the exact transport scalar flux ϕ_j arises as the solution of these equations.

Therefore, the LM method is rapidly convergent, but it is not a true acceleration scheme: one does not usually obtain the unaccelerated S_N solution. (The exception occurs when a *consistent* discretization is used to solve the LM equations.) However, in the limit $\Sigma_t h \to 0$, the truncation errors tend to zero, so the two LM scalar fluxes and the unaccelerated discrete S_N solution all converge to the true solution of the S_N equations. In this sense, the LM method is a legitimate, rapidly-converging method for solving the S_N equations.

A difficulty with the LM Second Moment scheme is that the terms on the right side of the diffusion equation contain second derivatives of the second Legendre moment ϕ_2, which can be negative. Therefore, it is very difficult to guarantee that the numerical expression for ϕ that comes from solving this equation is positive. (This problem has been addressed, but at the price of introducing a nonlinearity [90].) Another difficulty is that the accuracy of the LM scalar fluxes depends on how accurately both the S_N and diffusion equations are discretized. In other words, from an accuracy point of view, one must be concerned with both the S_N and the diffusion discretizations.

The LM First-Moment scheme was tested by Lewis and Miller [61]; a related nonlinear version of this method has recently been implemented and tested by Smith and Rhodes [283]. These authors report fast (DSA-like) convergence for neutronics-style problems.

III.G. The Quasidiffusion (QD) Method

In Chapter II we showed that when the continuous QD equations are linearized about a spatially flat solution, the QD method reduces to the LM method. The same is true for the discretized QD and LM methods. Therefore, the discrete Fourier analysis predicts that the LM and (linearized) QD methods have the same rapid convergence rates. In practical problems, the QD, LM, and consistently-discretized DSA schemes all converge with approximately the same rapid rate of convergence.

As with the LM scheme, the QD solution usually yields two estimates of the scalar flux: one from the spatially discretized S_N equations, and one from the low-order quasi-diffusion equation. These two solutions and the solution of the unaccelerated S_N equations differ by a spatial truncation error. (Thus, as with the LM method, the QD method is not usually a true acceleration scheme. The exception is when consistent discretizations are

used.) However, as the optical width of the spatial cells $\Sigma_t h$ tends to zero, all three of these solutions converge to the solution of the spatially continuous S_N equations.

III.H. The Weighted Alpha (WA) Methods

In Chapter II we stated that when the continuous WA equations are linearized about a spatially flat solution, the nonlinear WA method reduces to linear equations that are very similar to the S_2SA equations. The same is true for the discretized WA scheme. Thus, just as with the QD scheme, spatial and angular discretizations have a minor effect on the rates of convergence. However, spatial and angular discretizations do have an effect on the numerical solution; if one uses different discretization schemes for the S_N and WA equations, one does not achieve the unaccelerated solution of the discretized S_N equations, but obtains instead a different approximate S_N solution.

III.I. Second-Order Forms of the Transport Equation

We have seen that discretization details can have a crucial impact on the behavior of iterative methods. For example, given the DD transport discretization, three different discretizations of the low-order diffusion equation produce three very different iterative schemes. One (consistent) is always rapidly convergent, a second (edge-centered inconsistent) is convergent but ineffective for thick cells, and a third (cell-centered inconsistent, as analyzed by Reed [51]) is divergent for thick cells.

Because the second-order forms of the transport equation (discussed in Section II.I) have the same structure as the diffusion equation, it is straightforward to discretize the two equations consistently. Consider, for example, the edge-centered discretization of the diffusion equation that is given by Eq. (3.32) – the discretization that we have already noted is *inconsistent* with the DD discretization of the first-order form of the transport equation. We can apply this edge-centered discretization to the even-parity transport equation. With iteration indices the result is:

$$-\mu_n^2 \frac{\psi_{n,j+3/2}^{+(\ell+1/2)} - \psi_{n,j+1/2}^{+(\ell+1/2)}}{\Sigma_{t,j+1} h_{j+1}} + \mu_n^2 \frac{\psi_{n,j+1/2}^{+(\ell+1/2)} - \psi_{n,j-1/2}^{+(\ell+1/2)}}{\Sigma_{t,j} h_j} + \frac{\Sigma_{t,j+1} h_{j+1} + \Sigma_{t,j} h_j}{2} \psi_{n,j+1/2}^{+(\ell+1/2)}$$

$$= \frac{\Sigma_{s,j+1} h_{j+1} + \Sigma_{s,j} h_j}{2} \phi_{j+1/2}^{(\ell)} + \frac{Q_j h_j + Q_{j+1} h_{j+1}}{2} \quad . \tag{3.89}$$

Let us consider the iteration scheme given by Eqs. (3.89), (3.32), and the following:

$$\phi_{j+1/2}^{(\ell+1/2)} = \sum_{n:\mu_n>0} \psi_{n,j+1/2}^{+(\ell+1/2)} w_n \quad , \tag{3.90}$$

$$\phi_{j+1/2}^{(\ell+1)} = \phi_{j+1/2}^{(\ell+1/2)} + F_{j+1/2}^{(\ell+1)} \quad . \tag{3.91}$$

This is much like a one-dimensional version of DSA scheme that Morel et al. first explored in three dimensions for the even-parity equations [165]. We can Fourier-analyze this scheme, assuming the same model problem (infinite, uniform) as before. Omitting the details, we obtain:

$$\omega_{\mathrm{DSA}}(\Lambda) = \omega_{\mathrm{SI}} - \frac{c(1-\omega_{\mathrm{SI}})}{1-c+\frac{1}{3}\Lambda^2} \quad , \tag{3.92}$$

where

$$\omega_{\mathrm{SI}}(\Lambda) = \frac{c}{2}\sum_{n=1}^{N}\frac{w_n}{1+\mu_n^2\Lambda^2} \quad , \tag{3.93}$$

$$\Lambda \equiv \frac{1}{\Sigma_t h}\left(2[1-\cos(\Sigma_t h\lambda)]\right)^{1/2} \quad . \tag{3.94}$$

ω_{DSA} is of the same form as the DSA eigenvalue for the equations without spatial discretization, and the same form as the eigenvalue of the DD DSA method with consistent differencing of the diffusion operator. (Only the definition of Λ is different.) Thus, we have the bound $\omega_{\mathrm{DSA}}(\Lambda) \leq 0.2247c$, which is independent of h.

We can also apply the $KP_1(1)P_2(0)$ method to the even-parity equations. In this case we retain the transport sweep, Eqs. (3.89) and (3.90), and the diffusion equation, Eq. (3.32), and we define:

$$\phi_{j+1/2}^{(\ell+2/3)} = \phi_{j+1/2}^{(\ell+1/2)} + F_{j+1/2}^{(\ell+1)} \quad , \tag{3.95}$$

$$(1-\beta c)\tilde{F}_{j+1/2}^{(\ell+1)} = \beta c\left[\phi_{j+1/2}^{(\ell+2/3)} - \phi_{j+1/2}^{(\ell)}\right] \quad , \tag{3.96}$$

$$\phi_{j+1/2}^{(\ell+1)} = \phi_{j+1/2}^{(\ell+2/3)} + \tilde{F}_{j+1/2}^{(\ell+1)} \quad . \tag{3.97}$$

The Fourier analysis in this case produces

$$\omega_{KP_1P_2}(\Lambda) = \frac{1}{1-\beta c}\left[\omega_{\mathrm{DSA}}(\Lambda) - \beta c\right] \quad . \tag{3.98}$$

This has the same form as the un-discretized case discussed in Chapter II; thus, if β is chosen to be $\approx 1/8.88$, the spectral radius is bounded less than $0.127c$.

The main point of this illustration is that there is a form of the transport equation – the even-parity form – for which it is simple and natural to obtain consistently discretized acceleration equations. In this case, spatial discretization has little or no effect upon the performance of the acceleration scheme – performance is often independent of mesh spacing. Most of Lebedev's work on KP methods was analyzed and implemented within the even-parity framework; this is one reason that he did not observe poor iterative behavior caused by inconsistent discretizations. When Lebedev did employ the first-order form of the transport equation, it was usually for neutronics calculations in which the mesh cells were optically thin [Section XI.21 of [10]], [280, 293]. The importance of consistent discretizations for first-order forms and coarser meshes was recognized by other researchers

in the former Soviet Union, including Troschiev's group [42] and Germogenova's group [106]. We are confident that if Lebedev had tested his KP methods for the first-order form of the transport equation on optically thick meshes, he would have observed poor iterative behavior, in agreement with western experience and analyses (such as our analysis in Section III.D).

A natural question is: why would anyone use a form other than even-parity for a problem that requires significant iterative acceleration? The answer is that the even-parity form (and other forms with second-order derivatives, such as the odd-parity, spherical harmonics or P_N, and SAAF equations) have strengths and weaknesses different from those of the first-order form. The first-order form leads to a discrete system of equations for each direction that can be ordered in block lower-triangular form, enabling a solution by "sweeping" the spatial grid. Second-order forms, on the other hand, produce banded matrix systems that usually require more effort to invert. Another factor is the accuracy of the solution on a given spatial grid. It can be difficult to discretize second-order forms accurately in some problems (with streaming through void regions, for example). It can also be difficult to discretize first-order forms accurately in other problems (such as optically thick, diffusive problems). Given these and other considerations, there is not a convincing argument at this time to focus exclusively on any one form; instead, research continues on discretization and iterative acceleration for both first- and second-order forms of the transport equation. [286, 264, 281, 198, 211].

III.J. Performance in Non-Model Problems

In this chapter we have Fourier-analyzed iterative methods for the discretized transport equation, but only for one particularly simple model problem: an infinite medium with constant cross sections and a uniform space-angle grid. Two obvious questions are: how do these iterative methods perform on realistic problems with nonuniform spatial grids, boundaries, and material heterogeneities, and does the infinite-medium Fourier analysis remain a good predictive guide for the convergence rates in these problems?

Until recently, it was generally believed that performance in realistic problems is almost identical to performance in the simple model problem, as predicted by the Fourier analysis. This belief was founded on practical experience, over many years, on a vast number of realistic transport problems with spatial heterogeneities, nonuniform spatial grids, and finite system boundaries. Indeed, the power of the Fourier analysis is not so much that it accurately predicts the behavior of transport iteration schemes in idealized problelms, but that it also predicts the behavior in realistic non-model problems as well. (Alternatively, one could say that the discretization/iteration schemes generally exhibit the same basic iterative performance on model and non-model problems.)

However, recent work by Azmy and co-workers has shown that "extreme" problems exist in which the performance of DSA and similar acceleration schemes [259, 260, 279] is significantly degraded. (We are not aware that any problems have been seen in which a "consistently-discretized" DSA scheme has actually become unstable.) These problems are characterized as being 2-D or 3-D (not 1-D), with strong spatial heterogeneities, and with spatial grids having large aspect ratios. It is believed that for such problems, the diffusion approximation to the transport equation is not sufficiently accurate to provide an efficient preconditioner. Researchers are now seeking to understand how severe this degradation can be, whether it is significant in problems of practical interest, if it occurs for non-DSA-like iterative methods, and whether there are ways to make iterative methods more resistant to it.

III.K. Summary of Chapter III

Here we summarize the results developed in this chapter:

1. Iterative methods that are algebraically equivalent for the continuous transport equation, such as the DSA and Lewis-Miller methods, are generally not equivalent for the discretized transport equation. This is because the discrete equations approximate the continuous equations, and the algebraic manipulations that demonstrate equivalence for the continuous equations are not possible for the discrete equations.

2. The spectral radius of an iteration scheme depends on the angular discretization (for discrete-ordinates, the choice of quadrature set) and the spatial discretization (the choice of the spatial discretization schemes and the spatial grid).

3. The discrete-ordinates approximation of the angular variable in the transport equation generally has only a minor effect on convergence rates, and this effect does not lead to divergence for standard symmetric angular quadrature sets.

4. For the first-order form of the transport equation, the choice of the spatial discretization schemes for the high-order and low-order DSA equations has a much more significant effect on convergence rates than the choice of the angular quadrature set.

5. For the first-order form of the transport equation, unless special steps are taken, the spatially discretized DSA method generally loses efficiency or becomes divergent (the spectral radius of the scheme grows to a value equal to or exceeding unity) as the optical thickness of a spatial cell increases. This can be prevented by choosing a spatial discretization scheme for the low-order diffusion equation that is *consistent* with the discretization scheme of the high-order transport equation. The four-step method is one way to achieve this consistency.

6. For the first-order form of the transport equation, the S_2SA, TSA and WA schemes are unconditionally rapidly convergent if the low-order equations use the same (transport) spatial discretization as the high-order S_N equations. However, the low-order equations in these schemes are usually more costly to solve than the low-order equations in the DSA scheme.

7. The LM, QD, and WA schemes, in which the low-order equation directly determines the next scalar flux iterate, do not generally experience iterative divergence. These schemes usually are rapidly-converging for all spatial grids, without requiring that the diffusion discretization be consistent with the transport discretization. However, if the high-order and low-order equations are not discretized consistently, then upon iterative convergence, a truncation error distinguishes the two scalar flux solutions that come from the low-order and the high-order calculations. Also, neither of these discrete scalar fluxes equals that of the unaccelerated discrete transport equation. In the limit $\Sigma_t h \rightarrow 0$, these discretization errors disappear, and all three solutions limit to the exact solution of the S_N equations. However truncation-error differences exist for any finite spatial grid. Thus, the LM, QD, and WA methods converge rapidly, but unlike preconditioning methods, they are not true acceleration methods; upon iterative convergence, they do not yield the unaccelerated solution of the spatially discrete S_N equations. (The exception is when the equations are discretized consistently.) One can view this either as a difficulty (the discrete S_N solution is "contaminated") or an opportunity (a good low-order discretization can produce improvements over the unaccelerated solution). In problems containing important void or streaming regions, the former is likely to be true, whereas in diffusive problems the latter is likely to be true.

8. For the even-parity transport equation, one can discretize the high-order transport equation and the low-order diffusion equation using the same spatial differencing schemes. If this is done, DSA and the various KP iterative methods generally exhibit very rapid convergence with a rate that is mesh-independent, or nearly so.

9. The behavior of DSA and related acceleration schemes for realistic problems is generally well-predicted by the Fourier analysis of the idealized infinite homogeneous-medium problem. However, for certain extreme problems, in which diffusion theory does not accurately describe the behavior of the slowly-converging error modes, DSA and related schemes degrade in performance.

10. We have theoretically estimated the convergence rates of transport iteration schemes for various values of $\Sigma_t h$, and we have expressed a desire for iteration schemes that

are rapidly convergent for all values of $\Sigma_t h$. However, there are many practical radiation transport problems – such as neutron transport problems in nuclear reactors – in which, to achieve acceptable accuracy, spatial cells are rarely more than a few mean free paths thick. If for a desired application one knows that the spatial cells are not optically thick, then it is sensible to use an acceleration scheme that is convergent and efficient for optically thin spatial cells, even if it is less efficient for thick cells. However, the code user must be aware that if the code is applied to problems with increasingly thick spatial cells, the rate of iterative convergence of the code will degrade.

IV. OTHER DIFFERENCING SCHEMES AND GEOMETRIES

In Chapters II and III of this Review, we used the simplest geometry (1-D Cartesian) and one of the simplest spatial discretization schemes [diamond differencing (DD)] to illustrate some key concepts and properties of modern iterative methods for transport calculations. In this and subsequent chapters, we discuss, in less detail, the complications associated with more accurate spatial discretization schemes, more challenging geometries, and more complex physics. For now, we continue to assume steady state problems with isotropic scattering and one energy group. We find, not surprisingly, that as the discrete transport problem becomes more geometrically complex (and realistic), the task of devising a robust and efficient iterative method becomes more difficult.

IV.A. 1-D Planar Geometry

A 1-D planar spatial discretization that is more accurate and more complicated than DD is the one-parameter family of *linear discontinuous finite-element* (LD) methods or *generalized corner balance* (GCB) methods [195, 238]. This family, with the SI iteration scheme, is defined by:

$$\frac{2\mu_n}{\Sigma_{t,j}h}\left(\frac{1}{2}\left[\psi_{n,j,L}^{(l+1/2)}+\psi_{n,j,R}^{(l+1/2)}\right]-\psi_{n,j-1/2}^{(l+1/2)}\right)+\psi_{n,j,L}^{(l+1/2)}=\frac{c_j}{2}\phi_{j,L}^{(l)}+\frac{1}{2}\frac{Q_{j,L}}{\Sigma_{t,j}} \quad , \tag{4.1}$$

$$\frac{2\mu_n}{\Sigma_{t,j}h}\left(\psi_{n,j+1/2}^{(l+1/2)}-\frac{1}{2}\left[\psi_{n,j,L}^{(l+1/2)}+\psi_{n,j,R}^{(l+1/2)}\right]\right)+\psi_{n,j,R}^{(l+1/2)}=\frac{c_j}{2}\phi_{j,R}^{(l)}+\frac{1}{2}\frac{Q_{j,R}}{\Sigma_{t,j}} \quad , \tag{4.2}$$

$$\psi_{n,j+1/2}^{(l+1/2)}=\frac{1+\theta_{n,j}}{2}\psi_{n,j,R}^{(l+1/2)}+\frac{1-\theta_{n,j}}{2}\psi_{n,j,L}^{(l+1/2)} \quad , \quad \mu_n>0 \quad , \tag{4.3}$$

$$\psi_{n,j+1/2}^{(l+1/2)}=\frac{1+\theta_{n,j+1}}{2}\psi_{n,j+1,L}^{(l+1/2)}+\frac{1-\theta_{n,j+1}}{2}\psi_{n,j+1,R}^{(l+1/2)} \quad , \quad \mu_n<0 \quad . \tag{4.4}$$

$$\phi_{j,L}^{(\ell+1/2)}=\sum_{n=1}^{N}\psi_{n,j,L}^{(\ell+1/2)}w_n \quad , \tag{4.5}$$

$$\phi_{j,R}^{(\ell+1/2)} = \sum_{n=1}^{N} \psi_{n,j,R}^{(\ell+1/2)} w_n \quad , \tag{4.6}$$

with the "update" equations

$$\phi_{j,L}^{(\ell+1)} = \phi_{j,L}^{(\ell+1/2)} \quad , \tag{4.7}$$

$$\phi_{j,R}^{(\ell+1)} = \phi_{j,R}^{(\ell+1/2)} \quad . \tag{4.8}$$

In these equations, the subscripts "L" and "R" refer to the Left and Right halves of the spatial cell. For example, Eq. (4.1) [(4.2)] represents the balance equation for the left [right] half of the cell. If in Eqs. (4.3) and (4.4) we define $\theta = 3$, the scheme is equivalent to the standard LD method; if $\theta = 1$, the scheme is equivalent to the mass-lumped LD method and also to the "simple corner-balance" method [140, 195].

To analyze the convergence properties of the SI scheme with these methods, we consider the same infinite homogeneous-medium problem as before. A complication that immediately arises, relative to the analysis of SI for the DD method, in that *two* unknowns are needed to describe the scattering source in each cell. The description of a single Fourier error mode is now:

$$Q_{j,L} = Q_{j,R} = 0 \quad , \tag{4.9}$$

$$\phi_{j,H}^{(\ell)} = \omega^{\ell} A_H e^{i\Sigma_t \lambda x_j} \quad , \quad H = L,R \quad , \tag{4.10}$$

$$\psi_{n,j,H}^{(\ell+1/2)} = \omega^{\ell} a_{n,H} e^{i\Sigma_t \lambda x_j} \quad , \quad H = L,R \quad , \tag{4.11}$$

$$\psi_{n,j+1/2}^{(\ell+1/2)} = \omega^{\ell} b_n e^{i\Sigma_t \lambda x_{j+1/2}} \quad . \tag{4.12}$$

Using Eqs. (4.3)-(4.4) to eliminate the edge fluxes from Eqs. (4.1)-(4.2) and inserting the above description of a single error mode, we obtain:

$$\begin{bmatrix} 1 + \frac{\mu_n}{\Sigma_t h}\left(1 - [1-\theta_n]e^{-i\lambda\Sigma_t h}\right) & \frac{\mu_n}{\Sigma_t h}\left(1 - [1+\theta_n]e^{-i\lambda\Sigma_t h}\right) \\ -\frac{\mu_n}{\Sigma_t h}\theta_n & 1 + \frac{\mu_n}{\Sigma_t h}\theta_n \end{bmatrix} \begin{bmatrix} a_{n,L} \\ a_{n,R} \end{bmatrix} = \frac{c}{2} \begin{bmatrix} A_L \\ A_R \end{bmatrix} \quad , \mu_n > 0 \, , \tag{4.13}$$

$$\begin{bmatrix} 1 + \frac{|\mu_n|}{\Sigma_t h}\theta_n & -\frac{|\mu_n|}{\Sigma_t h}\theta_n \\ \frac{|\mu_n|}{\Sigma_t h}\left(1 - [1+\theta_n]e^{-i\lambda\Sigma_t h}\right) & 1 + \frac{|\mu_n|}{\Sigma_t h}\left(1 - [1-\theta_n]e^{-i\lambda\Sigma_t h}\right) \end{bmatrix} \begin{bmatrix} a_{n,L} \\ a_{n,R} \end{bmatrix} = \frac{c}{2} \begin{bmatrix} A_L \\ A_R \end{bmatrix} \quad , \mu_n < 0 \, . \tag{4.14}$$

More compactly,

$$T_n(\lambda) a_n = \frac{c}{2} A \quad , \tag{4.15}$$

where a_n and A are 2×1 vectors and $T_n(\lambda)$ is the obvious 2×2 matrix. It follows that

$$\omega A = \frac{c}{2} \left\{ \sum_{n=1}^{N} w_n [T_n(\lambda)]^{-1} \right\} A \quad . \tag{4.16}$$

Thus, for each value of λ the iteration eigenvalue ω satisfies a matrix eigenvalue problem. [The analog for DD is the 1×1 (scalar) Eq. (3.29).] The dimension of this matrix is the number of unknowns required to describe the scattering source in a cell. Thus, there generally are several error modes, one corresponding to each eigenvector A, for each value of λ. A consequence is that much more is asked of the low-order operator in a synthetic acceleration scheme (i.e., the preconditioner) for a transport discretization with several unknowns per cell than for a scheme with a single unknown per cell: the low-order operator has many more modes that it must attenuate. The transport discretizations with the most unknowns per cell are high-order schemes in multidimensional problems. *These are the schemes for which it is most difficult to create efficient acceleration methods.*

IV.A.1 Four-Step DSA

It is straightforward, although algebraically tedious, to apply the four-step procedure to the GCB equations in slab geometry. This has been reported [83] for the $\theta = 3$ case. Results are quite good; spectral radii are $< c/3$ for all values of c and cell thickness. The four-step procedure yields a diffusion discretization with one unknown at each cell edge, along with a local calculation in each cell that translates the edge-centered corrections to half-cell-average corrections. These calculations are much less computationally expensive than a GCB transport sweep; thus, the four-step procedure produces an extremely efficient acceleration scheme.

It is interesting that the four-step method can be applied to different (but equivalent) algebraic forms of a given transport discretization, such as GCB, with different results. For example, consider Eqs. (4.1)-(4.4) on one hand, and Eqs. (4.1)-(4.2) with the edge fluxes eliminated [by substitution of Eqs. (4.3)-(4.4)] on the other. The four-step procedure produces slightly different acceleration equations when applied to these two systems. In fact, using the four-step procedure on the second system is equivalent to using it on the first system after pre-multiplying Eqs. (4.3)-(4.4) by μ_n. This effectively changes the angular moments that are taken in step 1 of the procedure. We show later that this can make a significant difference in the performance of the method.

The following appears to be a general truth in slab geometry: *when applied to virtually any spatial discretization scheme with a symmetric angular quadrature set, the four-step procedure produces an efficient acceleration scheme.* With spatial discretizations more complicated than DD, it can be algebraically tedious to derive the discrete diffusion equations. However, with effort these equations can usually be manipulated into tridiagonal form, making them easy to solve. Spectral radii tend to be $< c/3$, which makes the resulting method very fast for problems with isotropic scattering.

IV.A.2 Other DSA Schemes

For transport discretizations that are more complicated than diamond differencing, the four-step procedure requires algebraic manipulations that can be daunting. Moreover, in multidimensional geometries it is not clear how to solve efficiently the resulting discrete low-order problems. Thus, there is motivation to develop DSA-like schemes with low-order equations that are easier to derive and solve. We now introduce one of these schemes, Adams and Martin's "modified four-step" (M4S) method, in the friendly setting of planar geometry.

The basic idea of the M4S method is to make an approximation in the angular first-moment equations that arise in the full four-step procedure. To illustrate, let us consider a GCB transport sweep. After this sweep, which produces fluxes at iteration $(l+1/2)$, the equations for the exact additive corrections f_n are:

$$\frac{2\mu_n}{\Sigma_{t,j}h_j}\left[\frac{1}{2}\left(f_{n,j,L}+f_{n,j,R}\right)-f_{n,j-1/2}\right]+f_{n,j,L}-\frac{c_j}{2}\sum_n w_n f_{n,j,L}=\frac{c_j}{2}\left(\phi_{j,L}^{(l+1/2)}-\phi_{j,L}^{(l)}\right)\ , \tag{4.17}$$

$$\frac{2\mu_n}{\Sigma_{t,j}h_j}\left[f_{n,j+1/2}-\frac{1}{2}\left(f_{n,j,L}+f_{n,j,R}\right)\right]+f_{n,j,R}-\frac{c_j}{2}\sum_n w_n f_{n,j,R}=\frac{c_j}{2}\left(\phi_{j,R}^{(l+1/2)}-\phi_{j,R}^{(l)}\right)\ , \tag{4.18}$$

$$f_{n,j+1/2}=\frac{1+\theta_{n,j}}{2}f_{n,j,R}+\frac{1-\theta_{n,j}}{2}f_{n,j,L}\ ,\quad \mu_n>0\ , \tag{4.19}$$

$$f_{n,j+1/2}=\frac{1+\theta_{n,j+1}}{2}f_{n,j+1,L}+\frac{1-\theta_{n,j+1}}{2}f_{n,j+1,R}\ ,\quad \mu_n<0\ . \tag{4.20}$$

These equations are the analog of Eqs. (3.46)-(3.47), previously shown for the DD method. Now we operate on the first two of these equations [(4.17) and (4.18)] by the discrete P_1 approximation: multiply by w_n (or $w_n\mu_n$), sum over n, and introduce the approximations

$$f_{n,j\pm1/2}=\frac{1}{2}\left(F_{j\pm1/2}+3\mu_n G_{j\pm1/2}\right)\ . \tag{4.21}$$

This yields the four equations:

$$\frac{2}{\Sigma_{t,j}h_j}\left[\frac{1}{2}\left(G_{j,L}+G_{j,R}\right)-G_{j-1/2}\right]+\left(1-c_j\right)F_{j,L}=c_j\left(\phi_{j,L}^{(l+1/2)}-\phi_{j,L}^{(l)}\right)\ , \tag{4.22}$$

$$\frac{2\mu_n}{\Sigma_{t,j}h_j}\left[G_{j+1/2}-\frac{1}{2}\left(G_{j,L}+G_{j,R}\right)\right]+\left(1-c_j\right)F_{j,R}=c_j\left(\phi_{j,R}^{(l+1/2)}-\phi_{j,R}^{(l)}\right)\ , \tag{4.23}$$

$$\frac{2}{3\Sigma_{t,j}h_j}\left[\frac{1}{2}\left(F_{j,L}+F_{j,R}\right)-F_{j-1/2}\right]+G_{j,L}=0\ , \tag{4.24}$$

$$\frac{2}{3\Sigma_{t,j}h_j}\left[F_{j+1/2}-\frac{1}{2}\left(F_{j,L}+F_{j,R}\right)\right]+G_{j,R}=0\ . \tag{4.25}$$

(Much of the remainder of this subsection is borrowed from Wareing [192].) For simplicity, we now assume that the parameter $\theta = 1$, which corresponds to the "lumped" linear discontinuous method or the "simple" corner balance method. Then, from Eqs. (4.19) and (4.20) we easily obtain

$$G_{j+1/2} = \frac{1}{2}\left(\gamma F_{j,R} + G_{j,R}\right) - \frac{1}{2}\left(\gamma F_{j+1,L} - G_{j+1,L}\right) \quad , \tag{4.26}$$

where $\gamma \approx 1/2$ is defined by Eq. (3.54). To this point the development is identical to the full four-step procedure. The full four-step procedure would now obtain an expression for the cell-edge scalar fluxes, $F_{j\pm1/2}$, in Eqs. (4.24) and (4.25) by taking an angular moment of Eqs. (4.19) and (4.20). The approximation made by Adams and Martin is to replace the cell-edge scalar fluxes in Eqs. (4.24) and (4.25) with values that are constructed entirely from cell-j information. With a discontinuous finite-element method, this can always be done by simply evaluating the function expansion at the cell edges. It can also be done with GCB; in the $\theta = 1$ case, for example, we obtain the following approximations for Eqs. (4.24) and (4.25):

$$\frac{2}{3\Sigma_{t,j}h_j}\left[\frac{1}{2}\left(F_{j,L} + F_{j,R}\right) - F_{j,L}\right] + G_{j,L} = 0 \quad , \tag{4.27}$$

$$\frac{2}{3\Sigma_{t,j}h_j}\left[F_{j,R} - \frac{1}{2}\left(F_{j,L} + F_{j,R}\right)\right] + G_{j,R} = 0 \quad . \tag{4.28}$$

These equations yield very simple Fick's-Law expressions for the currents:

$$G_{j,R} = G_{j,L} = -\frac{1}{3\Sigma_{t,j}h_j}\left(F_{j,R} - F_{j,L}\right) \quad . \tag{4.29}$$

These expressions can be used with Eq. (4.26) to easily eliminate all currents from Eqs. (4.22) and (4.23). The result is a relatively simple system of two equations per cell for the scalar-flux corrections $F_{j,R}$ and $F_{j,L}$.

In contrast, the fully consistent four-step equations for the $F_{j\pm1/2}$ in Eqs. (4.24) and (4.25) contain G terms from neighboring cells. The $F_{j\pm1/2}$ terms in these equations arise from taking the quadrature sum of $\mu_n^2 f_{n,j\pm1/2}$:

$$\sum_{n=1}^{N} 3\mu_n^2 f_{n,j+1/2} w_n = \sum_{\mu_n>0} 3\mu_n^2 f_{n,j,R} w_n + \sum_{\mu_n<0} 3\mu_n^2 f_{n,j+1,L} w_n \quad . \tag{4.30}$$

Making the P_1 approximation for each f in Eq. (4.30) [as shown in Eq. (4.21) for $f_{j+1/2}$], we obtain

$$F_{j+1/2} = \frac{1}{2}\left(F_{j,R} + F_{j+1,L}\right) + \frac{9\alpha}{8}\left(G_{j,R} - G_{j+1,L}\right) \quad , \tag{4.31}$$

where

$$\alpha = 4\sum_{\mu_n>0} \mu_n^3 w_n \approx 1 \quad .$$

Fortunately, when Eq. (4.31) is substituted into Eqs. (4.24) and (4.25), it is possible to eliminate the G terms by solving two equations for two unknowns at each cell edge. (However, eliminating the G terms from the four-step DSA equation is simple only for this $\theta = 1$ scheme in the GCB family; other values of θ lead to much more algebra.)

Wareing introduced a different simplification of the four-step equations by approximating Eq. (4.31) as follows:

$$F_{j+1/2} = \frac{1}{2}\left(F_{j,R} + F_{j+1,L}\right) \quad . \tag{4.32}$$

Like the Adams-Martin scheme, Wareing's scheme enables the immediate elimination of G terms from the equations, but unlike Adams-Martin it produces a discrete diffusion system that has a symmetric coefficient matrix. We call this method the "simplified symmetric" scheme.

There is no *a priori* guarantee that the Adams-Martin or Wareing scheme produces a rapidly-convergent method; this issue must be addressed by analysis and testing. This has been done; in Figure 8 we show the Adams-Martin "modified," Wareing "simplified symmetric" and the "full" four-step spectral radii as a function of mesh spacing for the $\theta = 1$ GCB method. In all cases the S_8 Gauss-Legendre quadrature set was employed. The results are very good: the spectral radii approach the expected analytic value (0.2247c) for fine meshes, remain < 0.5 for all mesh spacings, and approach zero for thick cells.

We remarked earlier that one can obtain different four-step DSA methods depending on the form of the discrete transport equations that is used as a starting point (which basically affects which angular moments are taken). If instead of taking the μ^2 moment in Eq. (4.30)

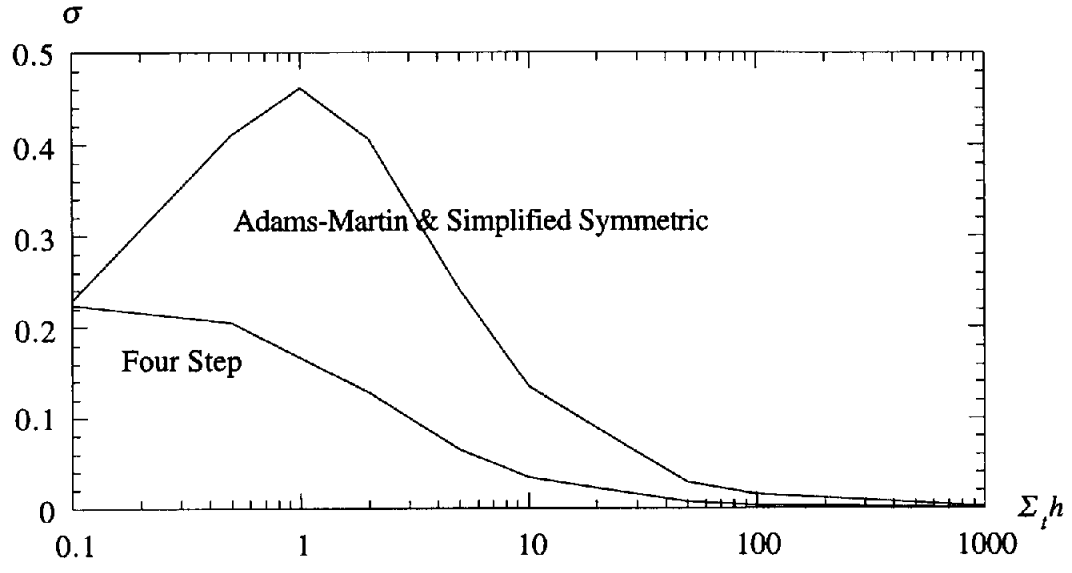

Figure 8: Spectral radius vs. mesh spacing; GCB $\theta = 1$ scheme, various DSA methods. ($c = 1$, S_{16} Gauss quadrature)

we had taken the $\mu^0 = 1$ moment, only the definition of α in Eq. (4.31) would change. However, this seemingly small change is enough to cause the spectral radius to remain roughly constant for all mesh spacings instead of limiting to zero for thick cells, as shown in Figure 8. This shows that *seemingly small details in a low-order operator can make a significant difference in its performance as an accelerator (i.e., preconditioner), particularly for large* $\Sigma_t h$.

IV.A.3 Transport Synthetic Acceleration (TSA)

The TSA scheme was introduced in Chapters II and III. This scheme eliminates the question of consistent discretizations of different operators, because the low-order operator is itself a transport operator. Thus, one simply uses the same spatial discretization for the high and low-order problems. This causes the performance of TSA to be essentially independent of the spatial discretization scheme.

The behavior of the TSA method in multiple space dimensions is similar to that in 1-D. The main difference is that in multi-D, it is possible for the TSA method to diverge if β is sufficiently close to unity [243]. Thus, greater care must be taken in the choice of β to ensure that the TSA method is not divergent.

IV.A.4 LM, QD, and WA Methods

As discussed in Chapters II and III, these methods do not require that the discretization of their low-order operators be consistent with the transport discretization – rapid convergence is attained even with independent discretizations. However, when independent discretizations are employed for the transport and low-order operators, the converged solution is not the same as the solution of the transport discretization, but is influenced by the discretization of the low-order operator. Thus, given a transport discretization whose solution has some highly desired properties, one should be cautious about "accelerating" that solution by using the LM, QD, or WA methods with inconsistent discretizations. It is possible to derive consistent discretizations for these methods, and these will indeed produce the same solution as the underlying transport discretization. However, the algebraic difficulties surrounding such consistent discretizations are just as severe as those associated with consistent DSA.

IV.B. 1-D Spherical Geometry

In 1-D spherical geometry, the angular flux depends only on the radial distance (r) from the origin and the angle (θ) between the outward radial direction and the direction of particle flight. This angle changes as a particle streams (unless the particle is moving directly toward or away from the origin), which means that in this geometry the streaming

term contains a derivative in the angle variable. If $\mu = \cos\theta$, the 1-D spherical geometry transport equation (with source-iteration indices included) can be written [9]:

$$\frac{\mu}{r^2}\frac{\partial\left(r^2\psi^{(\ell+1/2)}\right)}{\partial r}(r,\mu) + \frac{1}{r}\frac{\partial\left[(1-\mu^2)\psi^{(\ell+1/2)}\right]}{\partial\mu}(r,\mu) + \Sigma_t(r)\psi^{(\ell+1/2)}(r,\mu)$$

$$= \frac{\Sigma_s(r)}{2}\phi^{(\ell)}(r) + \frac{Q(r)}{2} \ , \ 0 < r < R \ , \ -1 \le \mu \le 1 \ , \tag{4.33}$$

$$\phi^{(\ell+1)}(r) = \int_{-1}^{1} \psi^{(\ell+1/2)}(r,\mu')d\mu' \ . \tag{4.34}$$

The angular derivative term in this equation significantly complicates the analysis of iteration methods. If we try to analyze source iteration for a simple model problem (infinite medium, uniform material properties) as we did in slab geometry by postulating that the error in ψ at a given iteration is a separable function of r and μ, we find that this algebraically does not work: the error is not separable. Thus, conventional wisdom has been that it is not possible to Fourier-analyze iteration schemes in spherical geometry.

Here we show that some Fourier analysis is in fact possible. As before, we set the source Q to zero and interpret the unknown functions as iteration errors. Then we analytically eliminate the angular variable to obtain an integral equation for the error in $\phi(r)$ [9]:

$$r\phi^{(\ell+1)}(r) = \frac{\Sigma_s}{2}\int_0^\infty r'\phi^{(\ell)}(r')[E_1(\Sigma_t|r-r'|) - E_1(\Sigma_t[r+r'])]dr' \ . \tag{4.35}$$

Here E_1 is the exponential integral:

$$E_1(z) = \int_z^\infty \frac{e^{-z'}}{z'}dz' = \int_0^1 \frac{1}{\mu}e^{-z/\mu}d\mu \ . \tag{4.36}$$

Defining $\phi(r)$ for negative r such that $\phi(r) = \phi(|r|)$ for $r < 0$, we can write Eq. (4.35) in the following form:

$$r\phi^{(\ell+1)}(r) = \frac{\Sigma_s}{2}\int_{-\infty}^\infty r'\phi^{(\ell)}(r')E_1(\Sigma_t|r-r'|)dr' \ . \tag{4.37}$$

Our definition of ϕ for negative arguments means that the product $r\phi(r)$ is an odd function of r. We therefore propose the following Fourier ansatz:

$$r\phi^{(\ell)}(r) = \omega^\ell \sin(\lambda\Sigma_t r) \ . \tag{4.38}$$

If the second definition of the E_1 function is substituted into Eq. (4.37) along with this ansatz, then the integral over r' can be performed, yielding the following expression for the iteration eigenvalue ω:

$$\omega(\lambda) \equiv c\int_0^1 \frac{d\mu}{1+\lambda^2\mu^2} = \frac{c}{\lambda}\tan^{-1}\lambda \ . \tag{4.39}$$

This is identical to the slab-geometry result, Eq. (2.12). Thus, in the absence of spatial and angular discretization, source iteration behaves the same way in 1-D spherical geometry as in 1-D Cartesian geometry.

We turn next to DSA. In the model problem (infinite uniform medium), the spherical-geometry equations for the iteration errors can be written as:

$$r\phi^{(\ell+1/2)}(r) = \frac{\Sigma_s}{2}\int_{-\infty}^{\infty} r'\phi^{(\ell)}(r')E_1(\Sigma_t|r-r'|)dr' \quad , \tag{4.40}$$

$$-\frac{1}{r^2}\frac{d}{dr}\frac{r^2}{3\Sigma_t}\frac{d}{dr}(F^{(\ell+1)}(r)) + \Sigma_a F^{(\ell+1)}(r) = \Sigma_s\left(\phi^{(\ell+1/2)}(r) - \phi^{(\ell)}(r)\right) \quad , \tag{4.41}$$

$$\phi^{(\ell+1)}(r) = \phi^{(\ell+1/2)}(r) + F^{(\ell+1)}(r) \quad . \tag{4.42}$$

It is possible to Fourier-analyze this scheme in spherical geometry. The ansatz is similar to Eq. (4.38), and the result is:

$$\omega(\lambda) = c\left[\frac{\lambda^2}{\lambda^2+3(1-c)}\right]\int_0^1 \frac{1-3\mu^2}{1+\lambda^2\mu^2}d\mu = \frac{3c}{\lambda^2+3(1-c)}\left[\left(\frac{\lambda^2}{3}+1\right)\frac{\tan^{-1}\lambda}{\lambda} - 1\right] \quad . \tag{4.43}$$

This is identical to the slab-geometry DSA result, Eq. (2.50). Thus, in the absence of spatial and angular discretization, the performance of DSA is the same in 1-D spherical geometry as in 1-D Cartesian geometry. To our knowledge, this analytic result is new.

The standard discrete-ordinates angular discretization of Eq. (4.33) is [9]:

$$\frac{\mu_n}{r^2}\frac{d\left(r^2\psi_n^{(\ell+1/2)}(r)\right)}{dr} + \frac{1}{r}\frac{\alpha_{n+1/2}\psi_{n+1/2}^{(\ell+1/2)}(r) - \alpha_{n-1/2}\psi_{n-1/2}^{(\ell+1/2)}(r)}{w_n} + \Sigma_t(r)\psi_n^{(\ell+1/2)}(r)$$

$$= \frac{\Sigma_s(r)}{2}\phi^{(\ell)}(r) + \frac{Q(r)}{2} \quad , \quad 0 < r < R \quad , \quad 1 \le n \le N \quad , \tag{4.44}$$

$$\psi_n^{(\ell+1/2)}(r) = \beta_n\psi_{n+1/2}^{(\ell+1/2)}(r) + (1-\beta_n)\psi_{n-1/2}^{(\ell+1/2)}(r) \quad , \tag{4.45}$$

where $\{\beta_n\}$ are chosen by various prescriptions [95] and $\{\alpha_n\}$ are defined by

$$\alpha_{n+1/2} = \alpha_{n-1/2} - 2w_n\mu_n \quad , \quad \alpha_{1/2} = 0 \, . \tag{4.46}$$

The scalar flux is given by a quadrature sum:

$$\phi^{(\ell+1/2)} = \sum_{n=1}^{N} \psi_n^{(\ell+1/2)} w_n \quad . \tag{4.47}$$

Unfortunately, with the angular variable discretized in this way, no Fourier analysis of source iteration or DSA seems to be possible. Spatial discretization adds further substantial complexity. Thus, the development of practical acceleration techniques for spherical-geometry problems has proceeded to date without the benefit of a sharp Fourier analysis.

In the absence of a Fourier analysis to guide the development of acceleration methods in spherical geometry, researchers have applied lessons from slab geometry and relied upon numerical testing. Experience has been that the techniques that work in slab geometry also work in spherical geometry. Thus, while spherical geometry makes it difficult to analyze iterative methods, it does not seem to hamper their effectiveness [144, 175].

IV.C. 1-D Cylindrical Geometry

In 1-D cylindrical geometry the angular flux depends upon the distance from the axis (r) and *two* angular variables. One angular variable, ξ, is the cosine of the angle between the axis and the direction of particle flight. The other angular variable, μ, is the angle between the outward radial direction and the radial-plane projection of the direction of particle flight. This latter variable changes continuously as a particle streams, as was the case in spherical geometry. Thus, there is once again a difficult angular derivative term [9].

As in spherical geometry, the practical development of acceleration schemes in cylindrical geometry has proceeded by applying the lessons learned from successful Cartesian approaches. As in spherical geometry, this strategy has been effective; cylindrical geometry has not yielded any major surprises [144, 175].

IV.D. Multidimensional Cartesian Geometries

IV.D.1. Source Iteration

The transport equation in multidimensional Cartesian geometry (still assuming isotropic scattering and one energy group) is:

$$\hat{\Omega}\cdot\vec{\nabla}\psi^{(l+1/2)}+\Sigma_t\psi^{(l+1/2)}\left(\vec{r},\hat{\Omega}\right)=\frac{\Sigma_s}{4\pi}\phi^{(l)}\left(\vec{r}\right)+\frac{Q\left(\vec{r}\right)}{4\pi}\ . \tag{4.48}$$

Here $\vec{r}$ is the position vector, $\hat{\Omega}$ is a unit vector in the direction of particle travel, and we have inserted iteration indices for a transport sweep. With source iteration, the new scalar flux is given by:

$$\phi^{(l+1)}\left(x,y,z\right)=\int_{4\pi}\psi^{(l+1/2)}\left(x,y,z,\hat{\Omega}\right)d\Omega\ , \tag{4.49}$$

where the integral is over all possible particle directions. One can again analyze the behavior of this iteration scheme given a simple model problem: infinite medium with constant material properties. As before, we set the source $Q=0$ and interpret the functions ψ and ϕ as iteration errors. The Fourier ansatz is then

$$\phi^{(l)}\left(\vec{r}\right)=\omega^l Ae^{i\Sigma_t\left(\lambda_x x+\lambda_y y+\lambda_z z\right)}=\omega^l Ae^{i\Sigma_t\vec{\lambda}\cdot\vec{r}}\ , \tag{4.50}$$

$$\psi^{(l+1/2)}\left(\vec{r},\hat{\Omega}\right)=\omega^l a(\hat{\Omega})e^{i\Sigma_t\vec{\lambda}\cdot\vec{r}}\ . \tag{4.51}$$

Inserting this ansatz into Eqs. (4.48) and (4.49) and manipulating the results, we obtain:

$$\omega\left(\vec{\lambda}\right) = \frac{c}{4\pi}\int_{4\pi}\frac{d\Omega}{1+\left(\vec{\lambda}\cdot\hat{\Omega}\right)^2} \ . \tag{4.52}$$

If we define the $s-$axis to be in the direction of $\vec{\lambda}$, $\lambda = |\vec{\lambda}| =$ length of $\vec{\lambda}$,

$$\hat{e}_s = \frac{\vec{\lambda}}{\lambda} \ ,$$

and $\mu = \hat{e}_s \cdot \hat{\Omega}$ to be the direction cosine along that axis, then we obtain

$$\omega\left(\vec{\lambda}\right) = \omega(\lambda) = \frac{c}{2}\int_0^1 \frac{d\mu}{1+\lambda^2\mu^2} \ . \tag{4.53}$$

This is identical to the slab-geometry source-iteration result. Thus, source iteration behaves identically in multidimensional and 1-D Cartesian geometries, at least in the absence of any discretization. The reason for this is fairly simple: each Fourier error mode is a plane wave along some axis, which means that a coordinate rotation produces one-dimensional equations for that mode. This remains true when we consider the DSA equations. Thus, in the absence of discretization, DSA in multidimensional Cartesian geometries behaves exactly like DSA in slab geometry, because each error mode is a plane wave and a coordinate rotation produces the slab equations. The behavior of an error mode depends only upon its wave number $\lambda = (\lambda_x^2+\lambda_y^2+\lambda_y^2)^{1/2}$, not on its orientation.

We now turn to the discrete-ordinates equations, in which there is angular discretization:

$$\hat{\Omega}_n \cdot \vec{\nabla}\psi_n^{(l+1/2)} + \Sigma_t \psi_n^{(l+1/2)}(\vec{r}) = \frac{\Sigma_s}{4\pi}\phi^{(l)}(\vec{r}) + \frac{Q(\vec{r})}{4\pi} \ , \tag{4.54}$$

$$\phi^{(l+1)}(\vec{r}) = \sum_{n=1}^{N_{tot}} w_n \psi_n^{(l+1/2)}(\vec{r}) \ . \tag{4.55}$$

The Fourier ansatz is essentially the same as before:

$$\phi^{(l)}(\vec{r}) = \omega^l A e^{i\Sigma_t(\lambda_x x+\lambda_y y+\lambda_z z)} = \omega^l A e^{i\Sigma_t\vec{\lambda}\cdot\vec{r}} \ , \tag{4.56}$$

$$\psi_n^{(l+1/2)}(\vec{r}) = \omega^l a_n e^{i\Sigma_t\vec{\lambda}\cdot\vec{r}} \ . \tag{4.57}$$

However, now one cannot perform a coordinate rotation to reduce the equations for a given error mode to slab-geometry equations. The reason for this is that the discrete-ordinates operator is not rotationally invariant. Thus, SI and DSA may perform differently for error modes that have the same wave number but different orientations. This implies that SI and DSA, applied to the 2-D and 3-D discrete-ordinates equations, may perform differently than in 1-D. If so, we would expect the largest differences to occur with quadrature sets that have few directions, because such sets are the least rotationally invariant.

The SI result is:

$$\omega\left(\vec{\lambda}\right) = \frac{c}{4\pi}\sum_{n=1}^{N_{tot}} \frac{1 - i\vec{\lambda}\cdot\hat{\Omega}_n}{1 + \left(\vec{\lambda}\cdot\hat{\Omega}_n\right)^2} w_n \ . \tag{4.58}$$

If the quadrature set has 180-degree rotational symmetry (the usual situation), then the imaginary term in the numerator vanishes because it is an odd function of $\hat{\Omega}$, while the denominator is even. Then the SI result is:

$$\omega\left(\vec{\lambda}\right) = \frac{c}{4\pi}\sum_{n=1}^{N_{tot}} \frac{w_n}{1 + \left(\vec{\lambda}\cdot\hat{\Omega}_n\right)^2} \ . \tag{4.59}$$

We note that the "flat" error mode, $\vec{\lambda} = \vec{0}$, produces the largest eigenvalue, whose value is c; this is the same as the result with no discretization. For other modes, let us more closely examine Eq. (4.59) for the standard quadrature set that has the fewest directions: the S_2 level-symmetric set, which has 8 directions in 3-D. Each direction cosine is $\pm 1/\sqrt{3}$ and each quadrature weight is $\pi/2$. We consider two different $\vec{\lambda}$'s that have the same magnitude, and explore how differently SI treats these two modes. We choose the first $\vec{\lambda}$ to be along a quadrature direction, $\vec{\lambda} = \lambda\hat{\Omega}_1$, and the second along a coordinate axis, $\vec{\lambda} = \lambda\hat{k}$. For the first we obtain:

$$\omega = c\frac{9 + 7\lambda^2}{(1+\lambda^2)(9+\lambda^2)} \ , \tag{4.60}$$

and for the second:

$$\omega = c\frac{3}{3+\lambda^2} \ . \tag{4.61}$$

For large λ, the first eigenvalue approaches $7c/\lambda^2$, while the second approaches $3c/\lambda^2$. This illustrates that given a finite discrete-ordinates quadrature set, SI does indeed treat different error modes differently, even when they have the same λ.

IV.D.2. Diffusion Synthetic Acceleration

We turn next to multidimensional DSA. The diffusion equation in multidimensional Cartesian geometry is rotationally invariant, and thus it treats identically all modes that have the same value of λ. However, when the diffusion equation is used to accelerate discrete-ordinates iterations, the full iteration operator is not rotationally invariant, and thus it performs differently for different modes that have the same λ.

Without spatial discretization, the DSA discrete-ordinates equations are Eq. (4.54) and:

$$\phi^{(l+1/2)}(\vec{r}) = \sum_{n=1}^{N_{tot}} w_n \psi_n^{(l+1/2)}(\vec{r}) \ , \tag{4.62}$$

$$-\vec{\nabla}\cdot\frac{1}{3\Sigma_t}\vec{\nabla}F + \Sigma_a F = \Sigma_s\left(\phi^{(l+1/2)} - \phi^{(l)}\right) \ , \tag{4.63}$$

$$\phi^{(l+1)}(\vec{r}) = \phi^{(l+1/2)}(\vec{r}) + F(\vec{r}) \ . \tag{4.64}$$

The Fourier ansatz is analogous to previous ones; the final result (again assuming 180-degree rotational symmetry of the quadrature set) is

$$\omega = \left(\frac{1}{\lambda^2 + 3(1-c)}\right) \frac{c}{4\pi} \sum_n \frac{\lambda^2 - 3(\vec{\lambda}\cdot\hat{\Omega}_n)^2}{1 + (\vec{\lambda}\cdot\hat{\Omega}_n)^2} w_n \ . \tag{4.65}$$

For $0 \leq c < 1$, one obtains a zero eigenvalue for the "flat" ($\vec{\lambda} = \vec{0}$) mode, as was the case without angular discretization. For other modes we more closely examine Eq. (4.65) given the S_2 quadrature set, considering again error modes with two orientations. The first is along a coordinate axis; the second is $\lambda_x = \lambda_y$ with $\lambda_z = 0$. For modes along a coordinate axis we obtain

$$\omega = 0 \ , \tag{4.66}$$

while the other considered modes produce

$$\omega = \left(\frac{\lambda^2}{\lambda^2 + 3(1-c)}\right)\left(\frac{c\lambda^2}{3 + 2\lambda^2}\right) \ . \tag{4.67}$$

The first result, Eq. (4.66) is the same as the S_2 result in one dimension – DSA converges immediately in that case. The second result is substantially different; as the wave number $\lambda \to \infty$, $\omega \to c/2$. We recall that in 1-D the DSA spectral radius is *zero* for the S_2 quadrature set and monotonically increases with increasing quadrature resolution up to approximately $0.2247c$ for S_∞. The situation in 2-D and 3-D is entirely different: the DSA spectral radius is $0.5c$ for the S_2 quadrature set and monotonically *decreases* with increasing quadrature order down to approximately $0.2247c$ for S_∞. Multidimensional DSA has been studied in detail by Adams and Wareing [181], who also considered asymmetric quadrature sets and anisotropic scattering. In addition, Marchuk and Lebedev studied the effects of anisotropic scattering (Section XI.19 of [10]) on Lebedev's $KP_1(1)$ preconditioning scheme, which is equivalent to DSA.

IV.D.3. S_2 Synthetic Acceleration

In 1-D without spatial discretization, S_2 Synthetic Acceleration (S_2SA) is equivalent to DSA. Given the preceding discussion, it is no surprise that this equivalence does not hold in 2-D or 3-D. Let us consider the S_2SA scheme given by Eq. (4.54), Eq. (4.62), the S_2 version of Eq. (4.63), and Eq. (4.64). If the high-order quadrature set in Eq. (4.54) is S_2, then the scheme converges in one iteration because the high- and low-order operators are the same. However, as the high-order quadrature order increases, the spectral radius of the S_2SA iteration scheme increases. In the limit as the high-order quadrature approaches an infinite number of directions, we have:

$$\sigma_{S2SA} \to \frac{c}{2-c} \ . \tag{4.68}$$

Obviously, this value approaches unity as $c \to 1$. Thus, in 2-D and 3-D, S_2SA and DSA have complimentary behavior: S_2SA is best for crude high-order quadratures and degrades as the quadrature set is refined, while DSA is at its worst for crude quadrature sets ($\sigma_{DSA} = c/2$ for the S_2 set) and improves for refined sets. [We remark that if the high-order quadrature is the S_{16} level-symmetric set, then the spectral radius of S_2SA is bounded below $0.86c$, which is substantially better than the limit of $c/(2-c)$.]

In the late 1960's, Gelbard and Hageman derived Eq. (4.68) [32]. Larsen later verified this result and further showed that S_4SA (one transport sweep followed by an S_4 low-order calculation) in 2-D has a spectral radius of $c/(6-c)$, which is always bounded below 0.2c [94]. Larsen also found that if *two* high-order sweeps precede each S_2 low-order calculation, then the spectral radius of the entire three-step iteration scheme is bounded below $0.153c$, with this maximum occuring as the high-order quadrature set becomes infinitely refined. [This three-step scheme is an example of Lebedev's general "K^2P" methods, in which two transport sweeps (Lebedev's K operations) are performed per low-order calculation (Section XI.12 of [10]).]

S_2SA and S_4SA have not received wide use in 2-D and 3-D calculations, mainly because the low-order equations have appeared to be too difficult to solve efficiently enough to make them worthwhile. The low-order equations have the same mathematical structure as the high-order equations; if an efficient technique existed for solving such equations, then that technique could be directly applied to the high-order equations. However, it might be that the hypothetical technique is efficient only when the number of angles is relatively small, as in the S_2 or S_4 equations. Then, given such a technique, S_2SA or S_4SA method could be efficient for accelerating S_N iterations, especially for large N.

Several authors have explored the use of low-order operators that are very similar to S_2 or S_4 operators. Nowak and Adams analyzed an S_2-like Boundary Projection Acceleration (BPA) method (Section V.B). They predicted that for spatially discretized problems, the spectral radii are smaller than those obtained previously for problems with no spatial discretization; thus, if efficient methods could be found for solving the S_2 problems, their S_2-like BPA method would have excellent performance even as $c \to 1$ [119], at least for problems whose spatial grids are not fine or whose quadrature orders are not high. Ramoné et al. developed and analyzed TSA methods (Sections II.E, III.E, IV.A.3), some of which employ S_2 low-order operators with modified cross sections [243], and found that these methods could be very effective if there existed efficient techniques for solving the S_2 equations. Hong and Cho have explored "angular rebalance" methods in 2-D (Section V.B), some of which have low-order equations that are much like S_2 equations [266, 267]. These authors found that their methods significantly reduce iteration counts, and they employed modern matrix iterative techniques to solve the low-order equations. These techniques are

reasonably efficient, at least for the test problems that Hong and Cho considered.

IV.D.4. Effects of Spatial Discretization: Regular Grids

For most spatial discretizations, the preconditioning (or "synthetic acceleration") of transport iterations in 2-D and 3-D is more complicated than in 1-D. The chief exception is the simple DD spatial discretization scheme on a rectangular grid; for that scheme, the four-step method can be applied to fairly readily produce a vertex-centered discretization of the diffusion equation that yields a DSA spectral radius equal to that without spatial discretization. This diffusion discretization has 9-point (27-point) coupling in two (three) dimensions. It is possible to approximate this consistent 9- or 27-point diffusion discretization with a simpler 5- or 7-point discretization; this makes the scheme lose effectiveness as the spatial mesh becomes coarse, but it significantly reduces the computational effort required to solve the diffusion equations [156]. This is the strategy employed in the DANTSYS codes [157, 232].

To illustrate the difficulties imposed by more complex spatial discretizations, let us consider the bilinear discontinuous (BLD) or corner-balance (CB) family [238] of schemes on rectangular grids in 2-D. (This is the 2-D analog of the 1-D GCB scheme discussed previously.) This family requires four fundamental unknowns per spatial cell to define the scattering source. Thus, there are four error modes and four eigenvalues per error-mode wave number $\vec{\lambda}$ in the simple model problem that is usually studied. The four-step DSA method produces a system of low-order equations with 12 unknowns per cell: four scalar-flux corrections and four corrections to each component of the net current. The corresponding 1-D system has 2 scalar flux and 2 net current unknowns per cell; we recall that it is possible to eliminate all of those in favor of one scalar flux unknown per cell edge. In 2-D, it is not generally possible to algebraically eliminate all unknowns in favor of a single scalar flux unknown per edge or vertex. For this reason, it is not known how to solve efficiently the four-step DSA equations.

Given the difficulties of deriving and implementing four-step DSA for complicated spatial discretizations in multidimensional geometries, many researchers have sought DSA approaches that are algebraically simpler, yet nearly as effective. One such approach was developed by Khalil [101, 128], primarily to accelerate "nodal" transport discretizations using "nodal" diffusion equations. Khalil discretized the diffusion equation directly, using approximations analogous to the approximations made in the given transport discretization. (In contrast, the four-step procedure derives DSA equations directly from the discrete transport equations.) Khalil's approach produced rapidly convergent DSA schemes for all spatial discretizations that he tested. To our knowledge, Khalil's procedure has not been applied to multidimensional transport discretizations other than "nodal" methods or to spatial

grids other than rectangular.

Another approach to simpler DSA equations is that of Adams and Martin [169], which we introduced previously in a 1-D setting. The authors showed that this modification of Larsen's four-step procedure could be applied to any discontinuous finite element (DFE) spatial discretization of the transport equation. Their "modification" is to replace the first-angular-moment equations with simple approximations; that is, to use a slightly "inconsistent" discrete Fick's Law. [In our 1-D example, this was the replacement of Eqs. (4.24) and (4.25) with Eqs. (4.27) and (4.28).] The result is a simple expression for each current-correction in terms of within-cell scalar-flux corrections, which makes it trivially easy to eliminate the current unknowns. Given the BLD/CB family of transport discretizations on rectangular grids in 2-D, for example, the Adams-Martin modification quickly reduces the system from 12 unknowns per cell to 4. The behavior of the Adams-Martin DSA scheme in XY geometry is much like that in slab geometry (see Figure 8).

Wareing introduced a different modification of the four-step equations that, like the Adams-Martin modification, makes it easy to eliminate the current unknowns in the acceleration equation [192]. (We illustrated this previously for one discretization scheme in slab geometry.) The Adams-Martin equations have an asymmetric coefficient matrix, which could hamper their efficient solution; Wareing's system is symmetric and positive definite. (Wareing called this "symmetric simplified" DSA.) The behavior of Wareing's DSA scheme in XY geometry is much like that in slab geometry (see Figure 8).

Wareing, Larsen, and Adams developed yet another approach to try to derive discrete diffusion equations that are simple yet effective when used for DSA [167]. Their logic was as follows. One can derive the analytic diffusion equation from the analytic transport equation by various procedures; two very different ones are (*i*) to make the P_1 approximation, and (*ii*) to take the asymptotic diffusion limit [140, 172]. Larsen's four-step DSA procedure derives discrete diffusion equations from discrete transport equations by making the P_1 approximation. Wareing et al. proposed to derive discrete diffusion equations by taking the asymptotic diffusion limit of the discrete transport equations [167]. That is, they determined a set of equations that the discrete transport solution satisfies in the limit of extreme optical thickness and high scattering ratio, and used those equations for DSA. This idea has strong intuitive appeal; the most difficult iterative problems are optically thick and highly scattering, and in such problems the low-order and high-order operators have nearly the same solutions. However, Fourier analysis shows that the scheme loses effectiveness (even in 1-D) in that limit. The cause is error modes that are discontinuous at cell edges; the diffusion-limit spatial discretization does not attenuate these modes, and their eigenvalues approach c for optically thick cells. Wareing et al. solved this problem by including a post-diffusion calculation that produces discontinuous scalar-flux correc-

tions. This post-diffusion calculation employs equations borrowed from the four-step or Adams-Martin method and is independent for each spatial cell – there is no cell-to-cell coupling. Thus, it does not add significantly to the computational cost. We call this scheme the "asymptotic" DSA scheme. The authors found that their asymptotic DSA scheme is very effective in 1-D and in 2-D for square cells. However, as the 2-D cell aspect ratio approaches infinity, the spectral radius of asymptotic DSA approaches c.

The DSA methods introduced by Khalil, Adams-Martin, Wareing, and Wareing-Larsen-Adams are all rapidly convergent, with the exception of the aspect-ratio problem encountered by the latter method. However, rapid convergence is only one piece of the puzzle; the other piece is the efficient solution of the acceleration equations. Khalil employed relatively straightforward iterative techniques to solve his diffusion discretization; these were sufficient for the reactor analysis problems that he considered. However, it is not clear that these techniques would remain efficient given optically thick spatial cells with c near unity. Adams and Martin used a brute-force matrix decomposition to solve their discrete diffusion equations (which are asymmetric) and noted that an efficient solution technique needed to be developed. Wareing solved his symmetric equations via the Conjugate Gradient method without a preconditioner. The asymptotic DSA of Wareing et al. is of a standard finite-difference form, with 9-point (27-point) coupling in 2-D (3-D), and thus is amenable to solution by standard diffusion solvers. However, as already noted, it suffers from loss of rapid convergence given cells with high aspect ratios. Thus, despite their successes, all of these efforts left something to be desired: none produced an unconditionally efficient iteration algorithm. At this point, the only acceleration algorithm that was known to be unconditionally efficient for multidimensional problems was four-step DSA applied to the DD equations on rectangular cells; this produces a standard diffusion discretization that can be accelerated using multigrid techniques. However, this unconditionally efficient algorithm was not implemented in production codes; the TWODANT code, for example, used a slightly *inconsistent* 5-point diffusion discretization instead of the consistent 9-point scheme in order to reduce the cost of solving the diffusion equation. This is a winning strategy for problems that are not too optically thick and highly scattering, but it does not work efficiently for the most difficult problems (optically thick cells, c close to unity).

This challenge was answered in 1993, at least for the BLD family of spatial discretizations on rectangular grids, by Morel, Dendy, and Wareing [190]. They developed an efficient technique for solving the Adams-Martin BLD equations on such grids, and thus implemented the first unconditionally efficient DSA scheme for (non-DD) multidimensional transport iterations. A full iteration in their scheme consists of several steps: a transport sweep, line relaxations on the Adams-Martin discontinuous diffusion equations, and fixed number (usually 1) of multigrid V-cycles on a bilinear continuous (BLC) diffu-

sion discretization. The entire scheme can be viewed as a generalized multigrid method: the highest level is BLD transport, the next is BLD diffusion, the next is BLC diffusion on the same grid, and the remaining levels are BLC diffusion on coarser grids. Results are excellent; the scheme converges any fixed-source one-group isotropic-scattering transport problem for the cost of a few transport sweeps.

Wareing, Walters, and Morel found that they could use the same acceleration equations – the Adams-Martin equations for the BLD scheme, solved with their multilevel technique – to accelerate the bilinear nodal transport discretization [201]. Adams and Wareing later used the same equations to accelerate the bilinear characteristic scheme [247]. Results in both cases are excellent, even though the acceleration equations are derived from the BLD transport scheme instead of the bilinear nodal or bilinear characteristic scheme. (We conjecture that this procedure works because the three different spatial discretization schemes all provide essentially the same solution in the asymptotic diffusion limit.) Thus, at the time of this writing, there exists an unconditionally efficient DSA methodology for several transport discretizations of practical interest, given rectangular grids in 2-D Cartesian geometry.

IV.D.5. Effects of Spatial Discretization: Unstructured Grids

In the preceding section we explained that there now exist unconditionally efficient DSA schemes for certain transport discretizations on certain kinds of grids. The picture is more clouded on unstructured grids, for which key questions remain unanswered:

1. Can one obtain a discrete preconditioner – a discretization of the diffusion equation, for example – that produces a small spectral radius?

2. If so, can one devise solution procedures for the discrete low-order operator that render the iteration scheme unconditionally efficient?

The answer to the first question is most likely affirmative. For example, we expect Larsen's four-step procedure to produce a discrete diffusion equation that would yield a small spectral radius. Recent work by Warsa et al., who have analyzed and tested consistent and inconsistent DSA for LD on tetrahedral grids in 3-D, supports this conjecture [300]. As another example, the Adams-Martin Boundary-Projection Acceleration procedure will almost certainly yield a low-order operator that provides rapid acceleration – one simply must choose a low-order angular space that approximates the iteration error reasonably well at cell surfaces [125]. However, despite the attractive logic behind our conjectures, arbitrary grids may yet offer surprises. For example, Warsa et al. show that the M4S method of Adams and Martin, which is rapidly convergent on orthogonal grids, is actually *divergent* on skewed tetrahedral grids [300]. This indicates that one should *not* assume that the orthogonal-grid behavior of an iterative scheme will automatically extend to arbitrary grids.

The problem posed by the second question is likely the more difficult one. For example, while Warsa et al. found that four-step DSA yields a small spectral radius for LD on tetrahedral grids, they also found that solving these consistent equations is extremely expensive relative to a transport sweep with a modest quadrature set, relative to solving the M4S or asymptotic DSA equations. Thus, their implementation of four-step DSA did not provide an unconditionally efficient iterative method for LD on tetrahedral grids.

Warsa et al. are not alone; to our knowledge no one has demonstrated an unconditionally efficient implementation of four-step DSA for any spatial discretization method of the first-order form of the transport equation on arbitrary grids. Considering a broader perspective, we note that all unconditionally efficient schemes devised to date rely on multigrid techniques to solve the low-order equations. Such techniques are not as readily available on unstructured grids as on structured grids, although the emerging class of "algebraic multigrid" (AMG) methods may solve this problem [107], [2]. Also, the efficient DSA method devised by Morel, Dendy, and Wareing [190] for BLD on rectangles relied upon line relaxations to attenuate discontinuous error modes. On an unstructured grid, the concept of a mesh line is not clearly defined; thus, even if AMG can efficiently solve standard diffusion problems on unstructured grids, it still may not be possible to generalize the Morel-Dendy-Wareing algorithm to such grids.

IV.E. Second-Order Forms in Multidimensional Geometries

If we consider the second-order forms of the transport equation, for which it is straightforward to obtain preconditioners that are standard discretizations of the diffusion equation, the picture is somewhat simpler. Let us suppose that the emerging AMG methods ultimately provide efficient techniques for solving standard diffusion discretizations on unstructured grids. Then we should find that the DSA equations for second-order forms yield a low spectral radius and are relatively inexpensive to solve. One remaining question would be whether the same AMG techniques could efficiently solve the high-order equations, which appear to be similar to diffusion equations, but which have important differences. A second question would be whether the solutions arising from discretizations of the second-order forms would be of sufficient accuracy and robustness for the applications of interest. If these questions are answered affirmatively, then the result will be an unconditionally efficient arbitrary-grid iterative method for a useful discretization of a second-order form of the transport equation.

To summarize: *at the time of this writing, an unconditionally efficient acceleration scheme for transport on unstructured grids has not been demonstrated.* This is an area of active research, for discretizations of both the first-order and second-order forms of the transport equation.

V. OTHER ITERATIVE METHODS

The methods describe in Chapters II and III make use of "low-order" operators that are closely related to diffusion or transport equations. In this chapter we discuss other low-order operators that have been used to accelerate transport iterations. Some of these produce additive corrections, while others produce multiplicative corrections.

V.A. Rebalance

Rebalance is one of the earliest acceleration schemes to be developed specifically for particle transport problems [15, 31]. This method has been employed in numerous production neutron transport codes [46]. It is quite imperfect in its performance [51, 69, 9], as discussed below. However, it is simple in both concept and implementation. Rebalance is usually presented as a nonlinear method, but like the Quasidiffusion scheme, it can be easily linearized. The linearized scheme can be Fourier-analyzed, and numerical experiments demonstrate that the nonlinear and linear forms of rebalance have very similar behavior, which is well-predicted by the Fourier analysis [127, 150].

Like many other acceleration methods, rebalance combines a "high-order" transport sweep with a "low-order" calculation. For rebalance, the low-order calculation is extremely simple – it contains no details of the "high-order" transport discretization. (Thus, rebalance can be applied to all S_N discretizations in basically the same way.) The price of this great simplicity is that to optimize performance, the code user must determine which *form* of rebalance to use. Typically, *fine mesh rebalance* (FMR) (in which rebalance factors are calculated on the fine transport spatial mesh) is divergent, although not always. *Coarse-mesh rebalance* (CMR), in which rebalance factors are calculated on groups of fine-mesh cells, is generally convergent if each coarse cell contains sufficiently many fine-mesh cells. If the coarse cells contain too many fine-mesh cells, the method will be convergent but inefficient. If the coarse cells contain too few fine-mesh cells, the method may be divergent. Thus, the code user must select an optimal coarse mesh to make the scheme convergent and maximize its efficiency. Yet, even if this is done, rebalance is often inefficient for the most challenging (optically thick, highly-scattering) problems. Because of these limitations, rebalance is often viewed with disfavor in comparison with more efficient and user-friendly schemes. Yet, because of its implementational simplicity, it is still used in some codes.

To describe the rebalance method, let us consider the planar-geometry diamond-differenced S_N problem defined by Eqs. (3.1)-(3.4). The j^{th} *fine-mesh* spatial cell consists of the interval:

$$x_{j-1/2} < x < x_{j+1/2} \quad , \quad 1 \leq j \leq J \quad .$$

The easiest way to define a coarse grid is to require that J, the number of fine-mesh cells,

be divisible by a smaller integer K:

$$J = pK \quad .$$

Then K is the number of coarse-mesh cells in the system, and p is the number of fine-mesh cells per coarse-mesh cell. (In practice, this definition of coarse-mesh cells need not be uniform.) Proceeding from left to right across the system, the first p fine-mesh cells constitute the first coarse-mesh cell, the next p fine-mesh cells constitute the second coarse-mesh cell, and so on. Thus, the k^{th} coarse-mesh cell consists of the interval

$$x_{p(k-1)+1/2} < x < x_{pk+1/2} \quad , \quad 1 \le k \le K \quad .$$

Often, *fine-mesh* or *coarse-mesh* cells are referred to as simply *fine* or *coarse* cells.

Now, let us assume that an estimate $\phi_j^{(\ell)}$ of the cell-average scalar fluxes is given on the fine spatial mesh, and that a transport sweep [Eqs. (3.10)-(3.14)] is performed on this mesh. At the completion of this sweep, new fine-mesh scalar flux estimates $\phi_j^{(\ell+1/2)}$ are stored. We also require that the exiting partial currents at the edge of each coarse cell be computed and stored:

$$\left.\begin{aligned} J_{pk+1/2}^{(\ell+1/2),+} &= \sum_{\mu_n>0} \mu_n \psi_{n,pk+1/2}^{(\ell+1/2)} w_n \\ J_{p(k-1)+1/2}^{(\ell+1/2),-} &= \sum_{\mu_n<0} |\mu_n| \psi_{n,p(k-1)+1/2}^{(\ell+1/2)} w_n \end{aligned}\right\} \quad 1 \le k \le K \quad . \tag{5.1}$$

Next, *rebalance factors* $A_k^{(\ell+1)}$ are introduced on each coarse cell, and accelerated partial currents and fine-mesh scalar fluxes are defined by multiplying the estimates obtained from the transport sweep by the appropriate rebalance factor. Specifically, the cell-average scalar flux estimates in fine-mesh cells contained in coarse cell k, and the partial currents exiting from coarse cell k, are multiplied by $A_k^{(\ell+1)}$. Thus, for each $1 \le k \le K$,

$$\phi_j^{(\ell+1)} = \phi_j^{(\ell+1/2)} A_k^{(\ell+1)} \quad , \quad p(k-1)+1 \le j \le pk \quad , \tag{5.2}$$

$$J_{pk+1/2}^{(\ell+1),+} = J_{pk+1/2}^{(\ell+1/2),+} A_k^{(\ell+1)} \quad , \tag{5.3}$$

$$J_{p(k-1)+1/2}^{(\ell+1),-} = J_{p(k-1)+1/2}^{(\ell+1/2),-} A_k^{(\ell+1)} \quad . \tag{5.4}$$

The constants $A_k^{(\ell+1)}$ are determined by requiring that the accelerated cell-averaged fluxes and partial currents satisfy the balance Eq. (3.1) "integrated" over all directions and each coarse cell:

$$\left(J_{pk+1/2}^{(\ell+1),+} - J_{pk+1/2}^{(\ell+1),-}\right) - \left(J_{p(k-1)+1/2}^{(\ell+1),+} - J_{p(k-1)+1/2}^{(\ell+1),-}\right) + \sum_{j=p(k-1)+1}^{pk} \Sigma_{a,j} \phi_j^{(\ell+1)} h_j$$

$$= \sum_{j=p(k-1)+1}^{pk} Q_j h_j \quad , \quad 1 \le k \le K \quad . \tag{5.5}$$

This is the *coarse-mesh balance equation*. Introducing Eqs. (5.2)-(5.4) into Eq. (5.5), we obtain the following linear tridiagonal system of equations for $A_k^{(\ell+1)}$:

$$A_k^{(\ell+1)}\left[J_{pk+1/2}^{(\ell+1/2),+}+J_{p(k-1)+1/2}^{(\ell+1/2),-}+\sum_{j=p(k-1)+1}^{pk}\Sigma_{a,j}\phi_j^{(\ell+1)}h_j\right]$$

$$-A_{k-1}^{(\ell+1)}\left[J_{p(k-1)+1/2}^{(\ell+1/2),+}\right]-A_{k+1}^{(\ell+1)}\left[J_{pk+1/2}^{(\ell+1/2),-}\right]$$

$$=\left[\sum_{j=p(k-1)+1}^{pk}Q_jh_j\right]\quad,\quad 1\le k\le K\quad, \tag{5.6}$$

where $A_0^{(\ell+1)}=A_{K+1}^{(\ell+1)}=1$. This system of equations is solved, $\phi_j^{(\ell+1)}$ are defined by Eqs. (5.2), and then one proceeds with the next transport sweep. If this iteration scheme converges, then

$$\lim_{\ell\to\infty}A_k^{(\ell)}=1\quad.$$

The rebalance method has several good features:

1. Any spatial discretization method that employs the balance equation, in conjunction with one or more auxilliary equations, can be run iteratively with rebalance. The algebraic form of the rebalance equations depends only on the balance equation, not on any of the auxilliary equations. This makes the application of rebalance extremely simple.

2. In multidimensional geometries, rebalance can easily be employed on problems with an unstructured spatial grid. It is only necessary that the coarse cells be simply-connected and disjoint, and that their union consist of the entire system.

3. Rebalance is easy to adapt to multigroup problems. Rebalance factors can be defined on coarse or fine energy-grids, as well as on coarse or fine spatial grids, depending on the decision of the code user.

4. Nonlinear rebalance is very easy to adapt to $k-$eigenvalue problems. In this case, the set of "low-order" equations for the rebalance factors A_k becomes an eigenvalue problem.

On the other hand, the ease with which rebalance can be implemented is often offset by its less-than-ideal performance and other poor features. (The following Figures 9-11 apply to the planar geometry diamond-differenced S_4 equations. The data in these figures was obtained from a Fourier analysis of the linearized fine and coarse-mesh rebalance methods. The predictions of this Fourier analysis agree very closely with numerical experiments of both the linearized and nonlinear methods [127, 150].)

1. Rebalance is generally divergent if the optical thickness of the spatial cells $\Sigma_t h$ is too small. In particular, rebalance is very difficult to employ effectively if the problem contains voided regions. (See Figures 9 and 10.)

2. Rebalance is usually convergent for scattering ratios c sufficiently small. However, as $c \rightarrow 1$, rebalance often becomes divergent. Unfortunately, these are the problems for which effective acceleration is most needed. (See Figures 9 and 10.)

3. Fine-mesh rebalance ($p = 1$) is usually divergent for $c \approx 1$, unless $\Sigma_t h \approx 1$. (See Figure 9.)

4. For sufficiently large p (i.e. sufficiently coarse coarse-mesh grids), coarse mesh rebalance (CMR) is convergent. If p becomes too large, CMR becomes increasingly inefficient (the convergence rate converges to that of source iteration). The optimal value of p is neither too small (for which CMR is divergent) nor too large (for which CMR is convergent but inefficient). (See Figure 11.)

5. The coarse-mesh rebalance equations do not limit to a physically or mathematically meaningful result as $\Sigma_t h \rightarrow 0$. (This is likely why rebalance becomes divergent in this limit.)

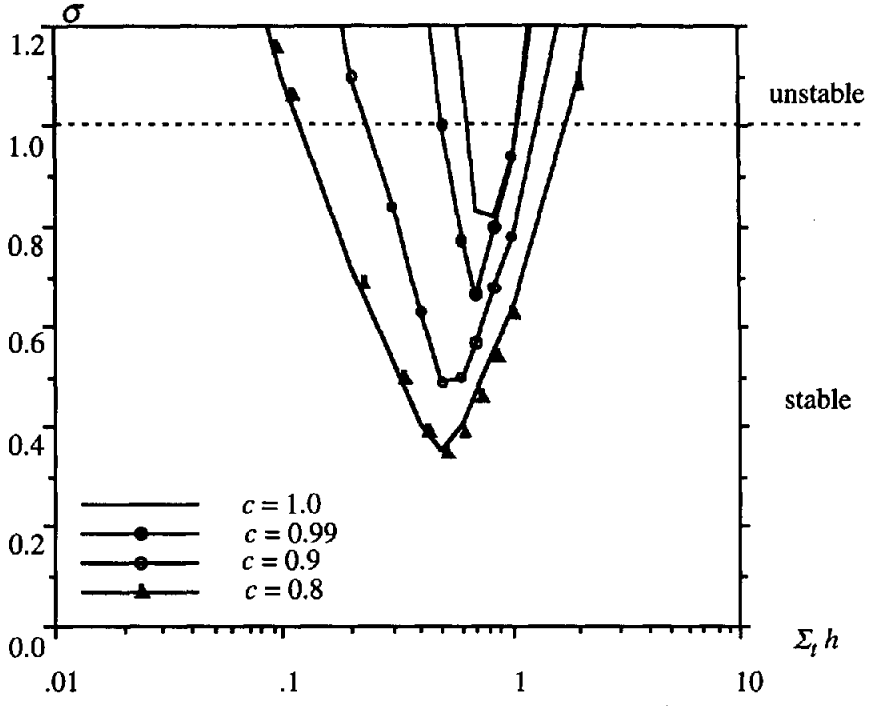

Figure 9: Spectral Radius (σ) vs. Optical Cell Thickness ($\Sigma_t h$), for Various Scattering Ratios (c) and Fine Mesh Rebalance ($p = 1$).

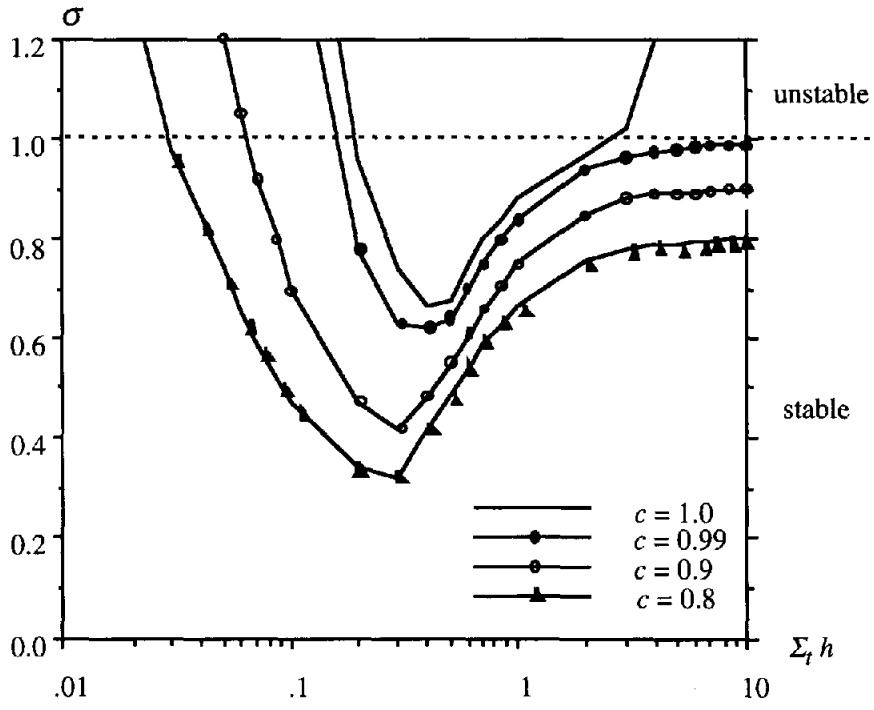

Figure 10: Spectral Radius (σ) vs. Optical Cell Thickness ($\Sigma_t h$), for Various Scattering Ratios (c) and Coarse Mesh Rebalance ($p = 4$).

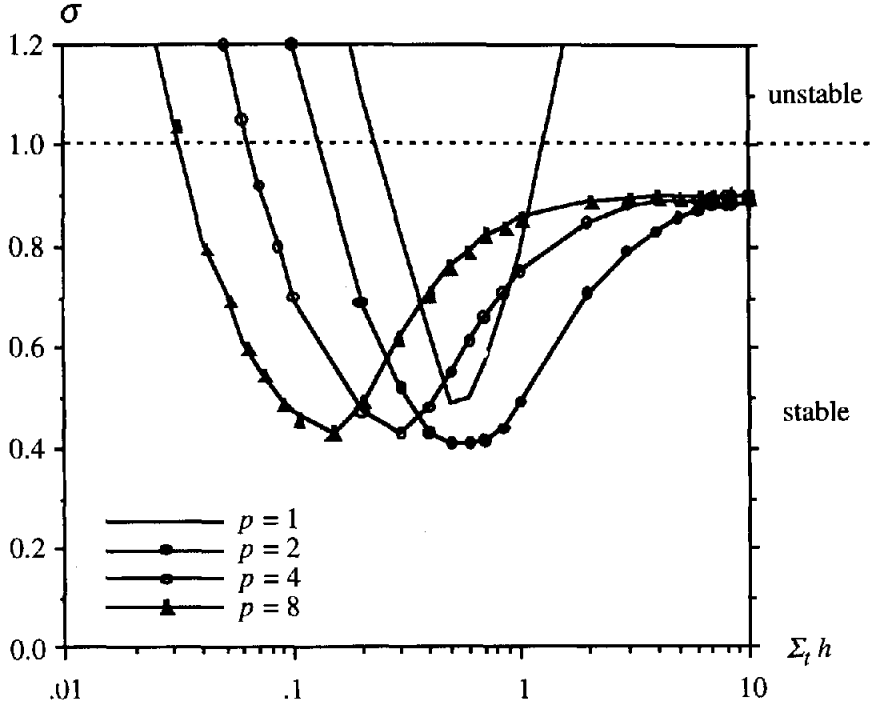

Figure 11: Spectral Radius (σ) vs. Optical Cell Thickness ($\Sigma_t h$), for Scattering Ratio $c = 0.9$ and Various Values of p.

In summary, rebalance is an iterative acceleration method that is easy to implement but requires careful input from the user to be effective. If the user chooses a coarse grid that is too fine, rebalance will generally be divergent. If the user chooses a coarse grid that is too coarse, rebalance will generally be convergent but ineffective. In many problems (containing voids, or with optically thick, highly-scattering regions) it is difficult or impossible to define coarse mesh cells whose rebalance factors render the rebalance scheme efficient. For these reasons, the particle transport community has generally come to prefer iterative acceleration methods such as DSA that are more complex in terms of concept, development, and implementation, but that offer more in terms of user-friendliness and efficiency.

V.B. Boundary Projection Acceleration (BPA)

In DSA, the low-order equation (i.e., the preconditioner) is constructed by making a crude approximation in the angular variable, i.e. by assuming that the solution is a linear function of that variable. It is possible to construct different low-order equations (and thus different preconditioners) by making different approximations to the angular variable. In fact, when considering spatially discretized transport equations, one encounters the interesting possibility of making these angular approximations only on cell surfaces and making no such approximations in cell interiors.

This possibility was first explored independently and simultaneously by Lawrence [111, 141] and Adams and Martin [104, 116, 125]. Lawrence devised low-order equations for additive corrections by making a "double-P_0" approximation of the correction at each cell surface. That is, his approximation was that on each cell surface in the problem, the corrections are half-range isotropic: the incoming-direction corrections are angle-independent and the outgoing-direction corrections are angle-independent. He found that no angular approximations were needed in cell interiors; he could obtain readily-solvable low-order equations without such approximations. After some manipulation, these low-order equations had the appearance of interface-current equations; thus, Lawrence termed the resulting scheme *Interface-Current Synthetic Acceleration* (ICSA). The structure of the ICSA low-order equations makes them easy to solve via a simple red-black procedure. (This red-black iteration may not be efficient for very difficult problems, but it is convergent and easy to implement.) Lawrence tested ICSA against DSA, SI, and coarse-mesh rebalance (CMR) on several problems including a 3-D reactor-analysis benchmark problem proposed by the International Atomic Energy Agency (IAEA). The spatial discretization schemes that he employed were so-called "nodal" methods. On a 3-D IAEA problem, he found that ICSA required fewer iterations than SI and CMR by factors of approximately 100 and 60, respectively, and less CPU time by factors of approximately 60 and 40, respectively. He found that for this and other problems, ICSA's performance was approximately the same

as that of Khalil's DSA scheme (discussed in Chapter IV above).

Working independently, Adams and Martin used a more general mathematical approach to develop a family of low-order equations that included Lawrence's ICSA scheme and was defined for essentially arbitrary spatial discretization schemes, geometries, and cell shapes. Because Adams and Martin's low-order equations are obtained by projecting the exact angular corrections on cell surfaces onto a low-order angular subspace, they called their methods *Boundary Projection Acceleration* (BPA) methods. They analyzed several members of the BPA family for various spatial discretization schemes in slab geometry and found some key results. First, even with only two low-order unknowns per cell surface (i.e., the "double-P_0" subspace), BPA methods can be defined that are rapidly convergent, with spectral radii monotonically decreasing from approximately $c/3$ toward zero as the cells ranged from optically thin to thick. Second, the choice of projection operators significantly affects the performance of a BPA method – with the "double-P_0" subspace, for example, different projection operators produced spectral radii of c/3, 0.2247c, and a value larger than unity (divergence). The chief open question that remained about BPA was how to solve efficiently the low-order equations in multidimensional problems. Again, it is straightforward to iterate on the interface unknowns in the low-order BPA equations, but it is easy to envision difficult problems for which this iteration will converge slowly.

Adams later devised a *nonlinear* version of BPA, which he called NLBPA [178]. This family of methods has much in common both with BPA and with the weighted-alpha (WA) methods described previously. Each NLBPA iteration consists of a high-order transport sweep and a low-order calculation, as is the case with most of the methods described in this Review. The low-order equations are obtained by replacing the full angular flux on cell surfaces with low-order unknowns that are multiplied by angular shape functions. The high-order sweep produces nothing but these angular shape functions; the low-order equations produce the scalar fluxes. (In this respect NLBPA is much like the QD and WA methods, discussed earlier in Chapters II and III.) Adams showed that if one linearizes the NLBPA equations about the exact solution of a model problem, one obtains the BPA equations for the corrections. Thus, a BPA method is the result of linearizing a NLBPA method, much as the Lewis-Miller method is the result of linearizing the Quasidiffusion method. The connection between the NLBPA and WA methods is that NLBPA makes essentially the same approximation as WA, except that it does so only on cell surfaces. As a result, NLBPA converges extremely rapidly when spatial cells become optically thick.

Adams also showed that one can use independent discretizations in the high- and low-order equations with NLBPA, and that there can be significant advantages in doing so. For example, he showed that in a number of problems, one could obtain a solution as accurate as a corner-balance solution by using the crude and inexpensive step-differencing method

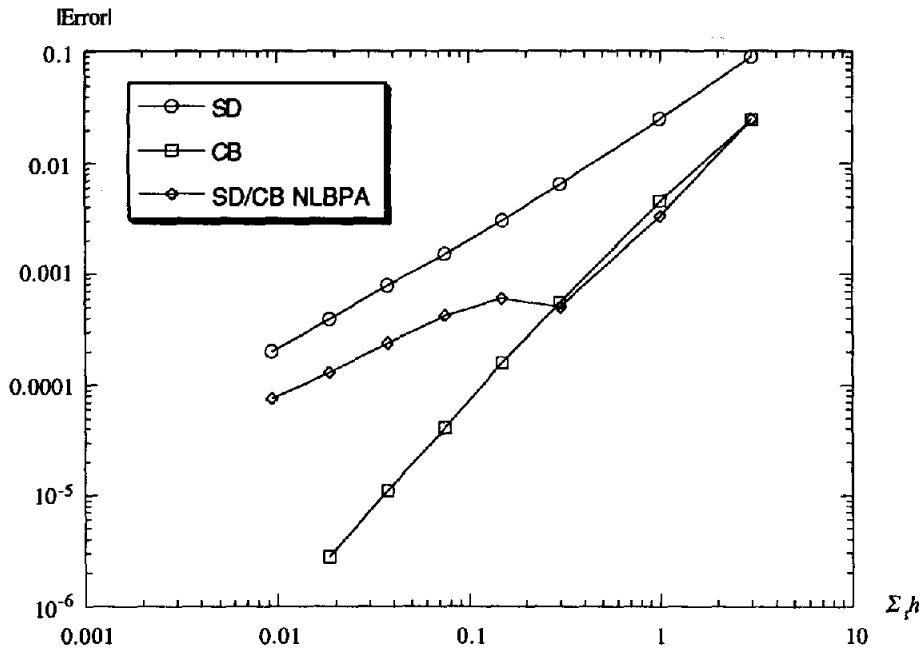

Figure 12: Error versus $\Sigma_t h$

for high-order sweeps in combination with the corner-balance method for the low-order equations (which have many fewer unknowns). In Figure 12 we plot for a specific problem the errors in (i) the Step solution, (ii) the Corner-Balance solution, and (iii) the NLBPA solution using Step Differencing for the high-order equations and the Corner-Balance method for the low-order equations. For optically thick spatial meshes, the NLBPA and Corner Balance solutions are nearly identical, even though the NLBPA method is much less costly computationally. For optically thin meshes, the NLBPA error is larger than the Corner Balance error, but is still significantly less than the Step solution error.

In this way, Adams obtained accurate solutions for (potentially) the cost of a "crude" solution. [However, he did not address the important question of how to efficiently solve the NLBPA equations in multidimensional problems.]

The same idea can be applied to any of the acceleration methods described in this Review in which the high- and low-order equations do not have to be discretized consistently. For example, Gol'din [82] and Anistratov [182] have demonstrated this for the QD method, using a relatively inaccurate discrete-ordinates scheme with a relatively accurate diffusion scheme, to achieve a solution that is much more accurate than is obtained by the unaccelerated transport scheme alone. Anistratov and Larsen [288] have also shown this for the WA Methods. Cooper and Larsen [292] have even shown that in the QD method, it is possible to use Monte Carlo to perform the transport sweeps – and estimate Eddington factors – in combination with an accurate diffusion discretization. The resulting scheme is not one in

which the transport simulation is inexpensive, but it is highly accurate, and the Eddington factors, while containing statistical errors, do not suffer from ray effects.

Cho and co-workers later developed a family of "angular rebalance" methods that also produce linear BPA methods when linearized [223, 240, 252, 266, 267]. (Adams's NLBPA method is a special 1-D member of this family.) They have shown that they can solve the two-dimensional low-order equations reasonably efficiently, at least for typical reactor neutronics problems. In their "angular rebalance" methods they solve the low-order equations for angle-dependent multiplicative factors that are applied to angular fluxes from the most recent transport sweep. Like Adams, Hong and Cho explored the use of independent discretizations in the high- and low-order equations, with similar results [240]. To solve the low-order equations (which are not symmetric), Hong and Cho have employed standard matrix iterative techniques such as Bi-Conjugate Gradient Stabilized (BCGSTAB). (We discuss such matrix iterative techniques in Chapter VI.) These perform reasonably well for the test problems that Hong and Cho have presented. For example, for a two-dimensional iron-water shielding problem, they achieved speedups of approximately a factor of 60 relative to SI.

We remark that Sanchez and Chetaine have introduced an "Asymptotic Synthetic Acceleration" (ASA) scheme [271, 282] that appears to have much in common with Lawrence's DP0 scheme, which is a particular linear BPA method described above. Sanchz and Chetaine applied ASA to a long-characteristics discretization of the transport equation and reported good results for assembly-level problems in reactor analysis.

V.C. Spatial Multigrid

The *spatial multigrid* (or simply *multigrid*) method has achieved spectacular success in the iterative solution of discretized elliptic problems [2, 11]. Thus, it is not surprising that researchers would investigate this method's application to transport iterations.

The observation that motivates multigrid is that it is often possible to devise simple iterative schemes that readily converge high-frequency error modes but not low-frequency modes. For example, let us consider source iteration (SI) for a spatially discrete transport problem. We recall that the SI eigenvalue depends on the scattering ratio c, the cell thickness $\Sigma_t h$, and a "frequency" variable $\theta \equiv \lambda \Sigma_t h$. When $\Sigma_t h$ is small, we find that the SI eigenvalue is reasonably small (say, less than $1/2$) for error modes that are "high-frequency" with respect to the spatial grid, i.e. modes such that $\pi/2 \leq \theta \leq \pi$. For example, in Figure 13 we plot the SI eigenvalue as a function of θ for the DD spatial discretization in slab geometry. We see that SI converges the high-frequency error modes (those with $\theta \geq \pi/2$) reasonably quickly, but it has little effect on the low-frequency modes.

Given this observation, the basic idea underlying multigrid is that some of the "low

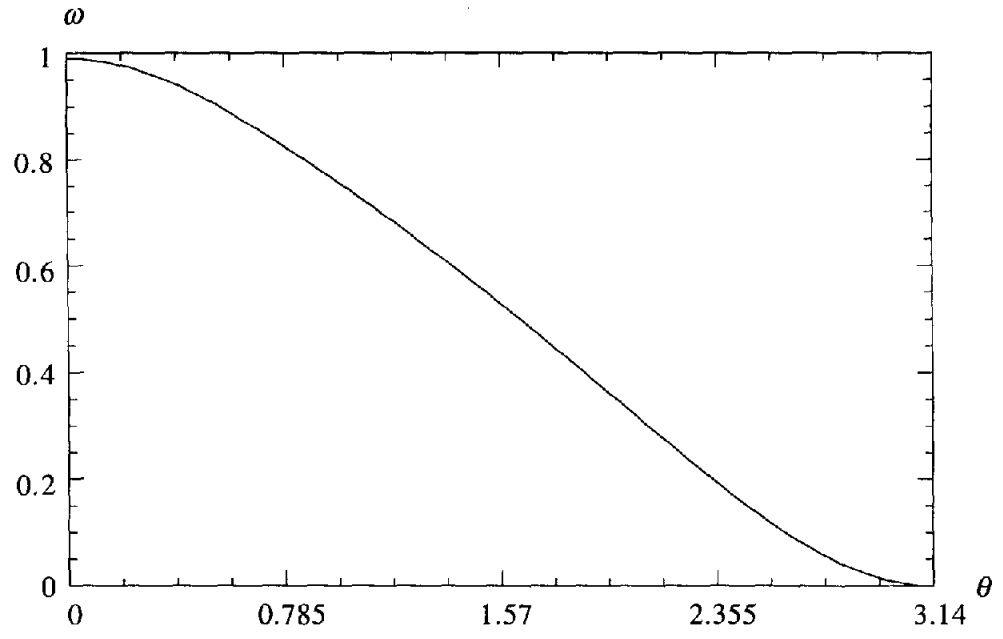

Figure 13: ω_{SI} versus θ
(c=0.99, $\Sigma_t h = 1$, Diamond Differencing in Slab Geometry)

frequency" error modes on a given grid are actually "high-frequency" on a coarser grid. For example, the modes $\pi/4 \leq \theta \leq \pi/2$ on a grid with $h = 1$ are the same as the modes $\pi/2 \leq \theta \leq \pi$ on a grid with $h = 2$. Thus, perhaps one could employ a "simple" iteration scheme on successively coarser spatial grids and effectively attenuate all error modes. To say this another way, after a few "simple" iterations, the remaining error may be well-approximated by a low-order operator defined on a coarser spatial grid. In multigrid terminology, the "simple" iteration scheme that attenuates high-frequency modes is the *smoother*; information is transferred from coarse grids to finer grids via *prolongation* operators; information is transferred from fine grids to coarser grids via *restriction* operators.

To our knowledge, the earliest work on spatial multigrid for the transport equation was reported by Nowak et al. for slab and XY geometries [120, 130], and by Barnett et al. for slab geometry [2, 137]. Nowak et al. first reported the Source-Iteration Multigrid (SIMG) method [120], in which the smoother was simply SI. These authors showed that for weighted diamond discretizations other than "pure" diamond differencing, SI is a reasonably efficient smoother, as follows. If M SI iterations attenuate high-frequency error modes by a factor of ρ on a given grid, then $2M$ iterations attenuate high-frequency error modes by the same factor on a grid twice as coarse. Since in 2-D geometries, "twice as coarse" means one-fourth the number of cells, the smoothing step on each coarser grid takes only half the time as on the previous grid. This renders the algorithm potentially efficient. Nowak's numerical results for the constant-constant (CC) "nodal" discretization were very encour-

aging. However, as the initial finest grid becomes coarser, the SIMG method becomes less attractive, for it requires more and more smoothing iterations to attenuate high-frequency errors on that grid.

Nowak et al. also reported results from a slightly more complicated method [130], which used BPA to accelerate the original transport iterations, and then used multigrid (with an improved smoother) to accelerate the iterative solution of the low-order BPA equations. Coarse-mesh discretizations were simply the fine-mesh discretization applied to the coarser cells with volume-weighted cross sections. Each "smoothing" iteration involved two steps: first an SI sweep, then a *one-cell inversion* independently in each cell. [A one-cell inversion means calculating the solution of the transport problem, including scattering, within each cell, given estimates for the incident fluxes on the cell.] The smoothing step can be written as:

$$\psi^{(\ell+1/2)} = L^{-1}\left(\hat{S}\phi^{(\ell)} + q\right) , \tag{5.7}$$

$$\phi_{SI}^{(\ell+1/2)} = K_0\psi^{(\ell+1/2)} , \tag{5.8}$$

$$\phi_{OCI}^{(\ell+1/2)} = R_{OCI}\psi^{(\ell+1/2)} , \tag{5.9}$$

$$\phi^{(\ell+1)} = \alpha\phi_{SI}^{(\ell+1/2)} + (1-\alpha)\phi_{OCI}^{(\ell+1/2)} . \tag{5.10}$$

Here K_0 is the same operator as in Eq. (1.45), i.e.

$$K_0\psi(x) = \int_{-1}^{1} \psi(x,\mu)d\mu ,$$

and R_{OCI} is a "response matrix" that gives ϕ inside a cell as a function of the angular flux incident upon the cell.

The authors found that $\alpha = 0.2$ provides the best smoothing, at least for the CC method in XY geometry, attenuating high-frequency errors by a factor of 0.6 per smoothing iteration. Their computational results were very good for the CC method. However, for more accurate spatial discretizations, such as bilinear discontinuous or linear nodal, the smoothing factor approaches unity as the spatial cells become optically thick, and thus the above smoothing strategy becomes inefficient.

Barnett et al. devised an effective spatial multigrid technique for iteratively solving the linear discontinuous (LD) equations in slab geometry. Unlike other spatial multigrid research, this work considered general anisotropic scattering. Like Nowak et al., Barnett et al. created a smoother from a combination of SI and cell inversions, although they employed overlapping two-cell inversions instead of one-cell inversions. Their smoother satisfied equations that are somewhat similar to Eqs. (5.7-5.10):

$$\psi_{SI}^{(\ell+1/2)} = L^{-1}\left(S\psi^{(\ell)} + q\right) , \tag{5.11}$$

$$\psi_{2CI}^{(\ell+1/2)} = R_{2CI}\psi_{SI}^{(\ell+1/2)} \quad , \tag{5.12}$$

$$\psi^{(\ell+1)} = \alpha\psi_{SI}^{(\ell+1/2)} + (1-\alpha)\psi_{2CI}^{(\ell+1/2)} \quad . \tag{5.13}$$

Here R_{2CI} is the two-cell response matrix that gives the angular flux inside two adjacent cells as a function of the angular flux incident upon the outer edges of the two-cell block. Barnett et al. found that $\alpha = 1/3$ yielded excellent results.

For the restriction (fine $\rightarrow$ coarse) operator, Barnett et al. used a Galerkin projection of the fine-mesh finite-element functions onto the coarse mesh functions. For the prolongation (coarse $\rightarrow$ fine) operator, they simply required that the coarse-mesh LD function be exactly replicated on the fine grid. Their method was successful; not only did it achieve rapid convergence for problems with isotropic scattering, it retained its effectiveness even in the presence of highly anisotropic scattering.

Manteuffel and co-workers also developed a spatial multigrid method for the LD equations in slab geometry, but they used a completely different approach to analysis and development [154, 173, 186, 196, 210, 225]. (They also considered only the isotropic-scattering equations.) Instead of using the Fourier-analysis techniques that have been described previously in this paper, they performed detailed algebraic studies of the LD equations. For example, let us consider the *two-cell inversion* process in a $c = 1$ problem: a complete solution of a two-cell problem subject to given incident fluxes on the outer edges. Manteuffel et al. were able to prove the following [210]:

1. Given a $c = 1$ problem and the S_2 quadrature set, the iteration error (difference between converged solution and current iterate) following a two-cell inversion is a continuous linear function of position within the two cells. This result is independent of mesh spacing.

2. Given a $c = 1$ problem and any quadrature set, the iteration error following a two-cell inversion is very nearly a continuous linear function of position within the two cells if the two cells are optically thin. In fact, it is a continuous linear function plus $O\left[(\Sigma_t h)^2\right]$.

3. Given a $c = 1$ problem and any quadrature set, the iteration error following a two-cell inversion is very nearly a continuous linear function of position within the two cells if the two cells are optically thick. In fact, it is a continuous linear function plus $O\left[1/(\Sigma_t h)\right]$.

These results mean that following a two-cell inversion on a given mesh, the remaining error can be calculated almost exactly using a mesh that is coarser by a factor of two (at least if $c = 1$). Manteuffel et al. used this fact to build an extremely efficient multigrid technique.

The smoother is simply a two-cell inversion for the pair of cells touching each cell edge; unlike previous spatial multigrid methods, there is no "transport sweep." (Their algebraic study showed that for thick cells, the transport sweep does not change the spatial shape of any isotropic error, and thus is not a good candidate for smoothing.) They employed a "V" cycle with one smoothing step per level, and they directly solved the coarsest (2-cell) level. For $c = 1$ problems, their method has a spectral radius that vanishes in the fine-mesh limit like $O\left((\Sigma_t h)^3\right)$ and in the coarse-mesh limit like $O\left(1/(\Sigma_t h)^2\right)$. The worst performance occurs for intermediate mesh spacings, where it is still exceptionally fast, with a spectral radius never exceeding 0.01 [210].

For problems with absorption ($c < 1$), Manteuffel et al. found that in the fine-mesh limit, the error following a two-cell inversion is linear across the two cells to $O\left[(\Sigma_t h)^2\right]$, just as in the $c = 1$ case. However, in the coarse-mesh limit the error is *not* linear when $c < 1$. It is continuous, but the error at the interior interface falls below a straight line drawn between the errors at the outer interfaces. The amount by which it falls below the straight line depends on the amount of absorption in the two cells. (In the limit as absorption goes to zero, the error approaches a straight line, as discussed above for $c = 0$.) Because of this, a direct application of the method that works so well for $c = 1$ to problems with $c < 1$ does not produce the same spectacular results. The authors showed that the spectral radius for such a method increases with increasing $\Sigma_t h$ and reaches a value of at least 0.85 when $\Sigma_t h = 10^4$. Not content with this, the authors devised a multigrid technique that accounts for the predicted shape of the error within two cells following a two-cell inversion. Their results with this new techniques were again spectacular: given uniform grids, the spectral radii are always less than 0.01; on a nonuniform grid (with $\Sigma_t h$ randomly varying across four orders of magnitude), they observed spectral radii only as high as 0.078 [225].

Manteuffel and co-workers have also applied multigrid to discretizations of second-order forms of the transport equation (which we introduced in Section II.I) [253]. They have developed a least-squares formulation of the transport equation that is very similar to the SAAF equation introduced in Section II.I. (One difference is that the least-squares formulation easily handles regions with $\Sigma_t = 0$; another is that it does not enforce cellwise particle conservation.) Because the second-order forms of the transport operator are similar to the diffusion operator, one might hope that a direct application of standard multigrid techniques developed for elliptic operators would be successful. Manteuffel and Ressel found that in slab geometry such a multigrid method applied to their least-squares formulation produced a spectral radius of approximately 0.1, independent of mesh spacing and scattering ratio [253]. However, they found later that because of the structure of the least-squares system, in multi-dimensional geometries standard multigrid methods do not give convergence rates independent of mesh spacing [281].

Thus, at the time of this writing, excellent multigrid methods have been demonstrated for both the first- and second-order forms of the transport equation in 1-D. Recent work has been aimed at extending these promising results to 2-D [263, 281, 289].

VI. ALGEBRAIC ITERATIVE METHODS

In the previous chapters, we have discussed iterative methods in which each full iteration contains two stages: a "high-order" stage that is either source iteration or some other "smoothing" step, and a "low-order" stage that solves some equations for additive corrections to or an accelerated estimate of the latest iterate. Here we consider methods that do not employ low-order equations, but rather try to obtain the converged solution by purely algebraic means.

VI.A. Asymptotic Source Extrapolation (ASE)

Asymptotic Source Extrapolation (ASE) [49] is based on a simple premise: that the remaining error consists only of the error mode associated with the unique iteration eigenvalue with the largest magnitude. If this were true, the following equation would hold:

$$\psi - \psi^{(\ell+1/2)} = \sigma\left(\psi - \psi^{(\ell)}\right) \quad , \tag{6.1}$$

where σ is the eigenvalue with the largest magnitude. This implies that the converged solution ψ can be obtained from two successive iterates from any convergent iterative method, including SI:

$$\psi = \psi^{(\ell+1/2)} + \frac{\sigma}{1-\sigma}\left(\psi^{(\ell+1/2)} - \psi^{(\ell)}\right) \quad . \tag{6.2}$$

In its simplest form, ASE proceeds by iterating with SI for several iterations and then extrapolating as shown above. This requires an estimate for σ, which can be obtained by taking the ratio of norms of two successive differences:

$$\sigma \approx \frac{\left\|\psi^{(\ell+1)} - \psi^{(\ell)}\right\|}{\left\|\psi^{(\ell)} - \psi^{(\ell-1)}\right\|} \quad . \tag{6.3}$$

In the Russian transport literature, ASE is known as Lyusternik's method [19, 10]. Unless care is taken in its implementation, ASE can be divergent. This is the case, for example, if ASE is applied after every source iteration in a problem with $c > 1/2$. Also, if there are many modes that are very slow to converge, as is the case with transport iterations in optically thick and highly scattering regions, then ASE by itself does not keep the iteration process from being unacceptably slow. The behavior of ASE is analyzed and discussed in Section XI.2 of [10]. To our knowledge, ASE is not used in modern S_N codes.

VI.B. Chebyshev Acceleration

To describe Chebyshev acceleration, we consider the general preconditioned Richardson iteration for the transport equation with isotropic scattering, which is given in Eq. (1.45). If we define the transport operator T:

$$T = [I - X_{SI}] \quad , \tag{6.4}$$

where X_{SI} is the SI iteration operator as defined in the Introduction, then the transport equation for the scalar flux is:

$$T\phi = \hat{q} \, , \quad \text{where} \quad \hat{q} = K_0 L^{-1} q \quad . \tag{6.5}$$

Here L is the streaming-plus-collision operator and K_0 is the integral over all directions. Given a preconditioner P, the preconditioned Richardson iteration for Eq. (6.5) is

$$\phi^{(\ell)} = (I - PT)\phi^{(\ell-1)} + P\hat{q} \quad . \tag{6.6}$$

Equivalently,

$$\phi^{(\ell)} = (I - A)\phi^{(\ell-1)} + \tilde{q} \quad , \tag{6.7}$$

where $A \equiv PT$ and $\tilde{q} \equiv P\hat{q}$. Subtracting the converged solution ϕ from both sides of this equation, and adding and subtracting $A\phi$ on the right side, we obtain an equation for the iteration error:

$$e^{(\ell)} = (I - A)e^{(\ell-1)} + (\tilde{q} - A\phi) = (I - A)e^{(\ell-1)} \quad , \tag{6.8}$$

where we have used $\tilde{q} = A\phi$. It follows that

$$e^{(\ell)} = (I - A)^{\ell} e^{(0)} \quad . \tag{6.9}$$

Now we introduce the eigenvalues and eigenvectors of A:

$$Av_k = \lambda_k v_k \quad . \tag{6.10}$$

We assume that the eigenvalues λ_k are real, positive, and distinct, and that the eigenvectors v_k form a basis for the vector space that contains the solution ϕ. Then the initial error can be expressed as a linear combination of the v_k:

$$e^{(0)} = \sum_k \gamma_k v_k \quad . \tag{6.11}$$

It follows from Eq. (6.9) that

$$e^{(\ell)} = \sum_k \gamma_k (I - A)^{\ell} v_k = \sum_k \gamma_k (1 - \lambda_k)^{\ell} v_k \quad . \tag{6.12}$$

Now we ask: Can we generate an improved estimate of the converged solution by taking a weighted average of all of the Richardson iterates that have been computed to this point? That is, if we form the average:

$$\tilde{\phi}^{(\ell)} = \sum_{i=0}^{\ell} \alpha_\ell^{(i)} \phi^{(i)} \quad , \tag{6.13}$$

with

$$\sum_{i=0}^{\ell} \alpha_\ell^{(i)} = 1 \quad , \tag{6.14}$$

can we choose the $\alpha_n^{(i)}$ such that the error $\tilde{e}^{(\ell)} = \tilde{\phi}^{(\ell)} - \phi$ is smaller than $e^{(\ell)}$? If we subtract the converged solution from both sides of Eq. (6.13) and use Eq. (6.14), we obtain

$$\begin{aligned} \tilde{e}^{(\ell)} &= \sum_{i=0}^{\ell} \alpha_\ell^{(i)} e^{(i)} = \sum_{i=0}^{\ell} \alpha_\ell^{(i)} \sum_k \gamma_k (1-\lambda_k)^i v_k \\ &= \sum_k \gamma_k \left(\sum_{i=0}^{\ell} \alpha_\ell^{(i)} (1-\lambda_k)^i \right) v_k \quad . \end{aligned} \tag{6.15}$$

We define the ℓ-th order polynomial

$$P_\ell(z) = \sum_{i=0}^{\ell} \alpha_\ell^{(i)} (1-z)^i \quad . \tag{6.16}$$

Then we find that our new averaged solution has an error given by

$$\tilde{e}^{(\ell)} = \sum_k \gamma_k P_\ell(\lambda_k) v_k \quad . \tag{6.17}$$

We now see that the error in our new "averaged" iterate depends directly upon the polynomial P_ℓ, and in particular upon its value at each of the eigenvalues of A. If a P_ℓ can be constructed that is small for each eigenvalue, or that is small across an entire domain that contains A's eigenvalues, then it would produce a small error. We note, though, that the restriction of Eq. (6.14) implies the restriction

$$P_\ell(0) = 1 \quad .$$

Thus, we are interested in a polynomial of order ℓ that is small in the range $(\lambda_{min}, \lambda_{max})$ but equals unity at $\lambda = 0$.

Of all possible polynomials of order ℓ that equal unity at $\lambda = 0$, a Chebyshev polynomial attains the smallest maximum value in the range $(\lambda_{min}, \lambda_{max})$ [7]. This is the basic idea behind Chebyshev acceleration.

It would be impractical to store all of the Richardson iterates $\phi^{(0)}, \ldots, \phi^{(\ell)}$ so that the linear combination could be taken as in Eq. (6.13). Fortunately, this is not necessary if

the polynomials P_ℓ satisfy a recursion relation. For example, if the polynomials satisfy a three-term recursion:

$$P_{\ell+1}(z) = c_0 P_{\ell-1}(z) + c_1(1-z)P_\ell(z) \quad , \tag{6.18}$$

then one can construct $\tilde{\phi}^{\ell+1}$ from the previous two iterates, $\tilde{\phi}^{(\ell)}$ and $\tilde{\phi}^{(\ell-1)}$. The Chebyshev polynomials do satisfy such a recursion relation (with $c_0 = -1$ and $c_1 = 2$). Thus, if one is willing to store two "old" scalar-flux iterates in a problem with isotropic scattering, one can apply Chebyshev acceleration to the standard Richardson (SI) or preconditioned Richardson (DSA, e.g.) iteration. The requirement is that one must know *a priori* an interval (a,b) that contains the interval $(\lambda_{min},\lambda_{max})$. In difficult iterative problems, λ_{min} tends to be very close to zero, while λ_{max} is usually approximately unity. The convergence rate will depend rather sensitively on a, which must be $\leq \lambda_{min}$. Asymptotically, in fact, the error reduction factor is

$$\sigma_{Cheby} = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} \quad , \tag{6.19}$$

where

$$\kappa \equiv b/a \quad .$$

If $a = \lambda_{min}$ and $b = \lambda_{max}$, then κ is the *condition number* of A, defined to be the ratio of the largest eigenvalue to the smallest. Because λ_{min} is not usually known, in practice one must choose a conservatively, so that $a < \lambda_{min}$ and κ is larger than the condition number. Obviously, the larger κ becomes, the slower is the convergence of the iteration. This leads to two conclusions. First, the performance of Chebyshev iteration depends sensitively on the value chosen for a; it needs to be as large as possible while not violating the requirement $a \leq \lambda_{min}$. Second, even with optimal a and b, Chebyshev iteration can be slow to converge if A has a high condition number. If A is the transport operator with no preconditioning, then $A = T = I - X_{SI}$, where X_{SI} is the source iteration matrix, and we can readily obtain a useful estimate of A's condition number. If σ_{SI} is the spectral radius of source iteration, and the smallest eigenvalue of X_{SI} is ω_{min}, then

$$\kappa = \frac{1-\omega_{min}}{1-\sigma_{SI}} \approx \frac{1}{1-\sigma_{SI}} \quad . \tag{6.20}$$

We note that when SI is very slow to converge, $\sigma_{SI} \approx 1$, and $\kappa \gg 1$. Thus, the statements "SI is slow to converge" and "T has a large condition number" are equivalent. In this case, Chebychev acceleration can converge much faster than SI, but for the most difficult problems it can still converge arbitrarily slowly. The way to make Chebyshev acceleration fast is to find a good preconditioner, so that A has a relatively small condition number. However, this is the same problem of finding a good low-order operator in a "synthetic" acceleration scheme – the problem that has been the subject of much of this paper.

A two-term cyclic form of Chebyshev acceleration exists that does not require storage of two old iterates, but instead uses the same storage that is required for Richardson iteration. The first $m-1$ steps of this scheme correspond to Eq. (6.13) with polynomials $\tilde{P}_\ell, \ell = 1,...,m-1$, which are not Chebyshev polynomials. However, the polynomial at the m^{th} step, $\tilde{P}_m$, is the m^{th}-order Chebyshev polynomial. This leads to an m-step cyclic iteration scheme with the same asymptotic error reduction factor per step, σ_{Cheby}, as the original Chebyshev scheme described above.

The two-term m-step cyclic scheme suffers from severe numerical instabilities in general. This problem was solved, independently and essentially simultaneously, by two teams: Lebedev and Finogenov [47], [48] and Samarsky and Nikolaev [13]. The solution found by these researchers is a careful ordering of the linear factors from which the polynomials $\tilde{P}_m$ are constructed, such that the two-term scheme is stable to roundoff errors. See Section X.18 of [10] for a discussion.

In summary, Chebyshev iteration has some intriguing properties but also several drawbacks. It is not widely used today to accelerate scattering iterations in transport computations. However, it is sometimes used to accelerate the convergence of eigenvalue iterations, as we discuss briefly in Section VIII.C.

VI.C. Conjugate Gradient (CG) Methods

It is not difficult to apply the Conjugate Gradient (CG) method [7, 199] to accelerate SI (Richardson) or a "synthetic" acceleration (preconditioned Richardson) method in a problem with isotropic scattering. Compared to Chebyshev iteration, CG converges with the same asymptotic rate as the Chebyshev scheme with optimally chosen parameters a and b, but CG does not require estimates of the eigenvalues of the matrix A. We do not explain here the theory behind CG; instead, we simply show how to apply this method to transport iterations.

We consider the matrix representation of the discretized transport problem with isotropic scattering, as shown in Eq. (6.5):

$$T\phi^{(\ell)} = \hat{q} \quad , \tag{6.21}$$

where T is the transport operator. The CG method begins with an initial guess $\phi^{(0)}$, which defines an initial residual $r^{(0)}$:

$$r^{(0)} = \hat{q} - T\phi^{(0)} \quad . \tag{6.22}$$

The first question that arises is how to obtain $T\phi^{(0)}$, for we certainly do not wish to construct the matrix T. It turns out that we do not need to form this matrix – we simply execute a transport sweep using $\phi^{(0)}$ in the scattering source, and then perform a simple manipulation.

In the notation used in a previous chapter, the transport sweep is:

$$\tilde{\psi} = L^{-1}[\hat{S}\phi^{(0)} + q] \ .$$

Now we can form $\tilde{\phi}$:

$$\begin{aligned} \tilde{\phi} = K_0\tilde{\psi} = K_0 L^{-1}[\hat{S}\phi^{(0)} + q] &\equiv X_{SI}\phi^{(0)} + \hat{q} \\ &= (I - T)\phi^{(0)} + \hat{q} \ . \end{aligned} \tag{6.23}$$

It follows that the initial residual is:

$$r^{(0)} = \hat{q} - T\phi^{(0)} = \tilde{\phi} - \phi^{(0)} \ . \tag{6.24}$$

Thus, we can generate our initial residual, $r^{(0)}$, by performing a transport sweep and then taking the difference between two scalar fluxes.

After finding the initial residual, CG defines an initial "search direction":

$$d^{(0)} = r^{(0)} \ . \tag{6.25}$$

With this search direction determined, each CG-SI iteration proceeds as follows. First a transport sweep determines the action of the operator T on the latest d:

$$\begin{aligned} \tilde{\psi} &= L^{-1}\hat{S}d^{(\ell)} \ , \\ \tilde{\phi} = K_0\tilde{\psi} &= (I - T)d^{(\ell)} \ , \\ \Rightarrow Td^{(\ell)} &= d^{(\ell)} - \tilde{\phi} \ . \end{aligned} \tag{6.26}$$

Again, operationally this is just a transport sweep followed by the difference of two vectors. The remainder of a CG-SI iteration is simple manipulation of vectors, which produces a new iterate, the associated residual, and a new search direction:

$$\alpha^{(\ell)} = \frac{\left\langle r^{(\ell)}, r^{(\ell)} \right\rangle}{\left\langle d^{(\ell)}, Td^{(\ell)} \right\rangle} \ , \tag{6.27}$$

$$\phi^{(\ell+1)} = \phi^{(\ell)} + \alpha^{(\ell)}d^{(\ell)} \ , \tag{6.28}$$

$$r^{(\ell+1)} = r^{(\ell)} - \alpha^{(\ell)}Td^{(\ell)} \ , \tag{6.29}$$

$$\beta^{(\ell+1)} = \frac{\left\langle r^{(\ell+1)}, r^{(\ell+1)} \right\rangle}{\left\langle r^{(\ell)}, r^{(\ell)} \right\rangle} \ , \tag{6.30}$$

$$d^{(\ell+1)} = r^{(\ell+1)} + \beta^{(\ell+1)}d^{(\ell)} \ . \tag{6.31}$$

Here the notation $\langle , \rangle$ denotes an inner product. The inner product must be chosen such that the operator T is self-adjoint; this leads to the following definition:

$$\langle f, g \rangle = \int_{r:c\Sigma_t>0} c(r)\Sigma_t(r)f(r)g(r)d^3r \ . \tag{6.32}$$

We note that the scattering cross section appears in the inner product; without this the operator T is not self-adjoint. (Another way to view this is that each row of the matrix T must be multiplied by a scattering cross section to make it symmetric. See [243] and [284] for a discussion.) We note also that the integral excludes any portions of the problem domain for which the scattering cross section is zero; without this we would not have a legitimate inner product, for it would be possible for the inner product of a non-zero vector and itself to be zero.

The CG error-reduction factor per iteration, σ_{CG}, is given by the same expression as the Chebyshev factor, given in Eq. (6.19). The difference is that the parameter κ in the CG expression is the true condition number, $\lambda_{max}/\lambda_{min}$, rather than the ratio a/b, where a and b are estimates that must be input into the Chebyshev algorithm.

CG is not difficult to implement; it adds only a few relatively simple vector operations to each SI iteration. Further, it can substantially reduce iteration count and computation cost relative to SI. However, CG has two characteristics that reduce its attractiveness for transport iterations. First, it requires a symmetric positive-definite (SPD) matrix T; this means that it can be applied to SI only if scattering is isotropic and the quadrature set is symmetric. (See reference [284] for a discussion of this point. We remark that Sanchez and Santrandea have devised a way to symmetrize the transport operator, even with anisotropic scattering [298], which could pave the way for more general application of CG to transport iterations. As early as the 1970's, Kuznetsov also worked on symmetrization of the transport operator and on applying CG to transport iterations [67].) In many transport problems of interest, scattering is not isotropic, and in some applications the quadrature set is not symmetric. Second, even though CG can offer substantial speedups over SI in isotropic-scattering problems, the performance of CG still degrades significantly in optically thick problems with $c \approx 1$. The reason for this degradation is that the condition number of the matrix T becomes large, as discussed earlier [see Eq. (6.20)].

Thus, while CG is potentially powerful, it is not by itself the final answer to transport iterations; its performance depends on having an SPD matrix and on that matrix having a condition number whiich is not large. Related methods, described briefly in the next section, do not require symmetric matrices; these could be applied to problems with anisotropic scattering, thus removing one difficulty. However, the problem of high condition numbers is more difficult; it can be addressed by finding a good "preconditioner." This is equivalently the problem of finding a good low-order operator in a "synthetic acceleration" scheme. Thus, as we have mentioned previously, synthetic acceleration can be

viewed as the application of a preconditioning operator, the effect of which is to reduce the condition number of the matrix T.

Derstine and Gelbard were perhaps the first to recognize that DSA is simply preconditioned Richardson iteration (see Introduction), and that it would be beneficial to replace this preconditioned Richardson method with the more powerful preconditioned Conjugate Gradient method [100]. The use of CG with DSA was an important step, partly because it is theoretically guaranteed to converge (neglecting roundoff), given SPD matrices. This means that with CG, even a very "inconsistent" diffusion discretization could be used without fear of a divergent iteration. This was potentially significant, because consistent discretizations are often much more difficult than simpler standard discretizations to derive, code, and solve (as we have discussed previously). Derstine and Gelbard tested CG-DSA using diamond differenced transport and cell-centered finite-differenced diffusion in XY geometry; they compared their results against the almost-consistent DSA of TWODANT. Some of their results are shown in Table 1.

It is clear that CG can dramatically improve the performance of inconsistent DSA: for some problems, inconsistent DSA diverges by itself but with CG it converges in less than 20 iterations! However, CG is less effective than the TWODANT treatment, and it is not clear from these results what happens with optically thicker cells, such as those typically encountered in radiative transfer problems.

Faber and Manteuffel, not aware of the work of Derstine and Gelbard, also recognized that SI is Richardson iteration and that DSA is preconditioned Richardson iteration [139]. Their work sparked further investigations by Ashby et al. [149, 158, 184, 204], who performed extensive theoretical and numerical investigations.

Considering the transport equation with *isotropic* scattering, Ashby et al.'s most important findings can be summarized as follows. First, CG can indeed be employed "on top of" SI or DSA to improve performance relative to Richardson iteration. Second, CG does indeed make inconsistent DSA converge even when by itself it would diverge. However, perhaps most importantly, a "good" DSA method is much faster to converge by itself than is a "poor" method with CG. Further, because a "good" DSA scheme (such as one arising from Larsen's Four-Step Method) converges so quickly, employing CG in addition

$\Sigma_t \Delta x$:	0.5	1.0	2.0	4.0
TWODANT DSA	6	6	7	12
Inconsistent DSA + CG	10	12	13	18
Inconsistent DSA	12	15	diverged	diverged

Table 1: Comparison of Iteration Counts.
$\{c = 0.99$ in part of the problem. (Taken from [100].)$\}$

generally reduces iteration counts by only one or two. Thus, it seems that while CG does help, it does not remove the need for good preconditioners – which is basically where DSA research had already been focusing.

For problems with *anisotropic* scattering, Ashby et al. recognized that the transport operator is not symmetric and that CG could not be directly employed. They then turned to more general Krylov-subspace methods and tested an adaptive Chebyshev method [65, 70]; we describe their results in Section VI.D below.

Ramoné et al. [243] used CG in their TSA method, but not in the same way that previous authors had used it for DSA. We recall that the low-order operator in TSA is contained in a transport equation with modified cross sections; the implementation of TSA requires that this low-order equation be solved (at least approximately) during each full iteration. In Ramoné's form of TSA, the low-order equation has isotropic scattering even when the original transport problem has anisotropic scattering. Ramoné et al. found that the most efficient implementation of TSA obtained its approximate low-order solution by using a fixed number of CG iterations "on top of" SI. Thus, these authors did not try to use CG to accelerate the overall iteration – which is what had been done previously with DSA. Instead, they used CG as a tool to help solve the low-order isotropic-scattering problem.

Building on these results, Zika and Adams [284, 285] employed CG to solve low-order problems arising from the application of TSA to assembly-level problems in reactor analysis. Because these problems have opposing reflecting boundaries, the low-order problem yields not only scalar-flux corrections, but also boundary angular-flux corrections. The resulting matrix equations for the combined scalar-flux and angular-flux solution is not symmetric. However, Zika and Adams recognized that there is an underlying symmetric problem (the infinite-medium problem simulated by the reflecting boundary conditions), and they were able to cast the problem in a way that was amenable to CG iteration. They found that despite the extra work needed to use CG in these problems, this still produced the most efficient implementation of TSA that they tested.

VI.D. Other Algebraic Methods

Given a linear system of the form

$$T\phi = \hat{q} \quad , \tag{6.33}$$

with T a symmetric and positive definite (SPD) matrix, then there is currently little reason to use an algebraic method other than CG, with a preconditioner if one is available. However, when T is not symmetric CG is not an option, and we must turn to other alternatives.

One family of alternative methods that has been used widely in recent years is that of *Krylov subspace* methods. Each such method uses the following equation for successive

iterates:

$$\phi^{(\ell+1)} = \phi^{(\ell)} + p^{(\ell)} \quad , \tag{6.34}$$

where $p^{(\ell)}$ is chosen from the Krylov space of dimension ℓ:

$$K_\ell\left(T, r^{(0)}\right) \equiv span\left\{r^{(0)}, Tr^{(0)}, T^2 r^{(0)}, \ldots, T^{\ell-1} r^{(0)}\right\} \quad , \tag{6.35}$$

$$r^{(\ell)} \equiv \hat{q} - T\phi^{(\ell)} \quad . \tag{6.36}$$

The CG method elegantly chooses the "best" value of $p^{(\ell)}$, in a certain sense, given an SPD matrix. With asymmetric matrices things do not happen quite as cleanly, but the basic goal is the same: try to find the "best" value of $p^{(\ell)}$, or some approximation thereto, from the space K_ℓ. There are many methods that differ in their approaches and their approximations; two of the more popular are *GMRES* (with name taken from "generalized minimum residual") and BCGSTAB (bi-conjugate gradient, stabilized). We will not discuss the details of these methods, which can be found in numerous references. (For an introduction to the application of these methods to transport problems, see for example [255] and [262].)

Ashby et al. seem to be the first to apply Krylov methods to transport problems with anisotropic scattering (which causes T to be asymmetric) [158, 204]. Building on the CG work of Faber and Manteuffel [139], they viewed DSA as a preconditioner and applied GMRES to accelerate its convergence. They also tested an adaptive Chebyshev iteration procedure [65, 70] designed for asymmetric systems. Much like Derstine and Gelbard had previously with isotropic scattering and the CG method [100], Ashby et al. studied whether or not various diffusion discretizations could lead to efficient iterative schemes if they were used with preconditioned GMRES or Chebyshev instead of preconditioned Richardson iteration. Their study took place in 1-D with the DD and standard LD spatial discretizations. They employed two different diffusion discretizations as preconditioners. One was the *consistent* discretization derived using Larsen's four-step procedure, as discussed previously. The other was a standard finite-element method (FEM) discretization using linear continuous elements. The latter differs only slightly from the consistent discretization in the case of the DD transport discretization. A sample of their numerical results is given in Table 2. The underlying test problem is a two-region slab with vacuum boundaries and isotropic scattering. The left region is 50 mean-free paths thick with scattering ratio $c_L = 0.99998$; the right region is 5×10^7 mean-free paths thick with scattering ratio $c_R = 0.8$. Each region uses 50 uniform spatial cells with the 16-point Gaussian quadrature set in angle. The iterations proceeded until a count of 50 was reached or the L_2 norm of the residual became lower than 10^{-8}.

For this test problem, all methods perform well for a consistent discretization of the diffusion equation, as expected. GMRES performs best and Richardson (standard DSA) the

Transport Discretization	Diffusion Discretization	Iterative Method	Iteration Count
DD	consistent	Richardson	11
	consistent	Chebyshev	8
	consistent	GMRES	7
DD	FEM	Richardson	>50
	FEM	Chebyshev	22
	FEM	GMRES	13
LD	consistent	Richardson	11
	consistent	Chebyshev	8
	consistent	GMRES	7
LD	FEM	Richardson	43
	FEM	Chebyshev	20
	FEM	GMRES	14

Table 2: Iteration Counts for Ashby's Problem.

worst. The more interesting results involve the inconsistent FEM preconditioner. With this preconditioner for this test problem, the improvement that GMRES provides over Richardson is more dramatic. We remark, however, that the FEM preconditioner is identical to the consistent one if $c = 1$; this is partially responsible for its reasonable behavior in this problem, for which the high-c region has c very nearly equal to unity. Ashby et al. studied a second test problem, a uniform slab 10^8 mean-free paths thick with $c = 0.998$. For this problem, all methods failed to converge in 50 iterations when the FEM diffusion discretization was employed, whereas all methods converged in no more than 2 iterations when the consistent discretization was used. Thus, while GMRES and Chebyshev are improvements over Richardson iteration, nothing takes the place of a good preconditioner (such as a consistent diffusion discretization).

A different application of Krylov methods to transport problems is to use them to solve the low-order problem; that is, to assist with the preconditioning step itself as opposed to being "outside" of that. If the low-order problem is asymmetric, this can be very important. The NLBPA method used by Hong and Cho has an asymmetric low-order operator [240, 252, 266, 267]; to solve the low-order equations in two-dimensional problems they have applied the BCGSTAB method and reported quite acceptable results [252].

Other authors have also employed Krylov methods to transport problems, and the literature on this subject is growing rapidly. Some examples are [255, 262, 209, 250, 263, 265].

VII. ACCELERATION OF OTHER SCATTERING ITERATIONS

In previous chapters we have discussed the iterative solution of problems with isotropic

or weakly anisotropic scattering in a single energy group. Here we address the iterative solution of problems with more difficult kinds of scattering. We first consider the "upscattering" problem commonly found in neutronics when there are many energy groups in the thermal energy range. Then we consider problems with very highly anisotropic scattering, which are commonly found in electron transport or in optical photon transport. Finally, we address the absorption-emission process that occurs in thermal radiative transfer.

VII.A. Upscattering

Most transport problems of practical interest contain particles with wide ranges of kinetic energies. Because the probability of interaction with the background matter often depends sensitively upon this energy, an accurate description of the transport process requires an energy-dependent transport equation. The most common method for discretizing the energy variable is the "multigroup" method, in which the particles are "grouped" by energy and are assumed to interact via cross sections that have been averaged over each group's energy range. Given isotropic scattering in slab geometry, the multigroup transport equations are:

$$\mu\frac{\partial\psi_g}{\partial x}(x,\mu)+\Sigma_{t,g}(x)\psi_g(x,\mu)=\frac{1}{2}\sum_{g'=1}^{G}\Sigma_{s,g'\to g}(x)\phi_{g'}(x)+\frac{Q_g(x)}{2}\ ,\ 1\le g\le G\ , \qquad (7.1)$$

where g is the energy-group index. Customarily, the g^{th} energy group is defined by $E_{g+1/2}\le E<E_{g-1/2}$, with (obviously) $E_{g+1/2}<E_{g-1/2}$. Thus, as the group index g increases, the energies in group g decrease.

In some neutron transport problems, the energy groups are chosen such that scattering from a given energy group to a group of higher energy is a negligibly rare event. In such problems the multigroup equations can be easily solved in sequence from the highest- to the lowest-energy group. In this case, each group can be treated using the techniques described in previous chapters, with the "downscattering" source known from the solution of the higher energy groups.

However, in many problems, particularly ones involving a detailed description of thermal neutrons, a non-negligible scattering from some thermal groups to thermal groups of higher energy occurs. This gives rise to an "upscattering" iteration. The simplest way to solve such problems is to use a Gauss-Seidel (GS) iteration in energy groups:

$$\mu\frac{\partial\psi_g^{(\ell+1)}}{\partial x}(x,\mu)+\Sigma_{t,g}(x)\psi_g^{(\ell+1)}(x,\mu)=\frac{1}{2}\sum_{g'=g+1}^{G}\Sigma_{s,g'\to g}(x)\phi_{g'}^{(\ell)}(x)$$

$$+\frac{\Sigma_{s,g\to g}}{2}\phi_g^{(\ell+1)}(x)+\frac{1}{2}\sum_{g'=1}^{g-1}\Sigma_{s,g'\to g}(x)\phi_{g'}^{(\ell+1)}(x)+\frac{Q_g(x)}{2}\ ,\ 1\le g\le G\ . \qquad (7.2)$$

One can Fourier-analyze this iteration scheme using an infinite homogeneous model problem, much like the analysis of the single-energy problem studied in previous chapters. One finds that for each spatial error mode with wave number λ, there are G eigenvalues $\omega(\lambda)$ that satisfy:

$$\omega(\lambda)\,[\mathbf{I}-\mathbf{L}]A = \mathbf{R}A \ , \tag{7.3}$$

where

$$\mathbf{L}_{g,g'} = \begin{cases} \alpha_g \Sigma_{s,g'\to g}, & g' \le g \ , \\ 0, & \text{otherwise,} \end{cases}$$

$$\mathbf{R}_{g,g'} = \begin{cases} \alpha_g \Sigma_{s,g'\to g}, & g < g' \ , \\ 0, & \text{otherwise,} \end{cases}$$

$$\alpha_g = \frac{1}{2}\sum_m \frac{w_m \Sigma_{t,g}}{\Sigma_{t,g}^2 + \lambda^2 \mu_m^2} \ .$$

(To obtain this expression for α_g we assumed a symmetric angular quadrature set.)

This Gauss-Seidel iteration can converge arbitrarily slowly if absorption is negligibly small. In fact, we can easily describe a limiting case in which an eigenvalue is unity in the infinite-medium problem, as follows. If there is no absorption, then $\Sigma_{t,g} = \Sigma_{s,g}$, which implies:

$$\Sigma_{t,g} = \Sigma_{s,g} = \sum_{g'} \Sigma_{s,g\to g'} \ . \tag{7.4}$$

If we consider the $\lambda = 0$ mode, then $\alpha_g = 1/\Sigma_{t,g}$, and the gth row of the matrix equation (7.3) can be multiplied by $\Sigma_{t,g}$ and rearranged to obtain

$$\omega(0)\Sigma_{t,g}A_g = \omega(0)\sum_{g'=1}^{g} \Sigma_{s,g'\to g}A_{g'} + \sum_{g'=g+1}^{G} \Sigma_{s,g'\to g}A_{g'} \ . \tag{7.5}$$

If the eigenvalue $\omega(0)$ is unity, then the associated eigenvector A_g must satisfy Eq. (7.5) with $\omega(0) = 1$. Eqs. (7.4) and (7.5) then give:

$$A_g \sum_{g'=1}^{G} \Sigma_{s,g\to g'} = \sum_{g'=1}^{G} \Sigma_{s,g'\to g}A_{g'} \ . \tag{7.6}$$

It is not difficult to show that this equation has a solution. (It is of the form $\mathbf{M}A = 0$. One can easily show that the adjoint of $\mathbf{M}$ has a zero eigenvalue, from which it follows that $\mathbf{M}$ itself has a zero eigenvalue.) Eq. (7.6) is a discrete version of a continuous problem whose solution A is a Maxwellian. Thus, in an infinite homogeneous medium with no absorption, the Gauss-Seidel iteration shown in Eq. (7.2) has an eigenvalue of unity for the $\lambda = 0$ mode, and the corresponding eigenvector is a discrete approximation of a Maxwellian. Because there are practical problems that have well-thermalized neutrons with little leakage and

little absorption, it follows that for such problems the Gauss-Seidel procedure is slow to converge the upscattering iteration.

B.T. Adams and J.E. Morel attacked this problem by devising a scheme whose low-order operator (preconditioner) produces a good approximation of the slowest-converging error mode of the Gauss-Seidel iteration [179, 180]. Independently and simultaneously, Averin and Voloschenko devised a similar scheme [193]. In the following, we describe the work of Adams and Morel and then briefly outline how the work of Averin and Voloschenko differs.

Adams and Morel began with a Fourier analysis as in Eq. (7.3), using tabulated cross section sets with 41 "thermal" energy groups (groups in which upscattering can occur) for heavy water, graphite, and iron. Considering both isotropic and anisotropic scattering cross sections, they found that the slowest-converging mode for each material occurs at $\lambda = 0$ and is isotropic in angle. This led them to propose the following "Two-Grid" (TG) iterative scheme, which we write only for the case of isotropic scattering:

$$\mu \frac{\partial \psi_g^{(\ell+1/2)}}{\partial x}(x,\mu) + \Sigma_{t,g}(x)\psi_g^{(\ell+1/2)}(x,\mu) = \frac{1}{2}\sum_{g'=g+1}^{G} \Sigma_{s,g'\to g}(x)\phi_{g'}^{(\ell)}(x)$$

$$+ \frac{\Sigma_{s,g\to g}}{2}\phi_g^{(\ell+1/2)}(x) + \frac{1}{2}\sum_{g'=1}^{g-1} \Sigma_{s,g'\to g}(x)\phi_{g'}^{(\ell+1/2)}(x) + \frac{Q_g(x)}{2} \ , \quad 1 \le g \le G \ , \tag{7.7}$$

$$R^{(\ell+1/2)} = \sum_{g=1}^{G}\sum_{g'=g+1}^{G} \Sigma_{s,g'\to g}\left[\phi_{g'}^{(\ell+1/2)} - \phi_{g'}^{(\ell)}\right] \ , \tag{7.8}$$

$$-\frac{d}{dx}D\frac{dE^{(\ell+1/2)}}{dx} + \Sigma_a E^{(\ell+1/2)} = R^{(\ell+1/2)} \ , \tag{7.9}$$

$$\phi_g^{(\ell+1)} = \phi_g^{(\ell+1/2)} + \xi_g E^{(\ell+1/2)} \ , \tag{7.10}$$

where

$$\Sigma_a(x) = \sum_{g=1}^{G} (\Sigma_{t,g} - \Sigma_{s,g})\,\xi_g \ , \tag{7.11}$$

$$D(x) = \sum_{g=1}^{G} \frac{\xi_g}{3\Sigma_{t,g}} \ . \tag{7.12}$$

Many terms in these equations depend on the function ξ_g, which in the Adams-Morel method is taken to be the spectral shape of the slowest-converging mode. This procedure requires the calculation of one such function for each unique material in the problem of interest. This calculation, which takes place before iteration begins, is a numerical solution of the eigenvalue problem given by Eq. (7.3) with $\lambda = 0$ (for each material in the problem). The function ξ_g in a given material is the eigenfunction corresponding to the largest eigenvalue of this problem, normalized such that $\sum_{g=1}^{G} \xi_g = 1$.

Adams and Morel found that their scheme is surprisingly efficient. For example, the GS spectral radius for an infinite medium of heavy water is 0.9998, but the TG method gives a spectral radius of 0.489. This is surprising, because the low-order operator is designed to remove only one error mode (it is a one-group operator). Adams and Morel investigated this result and found that the second-largest eigenvalue of the GS iteration operator at $\lambda = 0$ is much smaller than the largest, and in fact is 0.489. (This result holds for their 41-group cross-section set for heavy water.) This unexpected property of the scattering cross section makes the TG scheme work exceedingly well. Similarly, for graphite the second eigenvalue (given their 41-group cross-section set) is 0.622, and as a result the TG spectral radius for an infinite medium of graphite is 0.622. The only other material discussed in reference [180] is iron, for which both GS and TG give spectral radii close to 0.6.

Independently and almost simultaneously, Averin and Voloschenko developed a similar method for the iterative solution of upscattering problems [193]. The main differences are in the choice of the spectrum function ξ_g and update equation (7.10). These authors proposed two different options for ξ_g; their linear option takes simply $\xi_g = 1/G$ for all g, and their nonlinear option defines ξ_g such that system-wide particle balance is achieved in each energy group at the end of each iteration. Their update equation includes a correction to the first angular moment (net current density) and the zeroth moment (scalar flux). (Adams and Morel examined this variation and determined that it had no appreciable effect on the problems they were considering.) Finally, Averin and Voloschenko primarily used weighted diamond spatial differencing for their studies, whereas Adams and Morel used LD. Both sets of authors obtained good results for problems corresponding to the upscattering of thermal neutrons.

Regarding the effect of spatial discretizations in the upscattering problem, Adams & Morel and Averin & Voloschenko found that if the one-group diffusion problem is discretized consistently with the multigroup transport problem, then the behavior of the spatially discrete TG method is essentially identical to the behavior predicted by the Fourier Analysis of problems without spatial discretization. In other words, if one knows how to discretize DSA for a within-group scattering problem for a given transport discretization, one can apply the same discretization to Eq. (7.9) in the upscattering problem.

In heterogeneous-medium problems, a rigorous derivation of the one-group diffusion equation for the correction $E^{(\ell+1/2)}$ produces a first-derivative term that Adams and Morel decided to omit from their Eq. (7.9). They initially discarded this term for simplicity and then found via numerical testing that their method was effective without it; thus, there seems to be no motivation to include it.

VII.B. Highly Forward-Peaked Scattering

Previous sections of this Review have focused on problems with isotropic or mildly anisotropic scattering. However, highly anisotropic scattering makes the problem considerably more difficult. Such scattering arises in the transport of electrons, and of photons in the visible and near-visible frequency range.

Let us consider the slab-geometry discrete-ordinates equations with general anisotropic scattering [1], written with iteration indices for a transport sweep:

$$\mu_m \frac{\partial \psi_m^{(\ell+1/2)}(x)}{\partial x} + \Sigma_t(x)\psi_m^{(\ell+1/2)}(x) = \sum_{k=0}^{K} \frac{2k+1}{2}\Sigma_{sk}(x)P_k(\mu_m)\phi_k^{(\ell)}(x) + \frac{Q(x)}{2} \quad , 1 \le m \le N \ . \tag{7.13}$$

Here,

$$\phi_k(x) = \sum_{n=1}^{N} w_n P_k(\mu_n)\psi_n(x) \ ,$$

$$\Sigma_{sk}(x) = \int_{-1}^{1} \Sigma_s(\mu_0, x)P_k(\mu_0)d\mu_0 \ ,$$

where

$$\Sigma_s(\mu_0, x) = \sum_{k=0}^{K} \frac{2k+1}{2}\Sigma_{sk}(x)P_k(\mu_0)$$

is the differential scattering cross section for scattering through an angle whose cosine is μ_0, and P_k is the kth Legendre polynomial. Source iteration defines the next iterate as $\phi_k^{(\ell+1)} = \phi_k^{(\ell+1/2)}$. A simplified version of the Fourier analysis illustrates how SI behaves as a function of the scattering coefficients Σ_{sk}. First, let us consider Eq. (7.13) for *iteration errors* (which causes Q to disappear) and for a homogeneous medium (which implies that the cross sections are constants). If we consider only the $\lambda = 0$ modes (for which the spatial derivative term vanishes), multiply Eq. (7.13) by $w_m P_n(\mu_m)$, and sum over m, we obtain

$$\Sigma_t \phi_n^{(\ell+1)}(x) = \Sigma_{sn}\phi_n^{(\ell)}(x) \ . \tag{7.14}$$

Thus, for the $\lambda = 0$ modes, the iteration matrix is diagonal, with eigenvalues

$$c_n = \frac{\Sigma_{sn}}{\Sigma_t} \ .$$

We note that c_0 is simply the scattering ratio c, as defined in previous sections, because $\Sigma_{s0} = \Sigma_s$. We also note that as scattering becomes more forward-peaked, c_n for $n > 0$ become larger. In the limit of purely forward scattering [in which $\Sigma_s(\mu_0) = \Sigma_s\delta(\mu_0 - 1)$], $c_n = c_0$ for all n, which implies that all $K+1$ eigenvalues approach c_0 when $\lambda = 0$. Thus, in a problem with highly forward-peaked scattering, all $K+1$ of the $\lambda = 0$ error modes are potentially very slow to converge. This makes it very difficult to find a good preconditioner.

For example, the diffusion preconditioner that is so effective with isotropic scattering (i.e., the low-order operator of DSA) addresses only the ϕ_0 and ϕ_1 portions of the scattering source. Thus, if c_n is close to unity for $n > 1$, even DSA will not cause the iteration to converge quickly.

Manteuffel and Morel recognized that this problem could be solved using a multigrid method in the angular variable [164]. The basic idea is to use $S_{N/2}$ equations to approximate the exact additive correction to the solution from the latest S_N sweep, and to do this recursively. In more detail, the following is a description of the method applied (for example) to an S_{16} problem.

1. Perform a "high-order" S_{16} transport sweep. [This is Eq. (7.13) with N = 16.]

2. Perform an S_8 transport sweep with the total source equal to an 8-term expansion of the S_{16} scattering-source residual:

$$\mu_m \frac{\partial \psi_m^{[N]}(x)}{\partial x} + \Sigma_t^{[N]}(x)\psi_m^{[N]}(x) = \sum_{k=0}^{N-1} \frac{2k+1}{2} \Sigma_{sk}^{[2N]}(x) r_k^{[2N]}(x) \ , \qquad (7.15)$$

   where

$$r_k^{[2N]}(x) = \phi_k^{(\ell+1/2)}(x) - \phi_k^{(\ell)}(x) \ ,$$

   and where N = 8. The superscript [N] on ψ means that this equation is solved using the S_N quadrature set. The superscript on the cross sections is necessary because the cross sections actually change as a function of the number of terms in the scattering summation on the right-hand side, due to a type of "transport correction" that is employed. See reference [164] for details.

3. Perform an S_4 transport sweep with the total source equal to the P_3 expansion of the S_8 scattering-source residual. This is Eq. (7.15) with N = 4 and with

$$r_k^{[8]}(x) = \phi_k^{[8]}(x) \equiv \sum_{m=1}^{8} w_m^{[8]} \psi_m^{[8]}(x) P_k(\mu_m^{[8]}) \ .$$

4. Solve a P_1 problem whose fixed source equals the P_1 expansion of the S_4 scattering-source residual. This and the previous step constitute one full DSA iteration of an S_4 problem. In slab geometry, which is what Manteuffel and Morel considered, this step is equivalent to solving an S_2 problem (not just performing an S_2 sweep). We denote the resulting P_1 (or, equivalently, S_2) solution as $\phi_k^{[2]}$ for $k = 0$ and 1.

5. Obtain the next iterate by adding the P_1, S_4, and S_8 solutions to the result from the S_{16} sweep of step 1:

$$\phi_k^{(\ell+1)}(x) = \phi_k^{(\ell+1/2)}(x) + \phi_k^{[8]}(x) + \phi_k^{[4]}(x) + \phi_k^{[2]}(x) \ ,$$

where the superscript indicates not only the order of the calculation that produced the given set of moments, but also the number of nonzero moments in the set. For example, $\phi_k^{[4]}$ in this equation is defined to be zero for $k \geq 4$.

Manteuffel and Morel performed a Fourier analysis of their method with no spatial discretization and found that the spectral radius occurred for $\lambda = 0$ modes and was bounded by less than 0.6. This was the worst-case value, obtained in the limit as the quadrature order $\rightarrow \infty$, with scattering moments taken from the Fokker-Planck scattering operator [164]. They tested their method using the same spatial discretization for all of the transport sweeps at the various levels and a consistent-DSA discretization of the P_1 equations that constitute the coarsest level. They observed performance that was consistent with the analysis of the equations without spatial discretization; they concluded that if consistent discretizations are used for the P_1 step, then spatial discretization does not degrade the method's performance. Their consistent discretization was obtained using Larsen's four-step procedure. In addition, they tested the method with the Adams-Martin modified four-step version of discretized diffusion equations and again saw no degradation of performance.

Manteuffel and Morel considered only slab geometry. Pautz, Morel, and Adams later attempted to generalize the Manteuffel-Morel method to multidimensional problems. This led to the following changes to the one-dimensional algorithm:

1. In problems with highly forward-peaked scattering cross sections and solutions, it is best to use Morel's "Galerkin quadrature" [143], for reasons explained by Pautz and Adams [269]. In multidimensional problems with an order-N quadrature set, this requires that the scattering term contain more than just the moments of order N-1 and lower. In 2-D, some of the order-N moments must also be retained, while in 3-D some of the moments of orders N and N+1 must be retained. This necessitates a change in the residual that drives the transport sweep on a given level. For example, in an S_{16} calculation in 2-D, the residual on the right side contains some terms of order 8, in addition to all of the order-7 terms shown in Eq. (7.15).

2. Rather than solving a P_1 problem after the S_4 sweep, Pautz et al. perform an S_2 sweep and then solve a diffusion problem. The reason for this is that P_1 acceleration of S_4 calculations can be divergent in multidimensional problems for sufficiently highly forward-peaked scattering, as shown by Marchuk and Lebedev [10] and Adams and Wareing [181].

Pautz et al. first analyzed this method applied to S_N problems without spatial discretization. These authors found that the method has divergent high-frequency modes for which ordinary SI performs reasonably well; the multigrid method *amplifies* these error modes so

much that their eigenvalues exceed unity [270]. Fortunately, the multigrid method performs reasonably well for the low-frequency modes, much like it does in 1-D.

Thus, what one would like to have is the low-frequency portions of the corrections from the low-order equations *without* the high-frequency portions. With this in mind, Pautz et al. devised a procedure for using the diffusion equation to *filter out* the high-frequency portions of the additive corrections. For each moment $\phi_{k,n}$, all of the corrections calculated from the sweeps at each level are summed and used as a source in a diffusion equation:

$$-\vec{\nabla}\cdot\frac{\alpha_f}{\Sigma_f}\vec{\nabla}f_{k,n}+\Sigma_f(x)f_{k,n}(x)=\Sigma_f(x)\left[\phi_{k,n}^{[2]}+\phi_{k,n}^{[4]}+\ldots+\phi_{k,n}^{[N/2]}\right] . \qquad (7.16)$$

Here Σ_f is the "filter cross section" and α_f is the "filtering parameter." The solution of this equation is then used as the correction to the result of the high-order transport sweep:

$$\phi_{k,n}^{(\ell+1)}(x)=\phi_{k,n}^{(\ell+1/2)}(x)+f_{k,n}(x) .$$

Pautz et al. obtained very good results with $\alpha_f = 1$ and $\Sigma_f = \Sigma_{tr}$, the "transport" cross section. In the absence of spatial discretization, their procedure rendered the angular multigrid method rapidly convergent for a wide class of practical problems with highly forward-peaked scattering. However, their method's performance slowly degrades as the quadrature order increases. For example, the worst-case spectral radius is 0.90, 0.92, and 0.94 for the S_{10}, S_{12}, and S_{14} level-symmetric quadrature sets, respectively. More importantly, Pautz et al. found that for the bilinear discontinuous spatial discretization method, spatial discretization *improves* the performance of the angular multigrid scheme. In fact, for mesh cells greater than one transport mean-free path in thickness, the discretized method does not even need the high-frequency filter.

In summary, the angular multigrid method (with no filter) converges reasonably rapidly for highly anisotropic scattering problems with relatively coarse spatial meshes. The filtering step extends this performance to the fine-mesh limit. However, as the quadrature order increases, the filtered method's spectral radius approaches unity.

In this section we have focused on one approach – multigrid in angle – for solving problems with highly anisotropic scattering. Other approaches have also been studied; for example, Gol'din and co-workers have applied the quasidiffusion method to such problems [235, 239, 278], and Khattab et al. have developed iteration schemes whose low-order equations employ discrete approximations to the P_N equations [161], [241].

VII.C. Absorption-Emission in Radiative Transfer

Much of the development of rapidly convergent iterative methods for the transport equation has been motivated not by neutron transport problems, but by the problem of absorption and emission of thermal photons in radiative transfer. In slab geometry, the basic equations

(neglecting Compton scattering and assuming the multigroup approximation in frequency) are [246]:

$$\frac{1}{c}\frac{\partial\psi_g(x,\mu,t)}{\partial t}+\mu\frac{\partial\psi_g(x,\mu,t)}{\partial x}+\Sigma_g(x,t)\psi_g(x,\mu,t)=\Sigma_g(x,t)B_g\left(T(x,t)\right)\ , \tag{7.17}$$

$$C_p\frac{\partial T(x,t)}{\partial t}=\sum_{g=1}^{G}\Sigma_g(x,t)\int_{-1}^{1}\left[\psi_g(x,\mu,t)-B_g\left(T(x,t)\right)\right]d\mu+Q(x,t)\ , \tag{7.18}$$

where B_g is the Planckian integrated over a frequency (energy) group:

$$B_g(T)=\int_{\nu_{g-1/2}}^{\nu_{g+1/2}}\frac{4\pi h\nu^3}{c^2}\frac{1}{e^{h\nu/kT}-1}d\nu\ . \tag{7.19}$$

There are many ways to discretize the time variable in these equations. We choose a simple one for illustration; most other time discretizations lead to similar iterative difficulties. If the superscript n represents the beginning of the time step and the absence of a superscript represents the end, the time- and frequency-discretized equations are:

$$\frac{1}{c}\frac{\psi_g(x,\mu)-\psi_g^n(x,\mu)}{\Delta t}+\mu\frac{\partial\psi_g(x,\mu)}{\partial x}+\Sigma_g(x)\psi_g(x,\mu)=\Sigma_g(x)\tilde{B}_g(x)\ , \tag{7.20}$$

$$C_p\frac{T(x)-T^n(x)}{\Delta t}=\sum_{g=1}^{G}\Sigma_g(x)\int_{-1}^{1}\left[\psi_g(x,\mu)-\tilde{B}_g(x)\right]d\mu+Q\ . \tag{7.21}$$

Here $\tilde{B}_g$ is a linearized version of the Planckian:

$$\tilde{B}_g(x)=B_g^n(x)+\left[T(x)-T^n(x)\right]\dot{B}_g^n(x)\ , \tag{7.22}$$

with

$$B_g^n(x)=B_g\left(T^n(x)\right)\quad,\quad\dot{B}_g^n(x)=\frac{dB_g}{dT}\left(T^n(x)\right)\ .$$

The change in temperature, $[T(x)-T^n(x)]$, can be eliminated from Eqs. (7.20)-(7.21), producing the following steady-state equation for the unknown angular intensity:

$$\mu\frac{\partial\psi_g(x,\mu)}{\partial x}+\tilde{\Sigma}_g(x)\psi_g(x,\mu)=\frac{\chi_g(x)}{2}\sum_{g=1}^{G}\eta(x)\Sigma_g(x)\int_{-1}^{1}\psi_g(x,\mu')d\mu'+S_g(x,\mu)\ . \tag{7.23}$$

Here we have introduced:

$$\tilde{\Sigma}_g(x)=\Sigma_g(x)+\frac{1}{c\Delta t}\quad,\quad\left(\tilde{\Sigma}_g>\Sigma_g\right)\quad, \tag{7.24}$$

$$\eta(x)=\frac{\sum_{g=1}^{G}\Sigma_g(x)\dot{B}_g^n(x)}{\frac{C_p(x)}{2\Delta t}+\sum_{g=1}^{G}\Sigma_g(x)\dot{B}_g^n(x)}\quad,\quad(0<\eta<1)\quad, \tag{7.25}$$

$$\chi_g(x) = \frac{\Sigma_g(x)\dot{B}_g^n(x)}{\sum_{g'=1}^{G} \Sigma_{g'}(x)\dot{B}_{g'}^n(x)} \quad , \quad \left(\sum_{g=1}^{G} \chi_g = 1\right) \quad , \tag{7.26}$$

$$S_g(x,\mu) = \frac{1}{c\Delta t}\psi_g^n(x,\mu) + \Sigma_g B_g^n(x) + \eta\frac{\chi_g}{2}\left[Q(x) + 2\sum_{g'=1}^{G} \Sigma_{g'}(x)B_{g'}^n(x)\right] \; . \tag{7.27}$$

Equation (7.23) has the form of a subcritical neutron transport problem with fission but no scattering. The quantities $\chi_g(x)$, $\eta(x)$, $\Sigma_g(x)$, and $\tilde{\Sigma}_g(x)$ play the respective roles of fission spectrum, number of neutrons emitted per fission, fission cross section, and total cross section. Many radiative-transfer problems of practical interest have regions that are extremely optically thick in some frequency groups; thus, a typical photon's energy is absorbed and re-emitted many times before it escapes the problem domain. Therefore, a simple "source-iteration" approach (termed "lambda iteration" in the astrophysical community [115, 121]) would require many iterations to converge. If the time steps are sufficiently small that only a small number of source iterations are needed per step, then a very large number of steps is required. Unfortunately, larger time steps require many more source iterations per step. The preferred approach is to use (*i*) time steps that would require a very large number of source iterations per step, and (*ii*) a more rapidly converging iteration scheme than source iteration.

For a single frequency (energy) group, Eq. (7.23) becomes:

$$\mu\frac{\partial\psi(x,\mu)}{\partial x} + \tilde{\Sigma}(x)\psi(x,\mu) = \frac{1}{2}\eta(x)\Sigma(x)\int_{-1}^{1}\psi(x,\mu')d\mu' + S(x,\mu) \; . \tag{7.28}$$

This is the same as Eq. (1.1), with $\tilde{\Sigma}$ and $\eta\Sigma$ playing the roles of Σ_t and Σ_s, respectively. Thus, there is a close mathematical connection between the radiative transfer problem and the problems discussed in previous chapters. We note that in the limit of a large time step, the effective scattering ratio

$$\frac{\eta(x)\Sigma(x)}{\tilde{\Sigma}(x)} \approx 1 \; .$$

Given an optically thick problem domain, this implies a difficult iterative problem.

Let us return to the multigroup problem, Eq. (7.23), and examine the "emission" term (the first term on the right side). This term is the product of a specific energy shape ($\chi_g(x)$) and a term that depends only on position. Thus, the term that drives the iteration is independent of direction and energy. This is significantly different from the scattering term in the general multigroup problem of Eq. (7.1), which depends on both the spatial and energy variation of the unknown solution.

Larsen took advantage of this "one-group isotropic-scattering" nature of the driving term in Eq. (7.23) to develop a good preconditioner ("synthetic acceleration method") for

the problem [129]. His low-order equation in this *Grey Transport Acceleration* (GTA) method is a one-group (or "grey") transport equation of the form of Eq. (7.28). The cross sections in this equation are weighted averages of the multigroup cross sections in Eq. (7.23). The weight functions are the energy shapes of the slowest-converging error modes as determined by an infinite-medium Fourier analysis. Let us define:

$$\beta(x) = \sum_{g=1}^{G} \eta \Sigma_g(x) \int_{-1}^{1} \psi_g(x,\mu')d\mu' \ . \tag{7.29}$$

Then a single GTA iteration is given by

$$\mu \frac{\partial \psi_g^{(\ell+1/2)}(x,\mu)}{\partial x} + \tilde{\Sigma}_g(x)\psi_g^{(\ell+1/2)}(x,\mu) = \frac{\chi_g}{2}\beta^{(\ell)}(x) + S_g(x,\mu) \ , \tag{7.30}$$

$$\mu \frac{\partial f(x,\mu)}{\partial x} + \Sigma_t(x) f(x,\mu) = \frac{1}{2}\Sigma_s(x) \int_{-1}^{1} f(x,\mu')d\mu' + \frac{1}{2}\left[\beta^{(\ell+1/2)}(x) - \beta^{(\ell)}(x)\right] \ , \tag{7.31}$$

$$\beta^{(\ell+1)}(x) = \beta^{(\ell+1/2)}(x) + \Sigma_s(x) \int_{-1}^{1} f(x,\mu')d\mu' \ . \tag{7.32}$$

The quantities Σ_t and Σ_s in Eqs. (7.31) and (7.32) are weighted averages of the $\tilde{\Sigma}_g$ and Σ_g, respectively. Larsen showed via a Fourier analysis that his GTA method is convergent for a model analytic opacity, with a worst-case spectral radius of 0.868. The GTA method requires the solution of the low-order one-group problem, Eqs. (7.31) and (7.32), every full iteration. For this problem the one-group iteration methods discussed in previous chapters can be employed.

Gol'din and co-workers have also applied the Quasidiffusion method to the problem of radiative transfer [43, 82, 108, 216, 261]. The QD method is quite well-suited to this problem, especially when there is coupling to other physics, such as hydrodynamics. The basic ideas are illustrated by the following nested iteration scheme. The outermost iteration uses a previous value of $\beta(x)$ and produces an Eddington factor for each frequency group:

$$\mu \frac{\partial \psi_g^{(\ell+1/2)}(x,\mu)}{\partial x} + \tilde{\Sigma}_g(x)\psi_g^{(\ell+1/2)}(x,\mu) = \frac{\chi_g}{2}\beta^{(\ell)}(x) + S_g(x,\mu) \ , \tag{7.33}$$

$$E_g^{(\ell+1/2)}(x) = \frac{\int_{-1}^{1} \mu^2 \psi_g^{(\ell+1/2)}(x,\mu)d\mu}{\int_{-1}^{1} \psi_g^{(\ell+1/2)}(x,\mu)d\mu} \ . \tag{7.34}$$

For each outer iteration (index ℓ) an iterative calculation determines a new value of $\beta(x)$. In its simplest form this iteration consists of the solution of the Quasidiffusion equation for each group followed by the solution of a one-group Quasidiffusion system. Let us define

$$S_{k,g}(x) \equiv \int_{-1}^{1} \mu^k S_g(x,\mu)d\mu \ .$$

Then, for nested iteration s inside outer iteration ℓ, the multigroup Quasidiffusion equations are

$$\frac{d\phi_{1,g}^{(\ell+1/2,s+1/2)}}{dx}(x)+\tilde{\Sigma}_g(x)\phi_{0,g}^{(\ell+1/2,s+1/2)}(x)=\chi_g\beta^{(\ell,s)}(x)+S_{0,g}(x)\ , \tag{7.35}$$

$$\frac{d}{dx}\left[E_g^{(\ell+1/2)}\phi_{0,g}^{(\ell+1/2,s+1/2)}\right]+\tilde{\Sigma}_g(x)\phi_{1,g}^{(\ell+1/2,s+1/2)}=S_{1,g}(x)\ . \tag{7.36}$$

If these equations are summed over all groups, the result is a one-group Quasidiffusion system with solution-weighted frequency-averaged cross sections. The final part of iteration s is to solve this system with cross sections weighted by the latest solution:

$$\frac{d\Phi_1^{(\ell+1/2,s+1)}}{dx}+\Sigma_a^{(s+1/2)}(x)\Phi_0^{(\ell+1/2,s+1)}(x)=S_{0,sum}(x)\ , \tag{7.37}$$

$$\frac{d}{dx}\left[E^{(\ell+1/2)}\Phi_0^{(\ell+1/2,s+1)}\right]+\tilde{\Sigma}_t^{(s+1/2)}(x)\Phi_1^{(\ell+1/2,s+1)}$$
$$+\zeta^{(\ell+1/2)}(x)\Phi_0^{(\ell+1/2,s+1)}=S_{1,sum}(x)\ . \tag{7.38}$$

Here we have defined:

$$S_{k,sum}(x)\equiv\sum_{g=1}^{G}S_{k,g}(x)\ ,$$

$$\Phi_k(x)\equiv\sum_{g=1}^{G}\phi_{k,g}(x)\ ,$$

$$E^{(\ell+1/2)}(x)\equiv\sum_{g=1}^{G}E_g^{(\ell+1/2)}(x)\ ,$$

$$\Sigma_a^{(s+1/2)}(x)\equiv\frac{\sum_{g=1}^{G}\left[\tilde{\Sigma}_g(x)-\eta\Sigma_g(x)\right]\phi_{0,g}^{(\ell+1/2,s+1/2)}(x)}{\sum_{g=1}^{G}\phi_{0,g}^{(\ell+1/2,s+1/2)}(x)}\ ,$$

$$\tilde{\Sigma}_t^{(s+1/2)}(x)\equiv\frac{\sum_{g=1}^{G}\tilde{\Sigma}_g(x)|\phi_{1,g}^{(\ell+1/2,s+1/2)}(x)|}{|\phi_{1,g}^{(\ell+1/2,s+1/2)}(x)|}\ ,$$

$$\zeta^{(s+1/2)}(x)\equiv\frac{\sum_{g=1}^{G}\left[\tilde{\Sigma}_g(x)-\tilde{\Sigma}_t^{(s+1/2)}(x)\right]\phi_{1,g}^{(\ell+1/2,s+1/2)}}{\sum_{g=1}^{G}\phi_{0,g}^{(\ell+1/2,s+1/2)}(x)}\ .$$

The energy-averaging procedure that produces these equivalent one-group QD equations was first presented by Gol'din and Chetverushkin [43]; it was later refined by Gol'din and co-workers [108, 208]. While the latter two definitions look rather unusual, they achieve

the purpose of keeping the one-group system exact but avoiding average quantities with small quantities in denominators. We note that if each group's first angular moment, $\phi_{1,g}$, has the same sign, then $\tilde{\Sigma}_t$ is a simple $\phi_{1,g}$-weighted average and ζ is zero.)

The solution of this one-group system produces a new estimate for β:

$$\beta^{(\ell,s+1)}(x) = \Phi^{(\ell+1/2,s+1)}(x)\Sigma_s^{(\ell+1/2,s+1/2)}(x) \ , \tag{7.39}$$

where

$$\Sigma_s^{(\ell+1/2,s+1/2)} \equiv \frac{\sum_{g=1}^{G} \eta\Sigma_g(x)\phi_{0,g}^{(\ell+1/2,s+1/2)}(x)}{\sum_{g=1}^{G} \phi_{0,g}^{(\ell+1/2,s+1/2)}(x)} \ .$$

Upon convergence (or a pre-selected number) of the s iterations, the new β is declared to be the β at the next ℓ level:

$$\beta^{(\ell+1)}(x) = \beta^{(\ell,s_{max})}(x) \ , \tag{7.40}$$

where s_{max} is the number of "s" iterations taken on Eqs. (7.36)-(7.39).

Before leaving the subject of radiative transfer, we remark that the extreme optical thickness of typical problems places great stress on spatial discretization methods. Practical considerations usually require the use of a spatial grid whose cells are extremely optically thick, at least for certain frequency groups. In such problems, many "simple" spatial discretization methods (such as diamond differencing) exhibit unphysical behavior. A great deal of effort has gone into analyzing this behavior and developing spatial discretization methods with the correct behavior; we refer the reader to [140, 172, 247, 286] and references therein.

VIII. ACCELERATION OF k-EIGENVALUE PROBLEMS

The k-eigenvalue problem is of great interest in neutron transport calculations for nuclear reactor simulations. The one-group, slab-geometry, isotropic scattering version of this problem is:

$$\mu\frac{\partial\psi}{\partial x}(x,\mu) + \Sigma_t(x)\psi(x,\mu) = \frac{\Sigma_s(x)}{2}\phi(x) + \frac{1}{k}\frac{\nu\Sigma_f(x)}{2}\phi(x) \ , \tag{8.1}$$

where

$$\phi(x) \equiv \int_{-1}^{1} \psi(x,\mu)d\mu \ ,$$

and for simplicity we have omitted the (homogeneous) boundary conditions.

If we define the *loss* (L) and *production* (P) operators as:

$$L\psi \equiv \mu\frac{\partial\psi}{\partial x} + \Sigma_t(x)\psi(x,\mu) - \frac{\Sigma_s(x)}{2}\int_{-1}^{1} \psi(x,\mu')d\mu' \ , \tag{8.2}$$

$$P\psi \equiv \frac{\nu\Sigma_f(x)}{2}\int_{-1}^{1}\psi(x,\mu')d\mu' \ , \tag{8.3}$$

then the k-eigenvalue problem can be written

$$L\psi = \frac{1}{k}P\psi \ . \tag{8.4}$$

Equivalently,

$$k\psi = L^{-1}P\psi = A\psi \ . \tag{8.5}$$

Thus, the so-called *k-eigenvalues* are the eigenvalues of the operator

$$A \equiv L^{-1}P = [\text{loss}]^{-1}[\text{production}] \ .$$

Clearly, P, L^{-1}, and A are positive, bounded operators. Thus, the eigenvalues of A are bounded; generally the largest (in magnitude) of these eigenvalues is real and positive, and the corresponding eigenfunction is of one sign (positive). We denote the eigenvalues of $A = L^{-1}P$ by $\{k_n, n \geq 1\}$, the corresponding eigenfunctions by $\{u_n(x,\mu), n \geq 1\}$, and we assume that the eigenvalues are ordered such that $|k_{n+1}| \leq |k_n|$. Then the largest (in magnitude) eigenvalue is k_1, which is called the *multiplication factor*. This eigenvalue is of great practical importance and is the desired output of most reactor eigenvalue calculations.

The ratio

$$r \equiv \frac{|k_2|}{k_1} = \max_{n\geq 2}\frac{|k_n|}{k_1} \ , \tag{8.6}$$

which is strictly less than unity, is the *dominance ratio*. For systems with an optically thin fission region, r is usually small. However, for systems with optically thick or "loosely-coupled" fission regions, r is usually "large" (i.e., near unity). The dominance ratio r plays the same role for eigenvalue problems as the scattering ratio c does for fixed-source problems: if r is small, the simplest iteration scheme to determine k_1 (power iteration) converges rapidly, while if r is "large" (near unity), power iteration converges slowly.

VIII.A. Power Iteration (PI)

The simplest practical iterative procedure to determine k_1, and the associated eigenfunction u_1, is *Power Iteration* (PI) [132]. This can be defined for $n \geq 0$ by

$$L\psi^{(n+1/2)}(x,\mu) = P\psi^{(n)}(x,\mu) \ , \tag{8.7}$$

$$\psi^{(n+1)}(x,\mu) = \frac{\psi^{(n+1/2)}(x,\mu)}{||\psi^{(n+1/2)}||} \ , \tag{8.8}$$

$$k_1^{(n+1)} = ||\psi^{(n+1/2)}|| \ , \tag{8.9}$$

where $\psi^{(0)}$ is an arbitrary initial estimate and $||\ \ ||$ is any convenient norm. Equivalently,

$$\psi^{(n)}(x,\mu) = \frac{A^n\psi^{(0)}(x,\mu)}{||A^n\psi^{(0)}||} \ , \tag{8.10}$$

$$k_1^{(n)} = \frac{||A^n\psi^{(0)}||}{||A^{n-1}\psi^{(0)}||} \ . \tag{8.11}$$

In this scheme, the eigenfunction estimates $\psi^{(n)}(x,\mu)$ are normalized to satisfy $||\psi^{(n)}|| = 1$ for $n \geq 1$. Also, if $\psi^{(0)}(x,\mu) > 0$, then $\psi^{(n)}(x,\mu) > 0$ for $n \geq 1$.

Eq. (8.7) implies that power iteration requires one to solve, within each iteration (n), a fixed-source transport problem with scattering and a *specified* fission source. For many optically thick problems with weak absorption, such problems can be solved efficiently only using acceleration methods such as those described in the previous chapters of this Review.

To analyze the convergence properties of the PI scheme, let us assume that the eigenfunctions of A can be used to expand the initial estimate $\psi^{(0)}$:

$$\psi^{(0)}(x,\mu) = \sum_{j=1}^{\infty} a_j u_j(x,\mu) \ . \tag{8.12}$$

Then for all $n \geq 0$,

$$A^n\psi^{(0)}(x,\mu) = \sum_{j=1}^{\infty} a_j k_j^n u_j(x,\mu) \ , \tag{8.13}$$

so Eqs. (8.10) and (8.11) can be written

$$\psi^{(n)}(x,\mu) = \frac{a_1u_1(x,\mu) + \sum_{j=2}^{\infty} a_j \left(\frac{k_j}{k_1}\right)^n u_j(x,\mu)}{||a_1u_1 + \sum_{j=2}^{\infty} a_j \left(\frac{k_j}{k_1}\right)^n u_j||} \ , \tag{8.14}$$

$$k_1^{(n)} = k_1 \frac{||a_1u_1 + \sum_{j=2}^{\infty} a_j \left(\frac{k_j}{k_1}\right)^n u_j||}{||a_1u_1 + \sum_{j=2}^{\infty} a_j \left(\frac{k_j}{k_1}\right)^{n-1} u_j||} \ . \tag{8.15}$$

The summations in these two equations are $O(r^n)$. For large n,

$$\psi^{(n)}(x,\mu) = \frac{u_1(x,\mu)}{||u_1||} + O(r^n) \tag{8.16}$$

$$k_1^{(n)} = k_1 + O(r^n) \ . \tag{8.17}$$

Thus, r is the effective spectral radius of the PI scheme. If r is small, PI converges rapidly, but if r is close to unity, then PI converges slowly.

VIII.B. Shifted Power Iteration (SPI)

For many problems, *Shifted Power Iteration* (SPI) [131] significantly reduces the spectral radius of Power Iteration. For a suitable positive constant $\kappa > k_1$ (described below), let us write Eq. (8.4) as

$$\left(L - \frac{1}{\kappa}P\right)\psi(x,\mu) = \left(\frac{1}{k} - \frac{1}{\kappa}\right)P\psi(x,\mu) \ . \tag{8.18}$$

Then, analogous to Eqs. (8.7) - (8.9), SPI is defined by:

$$\left(L - \frac{1}{\kappa}P\right)\psi^{(n+1/2)}(x,\mu) = \left(\frac{1}{k} - \frac{1}{\kappa}\right)P\psi^{(n)}(x,\mu) \ , \tag{8.19}$$

$$\psi^{(n+1)}(x,\mu) = \frac{\psi^{(n+1/2)}(x,\mu)}{||\psi^{(n+1/2)}||} \ , \tag{8.20}$$

$$\frac{1}{k_1^{(n+1)}} - \frac{1}{\kappa} = ||\psi^{(n+1/2)}||^{-1} \ . \tag{8.21}$$

Equivalently,

$$\psi^{(n)}(x,\mu) = \frac{\left[\left(I - \frac{1}{\kappa}A\right)^{-1}A\right]^n \psi^{(0)}(x,\mu)}{||\left[\left(I - \frac{1}{\kappa}A\right)^{-1}A\right]^n \psi^{(0)}||} \ , \tag{8.22}$$

$$\frac{1}{k_1^{(n+1)}} - \frac{1}{\kappa} = \frac{||\left[\left(I - \frac{1}{\kappa}A\right)^{-1}A\right]^n \psi^{(0)}||}{||\left[\left(I - \frac{1}{\kappa}A\right)^{-1}A\right]^{n-1} \psi^{(0)}||} \ . \tag{8.23}$$

For this problem, the dominance ratio is easily shown to be

$$r = \frac{\left|\frac{k_2}{1-k_2/\kappa}\right|}{\left|\frac{k_1}{1-k_1/\kappa}\right|} = \left|\frac{\kappa - k_1}{\kappa - k_2}\right|\left|\frac{k_2}{k_1}\right| \ . \tag{8.24}$$

Because $|k_2| < k_1 < \kappa$, this dominance ratio is always less than that of simple power iteration. If a value of κ can be found satisfying

$$0 < \kappa - k_1 \ll |\kappa - k_2| \ , \tag{8.25}$$

then the SPI iteration converges very rapidly. For such values of κ, the fixed-source problems (8.19) that must be solved in each SPI iteration represent nearly-critical [or in the terminology of the previous chapters of this Review, very highly scattering] problems. Thus, the fixed-source acceleration techniques described earlier in this Review become even more important in solving SPI problems than in solving PI problems. Moreover, in multigroup

problems, the fission operator on the left side of the fixed-source problem, Eq. (8.19) introduces an effective upscattering, which further complicates its solution relative to that of the fixed-source problems encountered with PI.

The above results for the PI and SPI schemes are very general and hold for transport problems in general geometries, with anisotropic scattering, and with (multigroup) energy dependence. The effective spectral radius for PI is always given by Eq. (8.6), and the effective spectral radius for SPI is always given by Eq. (8.24), where κ is the shifting parameter. Unfortunately, for difficult problems in which $|k_2| \approx k_1$, it can be difficult to obtain a value of κ satisfying the inequalities (8.25). Also, as noted previously, the fixed-source problem that must be solved for each SPI iteration is considerably more difficult than is the problem that is solved for each PI iteration. For this reason, SPI is not a panacea, and other acceleration methods have been devised that do not directly require a shifting parameter κ. We turn to these methods next.

VIII.C. Chebyshev Iteration for k-Eigenvalue Problems

As we discussed in Section VI.B, it can be advantageous to replace the ℓ^{th} iterate in a fixed-source problem with a weighted average of all iterates through iteration ℓ. The weights in this weighted average can be chosen to correspond to a Chebyshev polynomial; this can significantly improve iterative convergence.

The same logic, applied to the k-eigenvalue problem, leads to the same conclusion. Rather than using only the nth iterate, $\psi^{(n)}$, we define an average of it and all previous iterates:

$$\tilde{\psi}^{(n)} = \sum_{i=0}^{n} \alpha_n^{(i)} \psi^{(i)} \quad . \tag{8.26}$$

As described in Section VI.B, it is not necessary to store all of the previous iterates. Instead, we can take advantage of a three-term recursion relation for Chebyshev polynomials, requiring us to store only two previous iterates while building the new one.

Chebyshev acceleration is used fairly widely in transport and diffusion codes to speed convergence of k-eigenvalue problems. For example, the DANT system of codes [232, 144, 92] employs Chebyshev acceleration in the solution of its low-order (diffusion) k-eigenvalue problems (see Section VIII.E below) and also in its transport k-eigenvalue problems in hexagonal geometry. The DIF3D code uses Chebyshev acceleration for its k-eigenvalue problems; the DIF3D manual nicely explains the method and its implementation [80]. For very difficult problems – those with dominance ratio $r \to 1$, Chebyshev acceleration can tremendously reduce the number of iterations compared to standard power iteration.

VIII.D. Quasidiffusion for k-Eigenvalue Problems

The QD method is excellently suited to the k-eigenvalue problem, as Gol'din and Kalitkin recognized very early [44], and Gol'din and Anistratov later exploited [82, 168]. Taking the 0^{th} and 1^{st} angular moments of the k-eigenvalue problem, Eq. (8.1), one obtains the QD k-eigenvalue equations:

$$\frac{d\phi_1}{dx}(x) + \Sigma_a(x)\phi_0(x) = \frac{1}{k}\nu\Sigma_f(x)\phi_0(x) \ , \tag{8.27}$$

$$\frac{d}{dx}\left[E(x)\phi_0(x)\right] + \Sigma_t(x)\phi_1(x) = 0 \ , \tag{8.28}$$

where E is the Eddington factor. There are various ways to proceed; a simple one begins with an initial guess for the Eddington factor:

$$E^{(1/2)} = \text{guess} \quad (\text{usually} = 1/3) \ . \tag{8.29}$$

Then the iteration proceeds as follows. In the first step of each iteration, one solves a QD k-eigenvalue problem, using the latest estimate for E:

$$\frac{d\phi_1^{(\ell)}}{dx}(x) + \Sigma_a(x)\phi_0^{(\ell)}(x) = \frac{1}{k^{(\ell)}}\nu\Sigma_f(x)\phi_0^{(\ell)}(x) \ , \tag{8.30}$$

$$\frac{d}{dx}\left[E^{(\ell-1/2)}(x)\phi_0^{(\ell)}(x)\right] + \Sigma_t(x)\phi_1^{(\ell)}(x) = 0 \ . \tag{8.31}$$

(These equations could be solved with PI or SPI, for example.) In the second step, one performs a transport sweep (with known scattering and fission sources from the previous step) to generate a new Eddington factor:

$$\mu\frac{\partial\psi^{(\ell+1/2)}}{\partial x}(x,\mu) + \Sigma_t(x)\psi^{(\ell+1/2)}(x,\mu) = \frac{\Sigma_s(x)}{2}\phi^{(\ell)}(x) + \frac{1}{k^{(\ell)}}\frac{\nu\Sigma_f(x)}{2}\phi^{(\ell)}(x) \ , \tag{8.32}$$

$$E^{(\ell+1/2)}(x) = \frac{\int_{-1}^{1}\mu^2\psi^{(\ell+1/2)}(x,\mu)d\mu}{\int_{-1}^{1}\psi^{(\ell+1/2)}(x,\mu)d\mu} \ . \tag{8.33}$$

This iteration continues until ϕ and k converge.

Contrasting this procedure with PI or SPI applied directly to the transport problem, as in Section VIII.A, we observe:

1. With PI or SPI applied directly to the transport problem, the number of transport sweeps is the number of k iterations times the average number of scattering iterations per k iteration. Transport sweeps, of course, solve for the full angle- and position-dependent angular flux. If the dominance ratio is close to unity, then the number of k iterations will be large and thus so will the number of transport sweeps (each of which is costly).

2. With QD, PI or SPI is applied only to a low-order problem. The number of transport sweeps depends not on the dominance ratio, but on how quickly the Eddington factor converges in the two-step iteration process described above. The potentially large number of PI or SPI iterations takes place only in the low-order problem, which has only position (not angle) as an independent variable. This is a central theme in the QD method: most of the work is done in the relatively inexpensive setting of a lower-dimensional problem.

We consider next the multigroup k-eigenvalue problem with isotropic scattering:

$$\mu\frac{\partial\psi_g}{\partial x}(x,\mu)+\Sigma_{t,g}(x)\psi_g(x,\mu)=\frac{1}{2}\sum_{g'=1}^{G}\left[\Sigma_{s,g'\to g}(x)+\frac{\chi_g}{k}\nu\Sigma_{f,g'}(x)\right]\phi_{0,g'}(x)\ . \tag{8.34}$$

Taking the 0^{th} and 1^{st} angular moments, we obtain the multigroup QD equations:

$$\frac{d\phi_{1,g}}{dx}(x)+\Sigma_{t,g}(x)\phi_{0,g}(x)=\sum_{g'=1}^{G}\left[\Sigma_{s,g'\to g}(x)+\frac{\chi_g}{k}\nu\Sigma_{f,g'}(x)\right]\phi_{0,g'}(x)\ , \tag{8.35}$$

$$\frac{d}{dx}\left[E_g(x)\phi_{0,g}(x)\right]+\Sigma_{t,g}(x)\phi_{1,g}(x)=0\ . \tag{8.36}$$

As we have shown in Section VII.C, it is possible to sum the QD equations over energy groups and obtain equivalent one-group equations in which the cross sections and other constants are weighted averages of the fine-group values:

$$\frac{d\Phi_1}{dx}(x)+\tilde{\Sigma}_a(x)\Phi_0(x)=\frac{1}{k}\widetilde{\nu\Sigma}_f(x)\Phi_0(x)\ , \tag{8.37}$$

$$\frac{d}{dx}\left[E_{sum}(x)\Phi_0(x)\right]+\tilde{\Sigma}_t(x)\Phi_1(x)+\zeta(x)\Phi_0=0\ , \tag{8.38}$$

where

$$\Phi_k(x)\equiv\sum_{g=1}^{G}\phi_{k,g}(x)\ ,$$

$$E_{sum}(x)\equiv\frac{\sum_{g=1}^{G}E_g(x)\phi_{0,g}(x)}{\sum_{g=1}^{G}\phi_{0,g}(x)}\ ,$$

$$\tilde{\Sigma}_a(x)\equiv\frac{\sum_{g=1}^{G}\left[\Sigma_{t,g}(x)-\sum_{g'=1}^{G}\Sigma_{s,g\to g'}(x)\right]\phi_{0,g}(x)}{\sum_{g=1}^{G}\phi_{0,g}(x)}\ ,$$

$$\tilde{\Sigma}_t(x) \equiv \frac{\sum_{g=1}^{G} \Sigma_{t,g}(x)|\phi_{1,g}(x)|}{\sum_{g=1}^{G} |\phi_{1,g}(x)|} ,$$

$$\zeta(x) \equiv \frac{\sum_{g=1}^{G} \left[\Sigma_{t,g}(x) - \tilde{\Sigma}_t(x)\right] \phi_{1,g}}{\sum_{g=1}^{G} \phi_{0,g}(x)} .$$

The multigroup k-eigenvalue QD iteration begins with a guess for multigroup Eddington factors, E_g:

$$E_g^{(1/2)} = \text{guess} \quad (\text{usually} = 1/3 \text{ for each } g) .$$

One also has an initial guess for the energy shapes of $\phi_{0,g}^{(1/2,1/2)}$ and $\phi_{1,g}^{(1/2,1/2)}$. Then the iteration proceeds as follows, beginning with $\ell = s = 0$.

1. Compute the one-group constants from the latest energy shapes:

$$E_{sum}^{(s-1/2)}(x) \equiv \frac{\sum_{g=1}^{G} E_g^{(\ell-1/2)}(x)\phi_{0,g}^{(\ell-1/2,s-1/2)}(x)}{\sum_{g=1}^{G} \phi_{0,g}^{(\ell-1/2,s-1/2)}(x)} ,$$

$$\tilde{\Sigma}_a^{(s-1/2)}(x) \equiv \frac{\sum_{g=1}^{G} \left[\Sigma_{t,g}(x) - \sum_{g'=1}^{G} \Sigma_{s,g\to g'}(x)\right] \phi_{0,g}^{(\ell-1/2,s-1/2)}(x)}{\sum_{g=1}^{G} \phi_{0,g}^{(\ell-1/2,s-1/2)}(x)} ,$$

$$\tilde{\Sigma}_t^{(s-1/2)}(x) \equiv \frac{\sum_{g=1}^{G} \Sigma_{t,g}(x)|\phi_{1,g}^{(\ell-1/2,s-1/2)}(x)|}{\sum_{g=1}^{G} |\phi_{1,g}^{(\ell-1/2,s-1/2)}(x)|} ,$$

$$\zeta(x)^{(s-1/2)} \equiv \frac{\sum_{g=1}^{G} \left[\Sigma_{t,g}(x) - \tilde{\Sigma}_t(x)\right] \phi_{1,g}^{(\ell-1/2,s-1/2)}(x)}{\sum_{g=1}^{G} \phi_{0,g}^{(\ell-1/2,s-1/2)}(x)} .$$

2. Solve the one-group QD k-eigenvalue problem with the latest group constants:

$$\frac{\partial \Phi_1^{(s)}}{\partial x}(x) + \tilde{\Sigma}_a^{(s-1/2)}(x)\Phi_0^{(s)}(x) = \frac{1}{k^{(s)}} \widetilde{\nu\Sigma}_f^{(s-1/2)}(x)\Phi_0^{(s)}(x) , \tag{8.39}$$

$$\frac{d}{dx}\left[E_{sum}^{(s-1/2)}(x)\Phi_0^{(s)}(x)\right] + \tilde{\Sigma}_t^{(s-1/2)}(x)\Phi_1^{(s)}(x) + \zeta^{(s-1/2)}(x)\Phi_0^{(s)} = 0 . \tag{8.40}$$

This produces a new estimate of the eigenvalue and the fission source distribution.

3. Solve a fixed-source multigroup QD problem driven by the new fission source:

$$\frac{\partial \phi_{1,g}^{(\ell-1/2,s+1/2)}}{\partial x}(x) + \Sigma_{t,g}(x)\phi_{0,g}^{(\ell-1/2,s+1/2)}(x)$$

$$= \sum_{g'=1}^{G} \Sigma_{s,g'\to g}(x)\phi_{0,g'}^{(\ell-1/2,s+1/2)}(x) + \frac{\chi_g}{k^{(s)}}\widetilde{\nu\Sigma}_f^{(s-1/2)}(x)\Phi_0^{(s)}(x) \ , \tag{8.41}$$

$$\frac{d}{dx}\left[E_g^{(\ell-1/2)}(x)\phi_{0,g}^{(\ell-1/2,s+1/2)}(x)\right] + \Sigma_{t,g}(x)\phi_{1,g}^{(\ell-1/2,s+1/2)}(x) = 0 \ . \tag{8.42}$$

4. Return to step 1 with the iteration counter s incremented by one, unless it is judged to be time to update the Eddington factors, in which case proceed to the next step.

5. Perform a transport sweep in which the fission and scattering sources are known from the latest QD calculations.

$$\mu\frac{\partial \psi_g^{(\ell+1/2)}}{\partial x}(x,\mu) + \Sigma_{t,g}(x)\psi_g^{(\ell+1/2)}(x,\mu)$$

$$= \frac{1}{2}\sum_{g'=1}^{G} \Sigma_{s,g'\to g}(x)\phi_{0,g'}^{(\ell-1/2,s+1/2)}(x) + \frac{\chi_g}{k^{(s)}}\widetilde{\nu\Sigma}_f^{(s-1/2)}(x)\Phi_0^{(s)}(x) \ . \tag{8.43}$$

Use the resulting angular fluxes to generate multigroup Eddington factors. Increment the iteration counter ℓ by one and return to step 1.

This continues until further changes in the Eddington factors and multigroup spectra cause sufficiently small changes in k and the scalar flux.

Many variations are possible on the above iteration scheme, but all are built around the fundamental QD philosophy of doing as much of the needed work as possible in a setting with the fewest number of independent variables. In this case, one solves the k-eigenvalue equations in the one-group QD setting, which has no independent variables in angle and energy.

VIII.E. Synthetic Acceleration Methods for k-Eigenvalue Problems

When Alcouffe introduced his consistent DSA method for the DD equations, he proposed several variants [63]. One was the source-correction scheme, which is linear; this scheme formed the basis for much of the later DSA work. However, Alcouffe recognized that for the acceleration of eigenvalue iterations it is advantageous to formulate a low-order problem that is itself an eigenvalue problem for the desired scalar flux, as opposed to an equation with an additive driving term. One of his variants, therefore, was a nonlinear

scheme in which the diffusion coefficient and the removal cross section in a consistently differenced diffusion equation are defined as nonlinear (rational) functionals of the transport solution. (We remark that such nonlinear schemes do not fit the definitions of synthetic acceleration or preconditioning methods that we have used throughout this paper. Historically, however, they have been called nonlinear synthetic acceleration methods.) For the one-group problem, Eq. (8.1), Alcouffe's DSA for k-eigenvalue problems is a discretized version of the following. First, there are initial guesses for the diffusion coefficient and removal cross section:

$$D^{(1/2)}(x) = \frac{1}{3\Sigma_t(x)} \quad ,$$

$$\Sigma_a^{(1/2)}(x) = \Sigma_a(x) \quad .$$

Then the iteration proceeds as follows:

1. Solve a diffusion k-eigenvalue problem with "corrected" diffusion coefficient and/or removal cross section:

$$-\frac{d}{dx}D^{(\ell-1/2)}\frac{d\phi_0^{(\ell)}}{dx} + \Sigma_a^{(\ell-1/2)}(x)\phi_0^{(\ell)}(x) = \frac{1}{k^{(\ell)}}\nu\Sigma_f(x)\phi_0^{(\ell)}(x) \quad . \tag{8.44}$$

   This discrete equation is solved using the discretization that is *consistent* with the DD transport discretization. (See Section III.B.)

2. Perform a transport sweep (with scattering and fission sources known from previous step), and generate a new corrected diffusion coefficient:

$$\mu\frac{\partial\psi^{(\ell+1/2)}}{\partial x}(x,\mu) + \Sigma_t(x)\psi^{(\ell+1/2)}(x,\mu) = \frac{\Sigma_s(x)}{2}\phi^{(\ell)}(x) + \frac{1}{k^{(\ell)}}\frac{\nu\Sigma_f(x)}{2}\phi^{(\ell)}(x) \quad , \tag{8.45}$$

$$D^{(\ell+1/2)}(x) = -\frac{\phi_1^{(\ell+1/2)}}{\left(\frac{d\phi_0^{(\ell+1/2)}}{dx}\right)} \quad . \tag{8.46}$$

   These equations are solved in discrete form using the DD discretization. Obviously, Eq. (8.46) can produce a negative or very large diffusion coefficient, which causes difficulties in the diffusion solution; to circumvent this, Alcouffe devised a nonlinear correction to the removal cross section. In practice (in the DANT series of codes [232]), Alcouffe's algorithm proceeds as follows when Eq. (8.46) produces an unacceptably large or negative diffusion coefficient:

$$D^{(\ell+1/2)}(x) = \frac{1}{3\Sigma_t(x)} \quad ,$$

$$\Sigma_a^{(\ell+1/2)}(x) = \Sigma_a(x) + \frac{\frac{d\phi_1^{(\ell+1/2)}}{dx} + \frac{d}{dx}\frac{1}{3\Sigma_t}\frac{d\phi_0^{(\ell+1/2)}}{dx}}{\phi_0^{(\ell+1/2)}} \quad . \tag{8.47}$$

During the iterative process in some problems, it is possible for Eq. (8.47) to generate a negative cross section in some cells. In practice in the DANTSYS codes, this is permitted unless it causes the discrete diffusion matrix to lose diagonal dominance. In such cases (which are rare in practice) the code simply turns off the acceleration in the offending energy group, and later turns it back on if and when diagonal dominance is restored. [287].

This process continues until convergence. For multidimensional problems, Alcouffe defines a diagonal diffusion tensor:

$$D_{uu}^{(\ell-1/2)} = -\frac{\phi_1^{(\ell-1/2)}}{\left(\frac{\partial \phi_0^{(\ell-1/2)}}{\partial u}\right)} , \tag{8.48}$$

where u is x, y, or z.

In [232], Alcouffe presented results from three two-dimensional k-eigenvalue test problems, comparing his DSA algorithm against fine-mesh and coarse-mesh rebalance. CMR diverged for the first two problems and required 369 iterations for the third; FMR required 48, 143, and 149 iterations for the three problems; DSA required 17, 24, and 80 iterations [63]. Alcouffe's DSA algorithm for the DD equations is implemented in the DANT code series [92], which has been widely used for decades to solve both fixed-source and eigenvalue problems. In recent versions of these codes, this DSA algorithm is employed for spatial discretization schemes other than DD, including linear discontinuous and linear nodal. However, for those schemes the diffusion discretization employed in the codes is not consistent, and it is used to accelerate only the cell-*averaged* scalar fluxes (not slopes). It therefore "quickly loses its effectiveness when the slope terms are important" in these non-DD schemes [287].

We now compare the QD scheme and Alcouffe's DSA scheme for k-eigenvalue problems. Alcouffe's diffusion-correction scheme is somewhat reminiscent of QD, in that the diffusion leakage term is transport-corrected. However, QD's nonlinear functional is stable and well-behaved, whereas the DSA functional can become negative or infinite. Either of these circumstances forces use of the *removal-correction* scheme. The DSA low-order problem is a true diffusion problem, and its matrix is symmetric positive definite; the QD equations are not symmetric and are thus more difficult to solve in general. The DSA scheme produces the unaccelerated solution, whereas QD does not. On the other hand, QD does not require consistent discretization. (See Section III.G.) Finally, both methods require the solution of low-order eigenvalue problems.

We have mentioned that eigenvalue problems are most naturally "accelerated" using low-order equations that are themselves eigenvalue problems. All such low-order eigenvalue problems that have been proposed make use of nonlinear functionals of the transport

solution. As a result, these methods require positive transport solutions, which almost always translates into a requirement for a negative-flux fixup in the transport algorithm. This has two unfortunate consequences. First, in eigenvalue problems, negative flux fixups tend to decrease solution accuracy. Second, fixups can cause a transport discretization to be inconsistent with a diffusion discretization that was carefully constructed to be consistent.

It is possible to devise DSA algorithms for k iterations without introducing nonlinearities and thus without forcing negative fluxes to be "fixed". Gelbard et al. created such a linear scheme and showed that it remained robust and fast (without negative flux fixups), even on problems for which negative fixups caused the DANT DD code to fail [81]. This scheme requires the solution of one adjoint low-order eigenvalue problem, and for each DSA iteration it requires the solution of a low-order problem with a singular operator.

VIII.F. Summary of Chapter VIII

With nonlinear methods (such as QD or DSA with a diffusion correction), eigenvalue problems can be accelerated in a relatively straightforward way. It is more difficult to devise linear methods for such problems, but this too can be done. With nonlinear methods, each "synthetic" iteration requires the solution of a low-order k-eigenvalue problem. This problem can be solved with PI or SPI iterations, possibly with Chebyshev or some other form of algebraic acceleration. Finally, we note that historically, much more effort has been spent on developing methods for accelerating the iterative convergence of fixed-source problems than on eigenvalue problems.

IX. DISCUSSION

This Review aims to provide a useful introduction to iterative acceleration methods for large-scale discrete-ordinates particle transport calculations. Chapter I describes the main historical events pertaining to this field. Chapters II and III present a "tutorial," to introduce the fundamental ideas that have led to important technical advances. Chapters IV-VIII discuss acceleration techniques associated with multidimensional geometries, advanced differencing schemes, unstructured spatial grids, etc.

In this Review, we have stressed the desire for methods that will accelerate robustly and efficiently for particle transport problems that are more difficult than nuclear reactor problems – problems containing spatial subregions with spatial cells that are *many* mean free paths thick, and with scattering ratios that are *exceedingly* close to unity. However, there are important problems in which acceleration is greatly needed, but the physical parameters are not so extreme. One common example is the simulation of neutron transport in nuclear reactors and shields. For these problems, spatial cells are typically on the order of

one mean free path in thickness, or less. If a code user is confident that a given discretized problem has spatial grids that are not optically thick, then there is no need to employ an acceleration method that is (unnecessarily complex because it is) designed to work effectively for problems with optically thick grids. Thus, acceleration methods that work well in the fine-mesh limit, but that degrade to the performance of source iteration for optically thick spatial cells, are viable candidates for efficient acceleration schemes for typical nuclear reactor problems. One example of such a scheme is DSA with (i) the diamond-differenced S_N equations, and (ii) a cell-edge diffusion equation employing a one-point removal term. This method, in 1-D geometry, is discussed in detail in Chapter III. Other "inconsistent" DSA schemes involving the diamond-differenced S_N equations in X,Y-geometry were studied in [156]. (This work was motivated by the slightly inconsistent form of DSA that is actually implemented in the DANT code.) A related method for DSA with the Linear Discontinuous differencing scheme in 1-D and 1-D geometries was developed in [167].

We have also stressed that linear and nonlinear acceleration schemes are often closely related. (For each nonlinear scheme, there seems to be a corresponding linear scheme, which can be derived by linearizing the nonlinear scheme around the flat infinite medium solution.) Linear schemes usually:

- involve a low-order (preconditioning) equation for an additive correction to the latest S_N iterate,
- if they converge, converge to the solution of the unaccelerated (source-iteration) equations (the converged numerical solution does not change),
- for unconditional convergence, require the low-order preconditioning equation to be discretized *consistently* with the discretization of the high-order transport sweeps,
- do not require the numerical solution to be positive (although, physically, it should be positive),
- are natural to apply to source-detector problems, but are not natural for eigenvalue problems.

Nonlinear schemes, on the other hand, usually:

- are not equivalent to preconditioning, and involve a low-order equation for the transport solution,
- produce *two* estimates for the solution (one from the high-order transport sweeps, one from the low-order equation), which usually differ from each other and from the unaccelerated solution by truncation errors,
- do not, for rapid convergence, require the low-order equations to be discretized consistently with the high-order equations (although, if the high and low-order equations *are* discretized consistently, then the two scalar flux estimates are identical and equal to the unaccelerated solution),

- generally require the converged solution and all iterates leading to this solution to be positive,
- are natural to apply to both source-detector and eigenvalue problems.

Thus, the linear and nonlinear acceleration schemes are somewhat complementary in terms of advantages and disadvantages.

An unfortunate aspect of DSA, which has been discussed already, is that as the spatial discretization scheme and the problem geometry become more complex, the implementation of a stable, efficient DSA method becomes more problematic. Here we wish to make one final observation concerning this fact. Typical advanced S_N differencing schemes involve a greater number of unknowns per spatial cell than simple S_N schemes. Often, low-order DSA equations are proposed for the advanced high-order S_N schemes that contain fewer scalar-flux unknowns per cell than the high-order S_N equations. Such low-order equations may be relatively easy to solve, but for some difficult problems, they can be incapable of producing a satisfactorily small overall spectral radius. On the other hand, low-order equations with the same number of scalar flux equations per cell as the high-order equations may yield a satisfactory overall spectral radius, yet be so expensive to solve that the overall cost is unacceptable [300]. Thus, while advanced spatial differencing schemes are more accurate, they usually involve multiple unknowns per cell; this adds to the basic storage and algebraic cost of implementing the scheme, and it *greatly* adds to the difficulties of DSA acceleration, particularly in multiple space dimensions.

Many open questions remain concerning practical iterative methods for transport problems. One that recently came to light is that the performance of DSA, even with fully consistent spatial discretizations, can degrade substantially in multidimensional problems with severe spatial heterogeneities. Azmy and co-authors have demonstrated this by Fourier analysis and by numerical results [260]. These authors showed numerically that spectral radii can grow as large as 0.88, even with methods that, for homogeneous problems, always produce spectral radii smaller than 1/3. We are not aware of a remedy to this interesting degradation.

A second general question pertains to the implementation of rapidly converging iterative transport schemes on massively parallel systems of computers. Is it possible to do this in a way that preserves *scalability*, i.e. does not degrade in parallel performance as the number of processors becomes very large? The answer to this question may be closely linked to the ability to solve elliptic equations efficiently on massively parallel systems. (This, of course, is because efficiently solving discrete diffusion problems is the basis of many of the rapidly converging transport iterative schemes.) At the present time, this is an active field of research.

Other open questions in the field of transport acceleration methods are related to the

solution of multidimensional transport problems on unstructured spatial grids. However, even for less-complicated problems, there is strong interest in new discretization methods that are more accurate, and new iteration methods that are efficient and easy to implement. We have tried to indicate in this Review that there is significant ongoing work on the development of alternative methods that seem to have the potential to overcome difficulties associated with present methods.

For example, *spatial multigrid* has found an extraordinarily wide audience in the mathematics and computational physics community. This method is still being extended and tested for multidimensional transport problems, but it is not yet known how efficient multigrid can be made for these applications.

A similar statement holds for the application of the Quasidiffusion method to radiative transfer problems. This method seems to have significant promise, but there is not a wealth of accessible literature on various issues associated with this application.

A trend that has received increasing attention for difficult problems – ones with, perhaps, severe spatial discontinuities, unstructured spatial grids, or even a slightly inconsistent acceleration scheme – is to employ an algebraic iterative method such as Conjugate Gradient (CG) or GMRES "outside of" DSA (i.e., to use CG or GMRES with a diffusion preconditioner). If the sweep + preconditioner has only "a few" slowly-converging or unstable error modes, then this approach can be quite advantageous. However, it remains true that for maximum overall efficiency, the diffusion preconditioner should suppress the maximum number of slowly converging error modes, without causing other modes to become slowly-converging or unstable, at the minimum cost. (If the diffusion preconditioner efficiently suppresses *all* error modes, then it is unnecessary – but probably not harmful – to combine it with an algebraic method such as CG or GMRES.)

Finally, we wish to emphasize two aspects of this Review that are of considerable importance to the authors – our attempts to (i) provide a complete list of English-language references on S_N acceleration schemes, and (ii) do justice to the extensive research on this topic performed since the early 1960's in the former Soviet Union.

In compiling the references for this Review (cited below), we performed an extensive search through the English-language technical literature. To our knowledge, the list of such references given below is complete, up to the time of the writing of this Review. Also, there has been significant work published on S_N acceleration schemes in the Russian literature, and we have tried to include in this reference list the most significant of these publications.

Unfortunately, little of the Russian-literature work is known in the west – even though a fair amount of it has been published in English – so this work has had relatively little influence on western research. However, the opening of communications between "east" and "west" that began a decade ago has had a beneficial effect on western awareness of

this research. We believe that it is now possible to place the Russian-literature work in a reasonable historical perspective, and we have attempted to do this in the present Review. In particular, it is now clear that during the 1960's, the research groups headed by Lebedev and Gol'din developed an understanding of the problem that was well in advance of western thinking. Either by insight or by serendipity, these two groups avoided the difficulties of "consistent discretization" between the high-order and low-order equations. Gol'din's group worked with QD, which does not require consistent discretization; Lebedev's group worked with the even-parity equations (for which a consistent diffusion discretization occurs naturally) or with very fine spatial meshes (for which a consistent discretization is not necessary). Thus, this early work did not (and did not need to) discuss the issue of numerical stability as a function of the size of the spatial grid. In the west, attention has historically been focused on synthetic acceleration, which *does* require some form of consistency between the high-and low-order discretizations, and on first-order forms of the S_N equations, for which consistent discretization is difficult. Thus, much of the western work since Alcouffe's publications in the mid-1970's has dealt with the subject of consistent discretization of the low-order operator. In the present Review, we have attempted to explain the differences and similarities in the "western" and "Russian" approaches. We wish to apologize for any omissions or errors, which we hope are minor.

In conclusion, we have tried in this Review to show that the subject of acceleration methods for particle transport simulations is a rich and self-consistent field, overlapping numerical analysis, computational physics, and nuclear engineering. We hope that that the Review will enable researchers and students to work on this subject more easily, and thereby help to advance it. In the future, this field may become very different, with discretization methods that are more accurate and iteration methods that are more efficient. Changes in computer architecture may drive some of these advances. However, even if all this change occurs, it seems likely that future simulation methods will be based on principles that, at least in part, are known today. It will be gratifying if this Review conntributes to the development of such methods.

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REFERENCES

General References

[1] Bell G.I. and Glasstone S. (1970) *Nuclear Reactor Theory*, Van Nostrand Reinhold, New York.

[2] Briggs W.L., Henson V.E., and McCormick S.F. (2000) "A Multigrid Tutorial," 2nd ed., SIAM, Philadelphia.

[3] Case K.M. and Zweifel P.F. (1967) *Linear Transport Theory*, Addison-Wesley, Reading, Mass.

[4] Davison B. (1957) *Neutron Transport Theory*, Oxford University Press, London.

[5] Duderstadt J.J. and Martin W.R. (1979) *Transport Theory*, Wiley-Interscience, New York.

[6] Greenbaum A. (1997) *Iterative Methods for Solving Linear Systems*, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, pp. 134-146.

[7] Hackbush W. (1994) *Iterative Solution of Large Sparse Systems of Equations*, Springer-Verlag, New York.

[8] Hageman L.A. and Young D.M. (1981) *Applied Iterative Methods*, Academic Press, New York.

[9] Lewis E.E. and Miller W.F., Jr. (1984) *Computational Methods of Neutron Transport*, Wiley-Interscience, New York. [Reprinted (1993). American Nuclear Society, LaGrange Park, Illinois.]

[10] Marchuk G.I. and Lebedev V.I. (1986) *Numerical Methods in the Theory of Neutron Transport*, Second Revised Edition, Harwood Academic Publishers, London. [Originally published (1971) in Russian by Isdatel'stvo Atomizdat, Moscow.]

[11] McCormick S. (editor) (1987) *Multigrid Methods*, Society for Industrial and Applied Mathematics, Philadelphia.

[12] Mihalas D. and Mihalas B. (1984) *Foundations of Radiation Hydrodynamics*, Oxford University Press, Oxford, 374-378.

[13] Samarsky A.A. (1971) *Introduction to the Theory of Difference Algorithms*, Publ. House "Nauka," Moscow (in Russian). See also: Samarsky A.A. and Nikolaev E.S. (1989) *Numerical Methods for Grid Equations, Vol. II: Iterative Methods*, Birkhauser, Basel.

[14] Stacey W.M. (2001) *Nuclear Reactor Physics*, Wiley-Interscience, New York.

[15] Wachspress E.L. (1966) *Iterative Solution of Elliptic Systems and Applications to the Neutron Diffusion Equations of Reactor Physics*, Prentice-Hall, Englewood Cliffs, New Jersey.

1900-59

[16] Eyges L. (1948) "Multiple Scattering with Energy Loss," *Phys. Rev.* **74**, 1534.

[17] Fermi E., cited in Rossi B. and Griessen K. (1949) "Cosmic Ray Theory," *Rev. Mod. Phys.* **13**, 240. (Fermi's work is cited on pp. 265-268.)

[18] Kuznetsov E.S. (1940). "On the Establishment of Equilibrium of Radiant Energy in an Absorbing and Scattering Atmosphere," *Izv. AN SSSR, Sev. Geol. and Geophysics.*, 813-842 (in Russian).

[19] Lyusternik L.A. (1947) "Remarks on Numerical Solution of the Boundary Value Problems for Laplace Equation and Calculation of Eigenvalues by the Mesh Method," *Trudy Matem. Inst. An. USSR* **20**, 49.

[20] Schmidt E. (1907) "Auflosung der allgemeiner linearen integralgleichungen," *Math. Ann.* **64**, 161 (in German).

[21] Vorobyov Yu.V. (1958). "Method of Moments in Applied Mathematics, Moscow, State Publishing House of Physical and Mathematical Literature (in Russian). English translation published by Gordon and Breach Science Publishers in *Russian Monographs and Texts on Advanced Mathematics and Physics* **9** (1965).

1960-64

[22] Crawford B.W. and Chambre P.L. (1964) "An Iterative Solution Method for the Neutron Transport Equation with Anisotropic Scattering," *Trans. Am. Nucl. Soc.* **7**, 254.

[23] Crawford B.W. and Friedman J.P. (1965) "A Two-Dimensional Application of an Iterative Method for Solving the Neutron Transport Equation with Anisotropic Scattering," *Trans. Am. Nucl. Soc.* **9**, 254.

[24] Feautrier P. (1964) "On the Numerical Solution of the Equation of Transfer," *Comptes Rendus Acad. Sci. Paris* **258**, 3189 (in French).

[25] Gol'din V.Ya. (1964) "A Quasi-Diffusion Method for Solving the Kinetic Equation," *Zh. Vych. Mat. I Mat. Fiz.* **4**, 1078 (in Russian). English translation published in: (1967) *USSR Comp. Math. and Math. Phys.* **4**, 136.

[26] Kopp H.J. (1963) "Synthetic Method Solution of the Transport Equation," *Nucl. Sci. Eng.* **17**, 65.

[27] Lebedev V.I. (1964) "The Iterative *KP* Method for the Kinetic Equation," Proc. *Conf. on Mathematical Methods for Solution of Nuclear Physics Problems*, Nov. 17-20, 1964, Dubna, 93 (in Russian).

[28] Morozov V.N. (1962) "On Solution of Kinetic Equations by the S_n Method," *Theory and Design of Nuclear Reactors*, Gosatomizdat, Moscow, p. 91 (in Russian).

[29] Pomraning G.C. and Clark M., Jr., "The Variational Method Applied to the Monoenergetic Boltzmann Equation. Part II," *Nucl. Sci. Eng.* **16**, 155.

[30] Vladimirov V.S. (1961) "Mathematical Problems in the One-Velocity Theory of Particle Transport," *Transactions of V.A. Steklov Mathematical Institute*, USSR Academy of Sciences, **61**. English translation published (as Tech. Report AECL-1661) by Atomic Energy of Canada Limited in 1963.

1965-69

[31] Froelich R. (1967) "A Theoretical Foundation for Coarse Mesh Variation Techniques," GA-7870, General Atomic (1967).

[32] Gelbard E.M. and Hageman L.A. (1969) "The Synthetic Method as Applied to the S_N Equations," *Nucl. Sci. Eng.* **37**, 288.

[33] Germogenova T.A. (1968) "Convergence of Some Approximate Methods of Solving the Transport Equation," *Soviet Math. Dokl.* **9**, 4, 855.

[34] Germogenova T.A. and Sushkevich T.A. (1969) "Solution of the Transport Equation by Means of the Method of Averaged Fluxes," *Problems of Shielding Physics*, Atomizdat, Moscow, **3**, 34 (in Russian).

[35] Gol'din V.Ya., Danilova G.V., and Chetverushkin B.N. (1969) "Approximate Method of Solving the Time-Dependent Kinetic Equation," Computational Methods in Transport Theory, Atomizdat, Moscow, 50-57 (in Russian).

[36] Lebedev V.I. (1966) "On Finding Solutions of Kinetic Problems," *USSR Comp. Math. and Math. Phys.* **6**, 895.

[37] Lebedev V.I. (1967) "An Iterative *KP* Method," *USSR Comp. Math. and Math. Phys.* **7**, 1250.

[38] Lebedev V.I. (1968) "Problem of the Convergence of a Method of Estimating Iteration Deviations," *USSR Comp. Math. and Math. Phys.* **8**, 1377.

[39] Lebedev V.I. (1969) "Convergence of the *KP* Method for Some Neutron Transfer Problems," *USSR Comp. Math. and Math. Phys.* **9**, 226.

[40] Lebedev V.I. (1969) "Construction of the *P* Operation in the *KP* Method," *USSR Comp. Math. and Math. Phys.* **9**, 762.

[41] Nikolaishvilli Sh.S. (1966) "On Solution of One-Velocity Transport Equation Based on Yvon-Mertens Approximation," *At. Energy* **20**, 344.

[42] Troshchiev V.E., Yudintsev V.F., and Fedyanin V.I. (1968) "Acceleration of the Convergence of Iterations in Solving the Kinetic Equation," *USSR Comp. Math. and Math. Phys.* **8**, 2, 298.

1970-74

[43] Gol'din V.Ya. and Chetverushkin B.N. (1972) "Methods of Solving One-Dimensional Problems of Radiation Gas Dynamics," *USSR Comp. Math. and Math. Phys.* **12**, No. 4, 177.

[44] Gol'din V.Ya. and Kalitkin N.N. (1973). "A Nonlinear Method for Determining of Critical Parameters of One-Dimensional Reactor," *USSR Comp. Math. and Math. Phys.*, **13**, No. 2.

[45] Kellogg R.B. (July, 1974) "First Derivatives of Solutions of the Plane Neutron Transport Equation," Technical Note BN-783, Institute for Fluid Dynamics and Applied Mathematics, University of Maryland.

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

[47] Lebedev V.I. and Finogenov S.A. (1971) "On the Order of Choosing Iteration Parameters in the Chebyshev Cyclic Iteration Method," *USSR Comp. Math. and Math. Phys.* **11**, 155.

[48] Lebedev V.I. and Finogenov S.A. (1973) "Solution of the Problems of Parameter Ordering in Chebyshev Iterative Methods, *USSR Comp. Math. and Math. Phys.* **13**, 21.

[49] Meneley D.A. (1971) "Acceleration of External Source Problems in Near-Critical Systems," Applied Physics Division Annual Report: July 1, 1970, to June 30, 1971, ANL-7910, 513-515, Argonne National Laboratory.

[50] Painter J.W., Ryden R.A., and Metcalf D.R. (1974) "Convergence Acceleration of Inner Iterations Using a Modified Synthetic Method," *Trans. Am. Nucl. Soc.* **18**, 143.

[51] Reed W.H. (1971) "The Effectiveness of Acceleration Techniques for Iterative Methods in Transport Theory," *Nucl. Sci. Eng.* **45**, 245.

[52] Rybicki G.B. (1971) "A Modified Feautrier Method," *J. Quant. Spectrosc. Radiat. Transfer* **11**, 589.

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

1975

[54] Alcouffe R.E. and Lewis E.E. (1975) "Synthetic Acceleration Methods for the Neutron Transport Equation," LA-UR-75-1561, Los Alamos Scientific Laboratory; also published in: (Nov. 1975) Proc. IAEA Specialist Meeting, *Methods of Neutron Transport Theory in Reactor Calculations*, Bologna, Italy, CONF-751152, International Atomic Energy Agency.

[55] Allen R.C. and Wing G.M., Jr. (1975) "A Study of the Synthetic Method as Applied to the Transport Equation in Slab Geometry - Some Analytical and Numerical Results," LA-UR-75-1104, Los Alamos Scientific Laboratory.

[56] Wing G.M., Jr. (1975) "An Analysis of the Synthetic Method of Transport Theory for the Case of Slab Geometry," LA-UR-75-1031, Los Alamos Scientific Laboratory.

1976

[57] Alcouffe R.E. (1976) "A Stable Diffusion Synthetic Acceleration Method for Neutron Transport Iterations," *Trans. Am. Nucl. Soc.* **23**, 203.

[58] Calahan J.E. (1976) "An Iterative Diffusion Theory Method for the Incorporation of Transport Effects in Fast Reactor Safety Neutronics," ANL/RAS 76-17, Argonne National Laboratory.

[59] Calahan J.E., Ott K.O., and Ferguson D.R. (1976) "A Nonlinear Iterative Diffusion-Transport Solution Technique for LMFBR Neutronics," *Trans. Am. Nucl. Soc.* **23**, 203.

[60] Gol'din V.Ya., Kuzyuk V.A., and Rakhmatulina A.K. (1976). "Nonlinear Method of Electron Transport Calculation," *USSR Comp. Math. and Math. Phys.* **16**, No. 2, 131.

[61] Lewis E.E. and Miller W.F., Jr. (1976) "A Comparison of P_1 Synthetic Acceleration Techniques," *Trans. Am. Nucl. Soc.* **23**, 202.

1977

[62] Alcouffe R.E. (1977) "The Diffusion Synthetic Acceleration Method Applied to Two-Dimensional Neutron Transport Problems," *Trans. Am. Nucl. Soc.* **27**, 346.

[63] Alcouffe R.E. (1977) "Diffusion Synthetic Acceleration Methods for the Diamond-Differenced Discrete-Ordinates Equations," *Nucl. Sci. Eng.* **64**, 344.

[64] Miller W.F., Jr. (1977) "Generalized Rebalance: A Common Framework for Transport Acceleration Methods," *Trans. Am. Nucl. Soc.* **27**, 346.

[65] Manteuffel T.A. (1977) "The TChebyshev Iteration for Nonsymmetric Linear Systems," *Numer. Math.***28**, 307.

1978

[66] Allen R.C. and Wing G.M., Jr. (1978) "A Method for Accelerating the Iterative Solution of a Class of Fredholm Integral Equations," *J. Optimization Th. Appl.* **24**, 5.

[67] Kuznetsov Yu.A. (1978). "On Symmetrization of Approximate Problems in the Transport Theory," *Computational Methods in Applied Mathematics, Geophysics and Optimal Control*, CC SB USSR Academy of Science, Novosibirsk, p. 125.

[68] Mihalas D. (1978) *Stellar Atmospheres* (second edition), Freeman, San Francisco.

[69] Miller W.F., Jr. (1978) "Generalized Rebalance: A Common Framework for Transport Acceleration Methods," *Nucl. Sci. Eng.* **65**, 226.

[70] Manteuffel T.A. (1978) "Adaptive Procedure for Estimating Parameters for the Nonsymmetric TChebyshev Iteration," *Numer. Math.* **31**, 183.

1979

[71] Aksenov N.N. and Gol'din V.Ya. (1979) "Computing of Two-Dimensional Steady Equation of Neutron Transport by Quasi-Diffusion Method," *USSR J. Comp. Math. and Math. Phys.* **19**, No. 5, 1341.

[72] Aull J.E. (1979) "The Stability of the Mesh-Cornered Synthetic Method of Diffusion Acceleration of the DOT-IV Transport Code," ORNL/TM-7097, Oak Ridge National Laboratory.

[73] Aull J.E., Rhoades W.A., and Dodds H.L. (1979) "A Modified Approach to Diffusion Acceleration in Neutron Transport Problems," *Trans. Am. Nucl. Soc.* **32**, 306.

[74] Rhoades W.A., Simpson D.B., Childs R.L., and Engle W.W., Jr. (1979) "The DOT-IV Two-Dimensional Discrete Ordinates Transport Code with Space-Dependent Mesh and Quadrature," ORNL/TM-6529, Oak Ridge National Laboratory.

[75] Rhoades W.A. and Tomlinson E.T. (1979) "Effectiveness of Three Rebalance Methods in Deep Penetration Problems," *Trans. Am. Nucl. Soc.* **33**, 717.

1980

[76] Aull J. (1980) "Acceleration of the Inner Iteration of the DOT-IV Transport Code Using a New Source-Correction Scheme," ORNL/TM-7404, Oak Ridge National Laboratory.

1981

[77] Alcouffe R.E., Brandt A., Dendy J.E., Jr., and Painter J.W. (1981) "The Multi-Grid Method for the Diffusion Equation with Strongly Discontinuous Coefficients," *SIAM J. Sci. Stat. Comput.* **2**, 430.

[78] Gelbard E.M., McCoy D.R., and Larsen E.W. (1981) "Finite Difference Effects in the Synthetic Acceleration Method," *Trans. Am. Nucl. Soc.* **39**, 462.

[79] Larsen E.W. and McCoy D.R. (1981) "An Unconditionally Stable Acceleration Method for Arbitrary Weighted Diamond Differencing Schemes," *Trans. Am. Nucl. Soc.* **39**, 469.

1982

[80] Derstine K.L. (1982) "DIF3D: A Code to Solve One-, Two-, and Three-Dimensional Finite-Difference Diffusion Theory Problems," Argonne National Laboratory Report ANL-82-64.

[81] Gelbard E.M., Adams C.H., McCoy D.R., and Larsen E.W. (1982) "Acceleration of Transport Eigenvalue Problems," *Trans. Am. Nucl. Soc.* **41**, 309.

[82] Gol'din V.Ya. (1982) "On Mathematical Modeling of Problems of Continuous Medium with Non Equilibrium Transfer," *Modern Problems of Mathematical Physics and Computational Mathematics*, Nauka, Moscow, 113 (in Russian).

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

[84] Larsen E.W. (1982) "Unconditionally Stable Diffusion Acceleration of the Transport Equation," *Transport Theory Statist. Phys.* **11**, 29.

[85] McCoy D.R. and Larsen E.W. (1982) "Unconditionally Stable Diffusion Synthetic Acceleration Methods for the Slab Geometry Discrete-Ordinates Equations. Part II: Numerical Results," *Nucl. Sci. Eng.* **82**, 64.

[86] Morel J.E. (1982) "A Synthetic Acceleration Method for Discrete Ordinates Calculations with Highly Anisotropic Scattering," *Nucl. Sci. Eng.* **82**, 34.

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

1983

[88] Alcouffe R.E. (1983) "The Multigrid Method for Solving the Two-Dimensional Multigroup Diffusion Equation," Proc. ANS Topical Meeting, *Advances in Reactor Computations*, March 28-30, 1983, Salt Lake City, **1**, 340.

[89] Gelbard E.M. and Khalil H. (1983) "Alternative Differencing Technique for the Synthetic Method," *Trans. Am. Nucl. Soc.* **45**, 322.

[90] Larsen E.W. (1983) "Rapidly Convergent Iterative Methods for Numerical Transport Problems," *Trans. Am. Nucl. Soc.* **45**, 317.

[91] Larsen E.W. (1983) "Diffusion Synthetic Acceleration Methods for Discrete-Ordinates Equations," Proc. ANS Topical Meeting, *Advances in Reactor Computations*, March 28-31, 1983, Salt Lake City, **2**, 705.

1984

[92] Alcouffe R.E., Brinkley F.W., Marr D.R., and O'Dell R.D. (October, 1984) "User's Guide for TWODANT: A Code Package for Two-Dimension, Diffusion Accelerated, Neutral- Particle Transport," Los Alamos National Laboratory manual LA-10049-M, Rev. 1.

[93] Larsen E.W. (1984) "Diffusion Synthetic Acceleration Methods for Discrete Ordinates Problems," *Transport Theory Statist. Phys.* **13**, 107.

[94] Larsen E.W. (October, 1984) "Acceleration of High-Order S_N Equations Using Low Order S_N Equations," LA-10189-PR (Progress Report, Radiation Transport, April 1, 1983 - December 31, 1983, R.D. O'Dell, editor), Los Alamos National Laboratory, p. 40.

[95] Morel J.E. and Montry G.R. (1984) "Analysis and Elimination of the Discrete Ordinates Flux Dip," *Transport Theory Statist. Phys.*, **13**, 615.

[96] Williams M. (1984) "The Acceleration of Anisotropic Transport Iterations," *Transport Theory Statist. Phys.* **13**, 127.

1985

[97] Alcouffe R.E., Clark B.A., and Larsen E.W. (1985) "The Diffusion Synthetic Acceleration of Transport Iterations with Application to a Radiation Hydrodynamics Problem," in *Multiple Time Scales*, J. Brackbill and B. Cohen, eds., Academic Press, Orlando, Florida, 73.

[98] Azmy Y.Y. and Dorning J.J. (1985) "Diffusion Synthetic Acceleration of the Multidimensional Discrete Nodal Transport Method," Proc. ANS *International Meeting on Advances in Nuclear Engineering Computational Methods*, April 9-11, 1985, Knoxville, Tennessee, **2**, 440.

[99] Clark B.A. (1985) "Nonlinear DSA Schemes for Radiative Transfer Applications," Proc. ANS *International Meeting on Advances in Nuclear Engineering Computational Methods*, April 9-11, 1985, Knoxville, Tennessee, **2**, 426.

[100] Derstine K.L. and Gelbard E.M. (1985) "Use of the Preconditioned Conjugate Gradient Method to Accelerate S_N Iterations," *Trans. Am. Nucl. Soc.* **50**, 260.

[101] Khalil H. (1985) "A Nodal Diffusion Technique for Synthetic Acceleration of Nodal S_N Calculations," *Nucl. Sci. Eng.* **90**, 263.

[102] Larsen E.W. (1985) "Projected Discrete Ordinates Methods for Numerical Transport Problems," Proc. ANS *International Meeting on Advances in Nuclear Engineering Computational Methods*, April 9-11, 1985, Knoxville, Tennessee, **2**, 413.

[103] Morel J.E., Larsen E.W., and Matzen M.K. (1985) "A Synthetic Acceleration Scheme for Radiative Diffusion Calculations," *J. Quant. Spectrosc. Radiat. Transfer* **34**, 243.

1986

[104] Adams M.L. and Martin W.R. (1986) "A New Approach to Synthetic Acceleration of Transport Calculations," *Trans. Am. Nucl. Soc.* **53**, 282.

[105] Anistratov D.Y. and Gol'din V.Ya. (1986) "Difference Scheme Comparison for Quasi-Diffusion Transport System of Equations," *Questions of Nuclear Science and Engineering (VANT)*, 2nd issue: Methods and Programs of Numerical Solving of Problems in Mathematical Physics, 17 (in Russian).

[106] Bass L.P, Voloshchenko A.M., and Germogenova T.A. (1986). "Methods of Discrete Ordinates in Radiation Transport Problems," preprint, Keldysh Institute of Applied Mathematics, Moscow, USSR, 231 pages (in Russian).

[107] Brandt, A. (1986) "Algebraic Multigrid Theory: The Symmetric Case," *Appl. Math. Comput.* **19**, 23.

[108] Gol'din V.Ya., Gol'dina D.A., Kolpakov A.V., and Shilkov A.A. (1986) "Mathematical Modeling of Gas Dynamic Processes with High Radiation Energy Densities," Problems of Atomic Science and Engineering: Methods and Codes for Numerical Solution of Mathematical Physics Problems, No. 2, 59 (in Russian).

[109] Larsen E.W. (1986) "Projected Discrete Ordinates Methods for Numerical Transport Problems," *Nucl. Sci. Eng.* **92**, 179. (This is an expanded version of [102].)

[110] Larsen E.W. and Miller W.F., Jr. (1986) "A Two-Step Acceleration Method for Transport Problems," *Trans. Am. Nucl. Soc.* **52**, 416.

[111] Lawrence R.D. (1986) "An Interface-Current Approach to Synthetic Acceleration of Three-Dimensional Discrete-Ordinates Transport Methods," *Trans. Am. Nucl. Soc.* **53**, 280.

[112] Lazo M.S. and Morel J.E. (1986) "A Linear Discontinuous Galerkin Approximation for the Continuous Slowing Down Operator," *Nucl. Sci. Eng.* **92**, 98.

[113] Lorence L.J., Jr., Larsen E.W., and Morel J.E. (1986) "An S_2 Synthetic Acceleration Scheme for the One-Dimensional S_N Equations," *Trans. Am. Nucl. Soc.* **52**, 417.

[114] Miller W.F., Jr. and Larsen E.W. (1986) "Modified Diffusion Synthetic Acceleration Algorithms," *Nucl. Sci. Eng.* **93**, 403.

[115] Olson G.L., Auer L.H., and Buchler J.R. (1986) "A Rapidly Convergent Iterative Solution of the Non-LTE Line Radiation Transfer Problem," *J. Quant. Spectrosc. Radiat. Transfer* **35**, 431.

1987

[116] Adams M.L. and Martin W.R. (1987) "Boundary Projection Acceleration: A New Approach to Synthetic Acceleration of Transport Calculations," Proc. ANS *International Topical Meeting on Advances in Reactor Physics, Mathematics and Computation*, April 27-30, 1987, Paris, **2**, 579.

[117] Azmy Y.Y. and Larsen E.W. (1987) "Fourier Analysis of the Diffusion Synthetic Acceleration Method for Weighted Diamond-Differencing Schemes in Cartesian Geometries," *Nucl. Sci. Eng.* **95**, 106.

[118] Morel J.E. and Barnett A. (1987) "S_N Multigrid Acceleration," in "Radiation Transport: April 1, 1986 - June 30, 1986," LA-10844-PR, R. D. O'Dell, A. Nagy, Eds., Los Alamos National Laboratory.

[119] Nowak P.F. and Adams M.L. (1987) "XY-Geometry Analysis of an 'S_2-like' Synthetic Acceleration Scheme" *Trans. Amer. Nucl. Soc.* **55**, 354.

[120] Nowak P.F., Larsen E.W., and Martin W.R. (1987) "Multigrid Methods for S_N Problems," *Trans. Am. Nucl. Soc.* **55**, 355.

[121] Olson G.L. and Kunasz P.B. (1987) "Short Charcteristic Solution of the Non-LTE Line Transfer Problem by Operator Perturbation - I. The One-Dimensional Planar Slab," *J. Quant. Spectrosc. Radiat. Transfer* **38**, 325.

[122] Palmiotti G., Rieunier J.M., Gho C., and Salvatores M. (1987) "Optimized Two Dimension S_N Transport (BISTRO)," Proc. ANS *International Topical Meeting on Advances in Reactor Physics, Mathematics and Computation*, April 27-30, 1987, Paris, **2**, 615.

[123] Stepanek J. and Davierwalla D.M. (1987) "Synthetic S_2 and DP_0 Acceleration Schemes for Inner Iterations," Proc. ANS *International Topical Meeting on Advances in Reactor Physics, Mathematics and Computation*, April 27-30, 1987, Paris, **2**, 605.

1988

[124] Adams M.L. and Larsen E.W. (1988) "Synthetic Acceleration of One-Group S_N k-Eigenvalue Problems," *Trans. Am. Nucl. Soc.* **57**, 105.

[125] Adams M.L. and Martin W.R. (1988) "Boundary Projection Acceleration: A New Approach to Synthetic Acceleration of Transport Calculations," *Nucl. Sci. Eng.* **100**, 177.

[126] Allen E.J. (1988) "Application of Richardson Extrapolation to Numerical Solution of the Neutron Transport Equation," *Nucl. Sci. Eng.* **99**, 123.

[127] Cefus G. and Larsen E.W. (1988) "Stability Analysis of Fine Mesh Rebalance," *Trans. Am. Nucl. Soc.* **56**, 309.

[128] Khalil H. (1988) "Effectiveness of a Consistently Formulated Diffusion Synthetic Acceleration Differencing Approach," *Nucl. Sci. Eng.* **98**, 226.

[129] Larsen E.W. (1988) "A Grey Transport Acceleration Method for Thermal Radiative Transfer Problems," *J. Comp. Phys.* **78**, 459.

[130] Nowak P.F., Larsen E.W., and Martin W.R. (1988) "A Multigrid Method for S_N Calculations in X-Y Geometry," *Trans. Am. Nucl. Soc.* **56**, 291.

[131] Surzhikov S.T. (1988) "Calculations of the Selective Radiative Transfer in Two-Dimensional Cylindrical Geometry. Zeroth Approximation of Quadramoments Method," *Preprint, Institute of Mechanics Problems, USSR Academy of Sciences*, No. 352 (in Russian).

[132] Sutton T.M. (1988) "Wielandt Iteration as Applied to the Nodal Expansion Method," *Nucl. Sci. Eng.* **98**, 169.

[133] Valougeorgis D. (1988) "Boundary Treatment of the Diffusion Synthetic Acceleration Method for Fixed-Source Discrete-Ordinates Problems in X-Y Geometry," *Nucl. Sci. Eng.* **100**, 142.

[134] Valougeorgis D., Williams M., and Larsen E.W. (1988) "Stability Analysis of Synthetic Acceleration Methods with Anisotropic Scattering," *Nucl. Sci. Eng.* **99**, 91.

[135] Yavuz M. and Larsen E.W. (1988) "Diffusion Synthetic Acceleration for S_N Problems with Reflecting Boundaries," *Trans. Am. Nucl. Soc.* **56**, 305.

1989

[136] Adams M.L. and Larsen E.W. (1989) "Linear Synthetic Acceleration of *k*-Eigenvalue Problems," Proc. ANS Topical Meeting, *Advances in Nuclear Engineering Computation and Radiation Shielding*, April 10-13, 1989, Santa Fe, **1**, 12:1.

[137] Barnett A., Morel J.E., and Harris D.R. (1989) "A Multigrid Acceleration Method for the 1-D S_N Equations with Anisotropic Scattering," *Nucl. Sci. Eng.* **102**, 1.

[138] Cefus G.R. and Larsen E.W. (1989) "Stability Analysis of Rebalance," Proc. ANS Topical Meeting, *Advances in Nuclear Engineering Computation and Radiation Shielding*, April 10-13, 1989, Santa Fe, **1**, 15:1.

[139] Faber V. and Mantueffel T.A. (1989) "A Look at Transport Theory From the Viewpoint of Linear Algebra," in *Transport Theory, Invariant Imbedding, and Integral Equations*, Lecture notes in Pure and Applied Mathematics **115**, P. Nelson et al., eds., Marcel Dekker, New York, p. 37.

[140] Larsen E.W. and Morel J.E. (1989) "Asymptotic Solutions of Numerical Transport Problems in Optically Thick, Diffusive Regimes II," *J. Comp. Phys.* **83**, 212. See also (1990) "Corrigendum," *J. Comp. Phys.* **91**, 246.

[141] Lawrence R.D. (1989) "Synthetic Acceleration of Integral Transport Methods," Proc. ANS Topical Meeting, *Advances in Nuclear Engineering Computation and Radiation Shielding*, April 10-13, 1989, Santa Fe, **1**, 13:1.

[142] Lorence L.J., Jr., Morel J.E., and Larsen E.W. (1989) "An S_2-Synthetic Acceleration Scheme for the One-Dimensional S_N Equations with Linear-Discontinuous Spatial Differencing," *Nucl. Sci. Eng.* **101**, 341.

[143] Morel J.E. (1989) "A Hybrid Collocation-Galerkin-Sn Method for Solving the Boltzmann Transport Equation," *Nucl. Sci. Eng.* **101**, 72.

[144] O'Dell R.D., Brinkley F.W., Jr., Marr D.R., and Alcouffe R.E. (1989) "Revised User's Manual for ONEDANT: A Code Package for One-Dimensional Diffusion-Accelerated, Neutral Particle Transport," LA-9184-M, Rev., Los Alamos National Laboratory.

[145] Parsons D.K. (1989) "INEL Experience with Damped DSA Algorithms," Proc. ANS Topical Meeting, *Advances in Nuclear Engineering Computation and Radiation Shielding*, April 10-13, 1989, Santa Fe, **1**, 16:1.

[146] Yavuz M. and Larsen E.W. (1989) "Spatial Domain Decomposition Methods for Discrete Ordinates Problems," Proc. ANS Topical Meeting, *Advances in Nuclear Engineering, Computation and Radiation Shielding*, April 10-13, 1989, Santa Fe, **1**, 14:1.

[147] Yavuz M. and Larsen E.W. (1989) "Spatial Domain Decomposition for Neutron Transport Problems," *Transport Theory Statist. Phys.* **18**, 205.

1990

[148] Alcouffe R.E. (1990) "A Diffusion-Accelerated S_N Transport Method for Radiation Transport on a General Quadrilateral Mesh," *Nucl. Sci. Eng.* **105**, 191.

[149] Ashby S.F., Brown P.N., Dorr M.R., and Hindmarsh A.C. (July, 1990) "Preconditioned Iterative Methods for Discretized Transport Equations," UCRL-JC-104901, Lawrence Livermore National Laboratory.

[150] Cefus G.R. and Larsen E.W. (1990) "Stability Analysis of Coarse Mesh Rebalance," *Nucl. Sci. Eng.* **105**, 31.

[151] Cefus G.R. and Larsen E.W. (1990) "Stability Analysis of the Quasidiffusion and Second Moment Methods for Iteratively Solving Discrete-Ordinates Problems," *Transport Theory Statist. Phys.* **18**, 493.

[152] Honrubia J.J. and Morel J.E. (1990) "A Synthetically Accelerated Weighted Diamond Scheme for Charged-Particle Transport Calculations," *Nucl. Sci. Eng.* **104**, 91.

[153] Larsen E.W. (1990) "Transport Acceleration Methods as Two-Level Multigrid Algorithms," in *Modern Mathematical Methods in Transport Theory (Operator Theory: Advances and Applications, Vol. 51)*, W. Greenberg and J. Polewczak, eds., Birkhäuser Verlag, Basel, 34.

[154] Manteuffel T., McCormick S.F., Morel J.E., and Yang G. (1990) "Fast Multigrid Solver for Neutron Transport Problems," Proc. IMACS First International Conference on Computational Physics, Boulder, Colorado, June 11-15, 1990.

[155] Palmiotti G., Rieunier J.M., Gho C., and Salvatores M. (1990) "Optimized Two-Dimensional S_N Transport," *Nucl. Sci. Eng.* **104**, 26.

1991

[156] AboAlfaraj T. and Larsen E.W. (1991) "The Efficiency of Linear and Nonlinear Implementations of Diffusion Synthetic Acceleration," *Proc. ANS Topical Meeting, Advances in Mathematics, Computations, and Reactor Physics*, April 29 - May 2, 1991, Pittsburgh, **3**, Sec. 11.1, p. 3-1.

[157] Alcouffe R.E. (1991) "A Multigrid Solution of the Three-Dimensional DSA Equation: A Question of Efficiency for Three-Dimensional Transport Iterations," Proc. ANS Topical Meeting, *Advances in Mathematics, Computations, and Reactor Physics*, April 29 - May 2, 1991, Pittsburgh, **3**, Sec. 11.1, p. 4-1.

[158] Ashby S.F., Brown P.N., Dorr M.R., and Hindmarsh A.C. (1991) "Preconditioned Iterative Methods for Discretized Transport Equations," Proc. ANS Topical Meeting, *Advances in Mathematics, Computations, and Reactor Physics*, April 29 - May 2, 1991, Pittsburgh, **2**, Sec. 6.1, p. 2-1.

[159] Azmy Y.Y. (1991) "Acceleration of the Second Angular Moment in Larsen's DSA Formalism," *Trans. Am. Nucl. Soc.* **63**, 183.

[160] Azmy Y.Y. (1991) "Optimal Diffusion Synthetic Acceleration of Discrete Ordinates Transport Calculations," *Trans. Am. Nucl. Soc.* **64**, 284.

[161] Khattab K. and Larsen E.W. (1991) "Synthetic Acceleration Methods for Linear Transport Problems with Highly Anisotropic Scattering," *Nucl. Sci. Eng.* **107**, 217.

[162] Kulas M.M. and Moses G.A. (1991) "Projected Discrete Ordinates Methods for S_N Problems in X-Y Geometry," Proc. ANS Topical Meeting, *Advances in Mathematics, Computations, and Reactor Physics*, April 29 - May 2, 1991, Pittsburgh, **3**, Sec. 11.2, p. 2-1.

[163] Larsen E.W. (1991) "Amplitude and Shape Function Formulations of Transport Problems," Proc. ANS Topical Meeting, *Advances in Mathematics, Computations, and Reactor Physics*, April 29 - May 2, 1991, Pittsburgh, **4**, Sec. 17.1, p. 4-1.

[164] Morel J.E. and Manteuffel T. (1991) "An Angular Multigrid Acceleration Technique for S_N Equations with Highly Forward-Peaked Scattering," *Nucl. Sci. Eng.* **107**, 330.

[165] Morel J.E., Olvey L.A., McGhee J.M., Claborn G.W., and Josef J.A. (1991) "Diffusion Accelerated Solution of the Even-Parity S_N Equations with Anisotropic Scattering," Proc. ANS Topical Meeting, *Advances in Mathematics, Computations, and Reactor Physics*, April 29 - May 2, 1991, Pittsburgh, **3**, Sec. 11.2, p. 3-1.

[166] Stepanek J. and Davierwalla C.M. (1991) "Synthetic Low-Order S_m Acceleration Scheme for Inner S_N Iterations of Two-Dimensional Finite Element Transport Method," Proc. ANS Topical Meeting, *Advances in Mathematics, Computations, and Reactor Physics*, April 29 - May 2, 1991, Pittsburgh, **3**, Sec. 11.2, p. 1-1.

[167] Wareing T., Larsen E.W., and Adams M.L. (1991) "Diffusion Accelerated Discontinuous Finite Element Schemes for the S_N Equations in Slab and X,Y Geometries," Proc. ANS Topical Meeting, *Advances in Mathematics, Computations, and Reactor Physics*, April 29 - May 2, 1991, Pittsburgh, **3**, Sec. 11.1, p. 2-1.

1992

[168] Anistratov D.Y. (1992) "Application of the Quasi-Diffusion Approach for Solving Neutron Transport Problems," Ph.D. Dissertation (Candidate of Physical and Mathematical Sciences), Scientific Advisor: V.Y. Gol'din (Dr. Sc.), Institute for Mathematical Modeling, Russian Academy of Sciences, Moscow.

[169] Adams M.L. and Martin W.R. (1992) "Diffusion Synthetic Acceleration of Discontinuous Finite Element Transport Iterations," *Nucl. Sci. Eng.* **111**, 145.

[170] Gol'din V.Ya. and Kolpakov A.V. (1992) "Combined Methods for Solving Multidimensional Steady System of Quasi-Diffusion Equations," *Computational Methods of Linear Algebra*, Moscow, (1993); Proceedings of 1992 all-union conference (in Russian).

[171] Hanebutte U.R. and Lewis E.E. (1992) "A Massively Parallel Discrete Ordinates Response Matrix Method for Neutron Transport," *Nucl. Sci. Eng.* **111**, 46.

[172] Larsen E.W. (1992) "The Asymptotic Diffusion Limit of Discretized Transport Problems," *Nucl. Sci. Eng.* **112**, 336.

[173] Manteuffel T., McCormick S.F., Morel J.E., Oliveira S., and Yang G. (1992) "Parallel Multigrid Methods for Transport Equations," Proc. Copper Mountain Conference on Iterative Methods, April 10-15, 1992.

[174] Miften M.M. and Larsen E.W. (1992) "A Symmetrized Quasidiffusion Method for Solving Multidimensional Transport Problems," *Trans. Am. Nucl. Soc.* **66**, 227.

[175] Palmer T.S. (1992) "Curvilinear Geometry Transport Discretizations in Thick Diffusive Regions," Ph.D. dissertation, University of Michigan.

[176] Wareing T. (November, 1992) "Asymptotic Diffusion Accelerated Discontinuous Finite Element Methods for Transport Problems," LA-12425-T, Los Alamos National Laboratory.

[177] Yavuz M. and Larsen E.W. (1992) "Iterative Methods for Solving X-Y Geometry S_N Problems on Parallel Architecture Computers," *Nucl. Sci. Eng.* **112**, 32.

1993

[178] Adams M.L. (1993) "New Nonlinear Methods for Linear Transport Calculations," Proc. ANS Topical Meeting, *Mathematical Methods and Supercomputing in Nuclear Applications, M&C + SNA '93*, April 19-23, 1993, Karlsruhe, Germany, **1**, 683.

[179] Adams B.T. and Morel J.E. (1993) "An Upscatter Acceleration Scheme for the Multigroup S_N Equations," Proc. ANS Topical Meeting, *Mathematical Methods and Supercomputing in Nuclear Applications, M&C + SNA '93*, April 19-23, 1993, Karlsruhe, Germany, **2**, 445.

[180] Adams B.T. and Morel J.E. (1993) "A Two-Grid Acceleration Scheme for the Multigroup S_N Equations with Neutron Upscattering," *Nucl. Sci. Eng.* **115**, 253.

[181] Adams M.L. and Wareing T.A. (1993) "Diffusion Synthetic Acceleration Given Anisotropic Scattering, General Quadratures, and Multiple Dimensions," *Trans. Amer. Nucl. Soc.* **68**, 203.

[182] Anistratov D.Y. and Gol'din V.Ya. (1993) "Nonlinear Methods for Solving Particle Transport Problems," *Transport Theory Statist. Phys.* **22**, 125.

[183] Aristova E.N. and Kolpakov A.V. (1993) "A Combined Finite Difference Scheme for an Elliptic Operator in an Oblique-Angled Cell," *Math. Modeling Comp. Exp.* **1**, 187.

[184] Ashby S.F., Brown P.N., Dorr M.R., and Hindmarsh A.C. (July, 1993) "A Linear Algebraic Analysis of Diffusion Synthetic Acceleration for the Boltzmann Transport Equation," UCRL-JC-110712 (Revision 1), Lawrence Livermore National Laboratory.

[185] Azmy Y.Y. (1993) "Cell-Centered Imposed Diffusion Synthetic Acceleration for Weighted Difference Transport Methods," *Nucl. Sci. Eng.* **115**, 265.

[186] Manteuffel T. and Ressel K. (1993) "Multilevel Methods for Transport Equations in Diffusive Regimes," Proc. Copper Mountain Conference on Multigrid Methods, April 5-9, 1993.

[187] Miften M.M. and Larsen E.W. (1993) "A Symmetrized Quasidiffusion Method for Solving Transport Problems in Multidimensional Geometries," Proc. ANS Topical Meeting, *Mathematical Methods and Supercomputing in Nuclear Applications, M&C + SNA '93*, April 19-23, 1993, Karlsruhe, Germany, **1**, 707.

[188] Miften M.M. and Larsen E.W. (1993) "The Quasi-Diffusion Method for Solving Transport Problems in Planar and Spherical Geometries," *Transport Theory Statist. Phys.* **22**, 165.

[189] Morel J.E., Dendy J.E., Jr., and Wareing T.A. (1993) "Diffusion Accelerated Solution of the 2-D S_N Equations with Bilinear-Discontinuous Differencing," Proc. ANS Topical Meeting, *Mathematical Methods and Supercomputing in Nuclear Applications, M&C + SNA '93*, April 19-23, 1993, Karlsruhe, Germany, **2**, 488.

[190] Morel J.E., Dendy J.E., Jr., and Wareing T.A. (1993) "Diffusion Accelerated Solution of the 2-D S_N Equations with Bilinear-Discontinuous Differencing," *Nucl. Sci. Eng.* **115**, 304.

[191] Nowak P.F. (1993) "A Grey Diffusion Acceleration Method for Time-Dependent Radiative Transfer Calculations: Analysis and Application," Proc. ANS Topical Meeting, *Mathematical Methods and Supercomputing in Nuclear Applications, M&C + SNA '93*, April 19-23, 1993, Karlsruhe, Germany, **1**, 33.

[192] Wareing T.A. (1993) "New Diffusion Synthetic Acceleration Methods for the S_N Equations with Corner Balance Spatial Differencing," Proc. ANS Topical Meeting, *Mathematical Methods and Supercomputing in Nuclear Applications, M&C + SNA '93*, April 19-23, 1993, Karlsruhe, Germany, **2**, 500.

1994

[193] Averin A.V. and Voloschenko A.M. (1994) "Consistent P_1 Synthetic Acceleration Method for Outer Iterations," *Transport Theory Statist. Phys.* **23**, 701.

[194] Azmy Y.Y. (1994) "Adjacent-Cell Preconditioners for Solving Optically Thick Neutron Transport Problems," Proc. ANS *Eighth International Conference on Radiation Shielding*, Arlington, Texas, April 24-28, 1994, **1**, 193.

[195] Eaton T.L. and Adams M.L. (1994) "A New Corner-Balance / Linear-Discontinuous Method for Transport in Slab Geometry," *Trans. Am. Nucl. Soc.* **70**, 158.

[196] Manteuffel T., McCormick S.F., Morel J.E., Oliveira S. and Yang G. (1994) "A Parallel Version of a Multigrid Algorithm for Isotropic Transport Equations," *SIAM J. Sci. Stat. Comp.* **15**, 474.

[197] Miften M. and Larsen E.W. (1994) "The SQD Method for S_N Problems on Equilateral Triangular Meshes," *Trans. Am. Nucl. Soc.* **70**, 156.

[198] Morel J.E. and McGhee J.M. (1994) "A Fission-Source Acceleration Technique for Time-Dependent Even-Parity S_N Calculations," *Nucl. Sci. Eng.* **116**, 73.

[199] Shewchuk J.R. (1994). " An Introduction to the Conjugate Gradient Method Without the Agonizing Pain," available online at: < http://www.cs.cmu.edu/-jrs/ >.

[200] Wareing T.A., Walters W.F., and Morel J.E. (1994) "Diffusion Accelerated Solution of the 2-D X-Y S_N Equations with Linear-Bilinear Nodal Differencing," Proc. ANS *Eighth International Conference on Radiation Shielding*, Arlington, Texas, **1**, 201.

[201] Wareing T.A., Walters W.F., and Morel J.E. (1994) "Diffusion Accelerated Solution of the Two-Dimensional X-Y S_N Equations with Linear-Bilinear Nodal Differencing," *Nucl. Sci. Eng.* **118**, 122.

[202] Wareing T.A., Walters W.F., and Morel J.E. (1994) "An S_2-Like Acceleration Method for the Nonlinear Characteristic Transport Scheme," *Trans. Am. Nucl. Soc.* **71**, 267.

1995

[203] Adams M.L. and Ramoné G. (August, 1995) "Acceleration Methods for Assembly-Level Transport Calculations," *Proc. X ENFIR (Tenth Brazilian Meeting on Reactor Physics and Thermal Hydraulics)*, August 7-11, 1995, Águas de Lindóia, Brazil, ABEN (Associação Brasiliera de Energia Nuclear), p. 501.

[204] Ashby S.F., Brown P.N., Dorr M.R., and Hindmarsh A.C. (1995) "A Linear Algebraic Analysis of Diffusion Synthetic Acceleration for the Boltzmann Transport Equation," *SIAM J. Numer. Anal.* **32**, 128. (This is the journal version of [184].)

[205] Brown P.N. (1995) "A Linear Algebraic Development of Diffusion Synthetic Acceleration for 3-D Transport Equations," *SIAM J. Numer. Anal.* **32**, 179.

[206] Brown P.N. and Dorr M.R. (January 1995) "Spherical Harmonic Solutions of Neutron Transport Systems via Discrete Ordinates," UCRL-JC-119761, Lawrence Livermore National Laboratory.

[207] Colombo V., Coppa G.G.M., Melisurgo V., and Ravetto P. (1995) "Improvements to the Diffusion Synthetic Acceleration Method in Neutron Transport with highly Anisotropic Scattering," Proc. ANS *International Conference on Mathematics and Computations, Reactor Physics, and Environmental Analyses*, April 30 - May 4, 1995, Portland, **2**, 1352.

[208] Gol'din V.Ya. and Anistratov D.Y. (1995). "Fast Neutron Reactor in a Self-Adjusting Neutron-Nuclide Regime," *Mathematical Modeling*, **7**, No. 10, 12-32 (in Russian).

[209] Kelley C.T. (1995) "Multilevel Source Iteration Accelerators for the Linear Transport Equation in Slab Geometry," *Transport Theory Statist. Phys.* **24**, 679.

[210] Mantueffel T., McCormick S.F., Morel J.E., Oliveira S., and Yang G. (1995) "A Fast Multigrid Algorithm for Isotropic Transport Problems I: Pure Scattering," *SIAM J. Sci. Comp.* **16**, 601.

[211] Morel J.E. and McGhee J.M. (1995) "A Diffusion Synthetic Acceleration Technique for Solving the Even-Parity S_N Equations with Anisotropic Scattering," *Nucl. Sci. Eng.* **120**, 147.

[212] Noh T. and Miller W.F. (1995) "The Comparison of P_1 and Simplified P_2 Synthetic Acceleration for Iterative Methods in Transport Solutions," Proc. ANS *International Conference on Mathematics and Computations, Reactor Physics, and Environmental Analyses*, April 30 - May 4, 1995, Portland, **2**, 1342.

[213] Oliveira S. (1995) "Krylov Subspace Methods for Transport Equations," *Proc. X ENFIR (Tenth Brazilian Meeting on Reactor Physics and Thermal Hydraulics)*, August 7-11, 1995, Águas de Lindóia, Brazil, ABEN (Associação Brasiliera de Energia Nuclear), p. 522.

[214] Wareing T.A., Walters W.F., and Morel J.E. (1995) "A Diffusion Accelerated Solution Method for the Nonlinear Characteristic Scheme," Proc. ANS *International Conference on Mathematics and Computations, Reactor Physics, and Environmental Analyses*, April 30 - May 4, 1995, Portland, **2**, 1335.

1996

[215] Anistratov D.Y., Adams M.L., and Larsen E.W. (1996) "Acceleration Method for the Nonlinear Corner-Balance Scheme," *Trans. Am. Nucl. Soc.* **75**, 156.

[216] Anistratov D.Y., Aristova E.N., and Gol'din V.Ya. (1996) "A Nonlinear Method for Solving the Problems of Radiation Transfer in Medium," *Mathematical Modeling* **8**, No. 12, 3 (in Russian).

[217] Anistratov D.Y. and Larsen E.W. (1996) "Alpha-Weighted Acceleration Methods for the Transport Equation," *Trans. Am. Nucl. Soc.* **75**, 154.

[218] Azmy Y.Y. (1996) "Adjacent-Cell Preconditioners for Accelerating Multidimensional Neutron Transport Methods," Proc. 1996 ANS Topical Meeting on Radiation Protection and Shielding, N. Falmouth, Mass., April 21-25, 1996, **1**, 390.

[219] Börgers C. and Larsen E.W. (1996) "Asymptotic Derivation of the Fermi Pencil Beam Approximation," *Nucl. Sci. Eng.* **123**, 343.

[220] Brantley P.S. and Larsen E.W. (1996) "Improved Iteration Strategy for the Simplified P_N Equations," *Trans. Am. Nucl. Soc.* **75**, 129.

[221] Coppa G.G.M., Ravetto P., and Colombo V. (1996) "On the Importance of Effective Convergence Velocity of Synthetic Acceleration Methods in Neutron Transport," *Prog. Nucl. Energy* **30**, 265.

[222] Dorr M.R. and Still C.H. (1996) "Concurrent Source Iteration in the Solution of Three-Dimensional, Multigroup Discrete Ordinates Neutron Transport Equations," *Nucl. Sci. Eng.* **122**, 287.

[223] Hong S.G. and Cho N.Z. (1996) "A Rebalance Nonlinear Iteration Method for Solving the Neutron Transport Equations," *Proc. Int. Conf. on the Physics of Reactors*, September 16-20, Mito, Japan, Vol. 1A, p. 250.

[224] Hunter M.A. and Haghighat A. (1996) "Comparison of Acceleration Schemes for Parallel S_N Algorithm Solution of Shielding Problems," *Trans. Am. Nucl. Soc.* **74**, 179.

[225] Manteuffel T., McCormick S.F., Morel J.E., and Yang G. (1996) "A Fast Multigrid Algorithm for Isotropic Transport Problems II: With Absorption," *SIAM J. Sci. Comp.* **17**, 1449.

[226] Oliveira S. (1996) "Parallel Multigrid Methods for Transport Equations: The Anisotropic Case," *Parallel Computing* **22**, 513. 1.

[227] Patton B.W. (1996) "Application of Krylov Subspace Iterative Techniques to the Numerical Solution of the Neutron Transport Equation," Ph.D. Dissertation, University of Michigan, Department of Nuclear Engineering and Radiological Sciences.

[228] Patton B.W. and Holloway J.P. (1996) "Application of Krylov Subspace Iterative Methods to the Slab Geometry Transport Equation," Proc. ANS Topical Meeting, Advancements and Applications in Radiation Protection and Shielding, Cape Cod, April 21-25, 1996, **1**, 384.

[229] Voloschenko A.M. (1996) "Completely Consistent P_1 Synthetic Acceleration Scheme for Charged-Particle Transport Calculations," Proc. 1996 ANS Topical Meeting on Radiation Protection and Shielding, N. Falmouth, Mass., April 21-25 1996, **1**, 408.

[230] Wareing T.A., McGhee J.M., and Morel J.E. (1996) "ATTILA: A Three-Dimensional, Unstructured Tetrahedral Mesh Discrete Ordinates Transport Code," *Trans. Am. Nucl. Soc.* **75**, 146.

[231] Wareing T.A., Walters W.F., and Morel J.E. (1996) "A Diffusion-Accelerated Solution Method for the Nonlinear Characteristic Scheme in Slab Geometry," *Nucl. Sci. Eng.* **124**, 72.

1997

[232] Alcouffe R.E., Baker R.S., Brinkley F.W., Marr D.R., O'Dell R.D., and Walters W.F. (1997) "DANTSYS: A Diffusion Accelerated Neutral Particle Transport Code System," Code manual, LA-12969-M. Available online at: < http://www-xdiv.lanl.gov/XTM/dant/la12969/dantsys.html >.

[233] Adams B.T. and Morel J.E. (1997) "An Acceleration Scheme for the Multigroup S_N Equations with Fission and Thermal Upscatter," Proc. ANS Topical Meeting, *Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications*, October 5-10, 1997, Saratoga Springs, New York, **1**, 343.

[234] Anistratov D.Y., Adams M.L., and Larsen E.W. (1997) "Acceleration of the Nonlinear Corner-Balance Scheme by the Averaged Flux Method," *J. Comp. Phys.* **135**, 66.

[235] Aristova E.N. and Gol'din V.Ya. (1997) "Method of Taking into Account Strong Anisotropy of Scattering in Transport Equation," *Mathematical Modeling* **9**, No. 6, 39 (1997) (in Russian).

[236] Azmy Y.Y. (1997) "Post Convergence Automatic Differentiation of Iterative Schemes," *Nucl. Sci. Eng.* **125**, 12.

[237] Azmy Y.Y (1997) "Analysis and Performance of Adjacent-cell Preconditioners for Accelerating Multidimensional Transport Calculations," Proc. *OECD/NEA Meeting on 3D Deterministic Radiation Transport Computer Programs, Features, Applications, and Perspectives*, Paris, France, December 2-3, 1996, p. 197, Organization for Economic Cooperation and Development, Paris.

[238] Adams M.L. (1997) "A Subcell Balance Method for Radiative Transfer on Arbitrary Spatial Grids," *Transport Theory & Stat. Phys.* **26**, Nos. 4 & 5, 385.

[239] Gol'din V.Ya. and Aristova E.N. (1997) "The Method of Consideration of a Strong Scattering Anisotropy in Transport Equation," Proc. ANS Topical Meeting, *Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications*, October 5-10, 1997, Saratoga Springs, New York, **2**, 1507.

[240] Hong S.G. and Cho N.Z. (1997) "A Rebalance Approach to Nonlinear Iteration for Solving the Neutron Transport Equation," *Ann. Nucl. Energy* **24**, 147.

[241] Khattab K.M. (1997) "The Generalized P_N Synthetic Acceleration Method for Linear Transport Problems with Highly Anisotropic Scattering," *Nucl. Sci. Eng.* **125**, 171.

[242] Lewis E.E. and Palmiotti G. (1997) "An Acceleration Technique for Red Black Response Matrix Algorithms," Proc. ANS Topical Meeting, *Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications*, October 5-10, 1997, Saratoga Springs, New York, **1**, p. 51.

[243] Ramoné G.L., Adams M.L., and Nowak P.F. (1997) "A Transport Synthetic Acceleration Method for Transport Iterations," *Nucl. Sci. Eng.*, **125**, 257.

[244] Voloschenko A.M. (1997) "Consistent P_1 Synthetic Acceleration Scheme for Transport Equation in Two-Dimensional R,Z Geometry," Proc. ANS Topical Meeting, *Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications*, October 5-10, 1997, Saratoga Springs, New York, **1**, 364.

[245] Zika M.R. and Adams M.L. (1997) "Transport Acceleration for the Long Characteristics Discretization," Proc. ANS Topical Meeting, *Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications*, October 5-10, 1997, Saratoga Springs, New York, **1**, 353.

1998

[246] Adams M.L. and Nowak P.F. (1998) "Asymptotic Analysis of a Computational Method for Time- and Frequency-Dependent Radiative Transfer," *J. Comput. Phys.* **146**, 366.

[247] Adams M.L., Wareing T.A., and Walters W.F. (1998) "Characteristic Methods in Thick Diffusive Problems," *Nucl. Sci. Eng.* **130**, 18.

[248] Azmy Y.Y. (1998) "Impossibility of Unconditional Stability and Robustness of Diffusive Acceleration Schemes," Proc. ANS Topical Meeting, *Radiation Protection and Shielding*, Nashville, TN, April 19-23, 1998, Vol. 1, p. 480, American Nuclear Society, La Grange Park, Illinois.

[249] Baker R.S. and Koch K.R. (1998) "An S_N Algorithm for the Massively Parallel CM-200 Computer," *Nucl. Sci. Eng.* **128**, 312.

[250] Banoczi J.M. and Kelley C.T. (1998) "A Fast Multilevel Algorithm For The Solution of Nonlinear Systems of Conductive-Radiative Heat Transfer Equations," *SIAM J. Sci. Comput.* **19**, 266.

[251] Castrianni C.L. and Adams M.L. (1998) "A Nonlinear Corner-Balance Spatial Discretization for Transport on Arbitrary Grids," *Nucl. Sci. Eng.* **128**, 278.

[252] Hong S.G. and Cho N.Z. (1998) "Angle-Dependent Rebalance Factor Method for Nodal Transport Problems in XY Geometry," *Trans. Am. Nucl. Soc.* **79**, 139.

[253] Manteuffel T.A. and Ressel K. (1998). "Least-Squares Finite-Element Solution of Neutron Transport Equations in Diffusive Regimes," *SIAM J. Numer. Anal.* **35**, 806.

[254] Oliveira S. (1998) "Analysis of a Multigrid Method for a Transport Equation by Numerical Fourier Analysis, *Comp. and Math. with Appl.* **35**, 7.

[255] Oliveira S. and Deng Y. (1998) "Preconditioned Krylov Subspace Methods for Transport Equations," *Prog. Nucl. Energy* **33**, 155.

[256] Pautz S. (April, 1998) "Discrete Ordinates Transport Methods for Problems with Highly Forward-Peaked Scattering," LA-13444-T, Los Alamos National Laboratory.

[257] Zika M.R. and Larsen E.W. (1998) "Fourier Mode Analysis of Source Iteration in Spatially Periodic Media," *Trans. Am. Nucl. Soc.* **79**, 135.

[258] Zika M.R. and Larsen E.W. (1998) "Half-Range Acceleration for One-Dimensional Transport Problems," *Trans. Am. Nucl. Soc.* **79**, 137.

1999

[259] Azmy Y.Y. (1999) "Iterative Convergence Acceleration of Neutral Particle Transport Methods via Adjacent-Cell Preconditioners," *J. Comput. Phys.* **152**, 359.

[260] Azmy Y.Y., Wareing T., and Morel J. (1999) "Effect of Material Heterogeneity on the Performance of DSA for Even-Parity S_n Methods," Proc. ANS Topical Meeting, *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, 1999, Madrid, Spain, **1**, 55.

[261] Aristova E.N., Gol'din V.Ya, and Kolpakov A.V. (1999) "Multidimensional Calculations of Radiation Transport by Nonlinear Quasi-Diffusion Method," Proc. ANS Topical Meeting, *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, 1999, Madrid, Spain, **1**, 667.

[262] Baldwin C., Brown P.N., Falgout R.D., Graziani F., and Jones J. (1999) "Iterative Linear Solvers in a 2D Radiation- Hydrodynamics Code: Methods and Performance," *J. Comp. Phys.* **154**, 1. Also available as a technical report, (1998) UCRL-JC-130933, Lawrence Livermore National Laboratory.

[263] Banoczi J.M. and Kelley C.T. (1999) "A Fast Multilevel Algorithm For The Solution of Nonlinear Systems of Conductive-Radiative Heat Transfer Equations in Two Space Dimensions," *SIAM J. Sci. Comput.* **20**, 1214.

[264] Gesh C.J. and Adams M.L. (1999) "Even- and Odd-Parity Finite Element Solutions to Thick Diffusive Discrete Ordinates Problems," Proc. ANS Topical Meeting, *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, Madrid, Spain, **2**, 1175.

[265] Guthrie B., Holloway J.P., and Patton B.W. (1999) "GMRES as a Multi-Step Transport Sweep Accelerator," *Transport Theory Statist. Phys.* **28**, 83.

[266] Hong S.G. and Cho N.Z. (1999) "Convergence Analysis of the Angular Dependent Rebalance Iteration Method in XY Geometry," *Trans. Am. Nucl. Soc.* **80**, 115.

[267] Hong S.G. and Cho N.Z. (1999) "Angular Dependent Rebalance (ADR) Iteration for Discrete-Ordinates Transport Problems in Equilateral Triangular Meshes," Proc. ANS Topical Meeting, *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, 1999, Madrid, Spain, **1**, 74.

[268] Morel J.E. and McGhee J.M. (1999) "A Self-Adjoint Angular Flux Equation," *Nucl. Sci. Eng.* **132**, 312.

[269] Pautz S.D. and Adams M.L. (1999) "An Asymptotic Study of Discretized Transport Equations in the Fokker-Planck Limit," Proc. ANS Topical Meeting *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, Madrid, Spain, **1**, 637.

[270] Pautz S.D., Morel J.E., and Adams M.L. (1999) "An Angular Multigrid Acceleration Method for S_N Equations with Highly Forward-Peaked Scattering," Proc. ANS Topical Meeting, *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, 1999, Madrid, Spain, **1**, 647.

[271] Sanchez R. and Chetaine A. (1999) "Synthetic Acceleration for a 2-D Characteristic Method in Non Regular Meshes," Proc. ANS Topical Meeting, *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, 1999, Madrid, Spain, **2**, 1572.

[272] Voloschenko A.M. (1999) "Experience in the Use of the Consistent P_1 Synthetic Acceleration Scheme for S_n Transport Equation in 2-D Geometry," Proc. ANS Topical Meeting, *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, 1999, Madrid, Spain, **1**, 104.

[273] Wareing T.A., McGhee J.M., Morel J.E., and Pautz S.D. (1999) "Discontinuous Finite Element S_N Methods on 3-D Unstructured Grids," Proc. ANS Topical Meeting, *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, 1999, Madrid, Spain, **2**, 1185.

[274] Wareing T.A., Morel J.E., and McGhee J.M. (1999) "A Diffusion Synthetic Acceleration Method for the S_N Equations with Discontinuous Finite Element Space and Time Differencing," Proc. ANS Topical Meeting, *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, 1999, Madrid, Spain, **1**, 45.

[275] Wareing T.A. (1999) Private communication.

[276] Zika M.R. and Larsen E.W. (1999) "Fourier Mode Analysis of Slab-Geometry Transport Iterations in Spatially Periodic Media," Proc. ANS Topical Meeting, *International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis*, September 27-30, 1999, Madrid, Spain, **1**, 64.

2000

[277] Anistratov D.Y. (2000) "The Generalized Quasi-Diffusion Method for Solving Adjoint Transport Problems with Alternating Solutions," *Trans. Am. Nucl. Soc.* **83**, 348.

[278] Aristova E.N. and Gol'din V.Ya. (2000) "Computation of Anisotropic Scattering of Solar Radiation in the Atmosphere (Monoenergetic Case)," *J. Quant. Spectrosc. Radiat. Transfer* **67**, 139.

[279] Azmy Y.Y. (2000) "Acceleration of Multidimensional Discrete Ordinates Methods Via Adjacent-Cell Preconditioners," *Nucl. Sci. Eng.* **136**, 202.

[280] Lebedev V.I. (2000) Private communication.

[281] Manteuffel T.A., Ressel K.J., and Starke G. (2000) "A Boundary Functional for the Least-Squares Finite Element Solution of the Neutron Transport Equation," *SIAM J. Numer. Anal.* **37** No. 2, 556.

[282] Sanchez R. and Chetaine A. (2000) "A Synthetic Acceleration for a Two-Dimensional Characteristic Method in Unstructured Meshes," *Nucl. Sci. Eng.* **136**, 122.

[283] Smith K.S. and Rhodes J.D. III (2000) "Casmo-4 Characteristics Methods for Two-Dimensional PWR and BWR Core Calculations," *Trans. Am. Nucl. Soc.* **83**, 294.

[284] Zika M.R. and Adams M.L. (2000) "Transport Synthetic Acceleration for Long-Characteristics Assembly-Level Transport Problems," *Nucl. Sci. Eng.* **134**, 135.

[285] Zika M.R. and Adams M.L. (2000) " Transport Synthetic Acceleration with Opposing Reflecting Boundary Conditions," *Nucl. Sci. Eng.* **134**, 159.

2001

[286] Adams M.L. (2001) "Discontinuous Finite Element Transport Solutions in Thick Diffusive Problems," *Nucl. Sci. Eng.* **137**, 298.

[287] Alcouffe R.E. (2001) Private communication.

[288] Anistratov D.Y. and Larsen E.W. (2001) "Nonlinear and Linear α-Weighted Methods for Particle Transport Problems," *J. Comp. Phys.*, to appear.

[289] Balsara D. (2001) "Fast and Accurate Discrete Ordinates Methods for Multidimensional Radiative Transfer. Part I, Basic Methods," *Journal Quant. Spectrosc. Radiat. Transfer* **69**, 671.

[290] Ching B. and Palmer T. (2001) "An Acceleration Scheme for Binary Stochastic Mixture Deterministic Transport Equations in Slab Geometry," Proc. ANS Topical Meeting: *International Conference on Mathematical Methods to Nuclear Applications*, September 9-13, 2001, Salt Lake City, Utah, CD-ROM (ISBN: 0-89448-661-6, ANS Order No. 700286) available from the American Nuclear Society, 555 N. Kensington Avenue, La Grange Park, IL 60525.

[291] Cho N.Z. and Park C.J. (2001) "An Additive Angular Dependent Rebalance Acceleration Method for Transport Equations," *Trans. Am. Nucl. Soc.* **84**, 222.

[292] Cooper M.A. and Larsen E.W. (2001) "Automated Weight Windows for Global Monte Carlo Deep Penetration Neutron Transport Calculations," *Nucl. Sci. Eng.* **137**, 1.

[293] Germogenova T.A. (2001). Private communication.

[294] Patton B.W. and Holloway J.P. (2001) "Application of Preconditioned GMRES to the Numerical Solution of the Neutron Transport Equation," *Ann. Nucl. Energy*, to appear.

[295] Park C.J. and Cho N.Z. (2001) "Additive Angular Dependent Rebalance Acceleration of the Discrete Ordinates Transport Calculations," Proc. ANS Topical Meeting: *International Conference on Mathematical Methods to Nuclear Applications*, September 9-13, 2001, Salt Lake City, Utah, CD-ROM (ISBN: 0-89448-661-6, ANS Order No. 700286) available from the American Nuclear Society, 555 N. Kensington Avenue, La Grange Park, IL 60525.

[296] Park C.J. and Cho N.Z. (2001) "A Linear Multiple Balance Method with High Order Accuracy for Discrete Ordinates Neutron Transport Equations," *Ann. Nucl. Energy*, to appear.

[297] Santandrea S. and Sanchez R. (2001) "Acceleration Techniques for the Characteristic Method in Unstructured Meshes," *Ann. Nucl. Energy*, to appear.

[298] Sanchez R. and Santandrea S. (2001) "Symmetrization of the Transport Operaor and Lanczos' Iterations," Proc. ANS Topical Meeting: *International Conference on Mathematical Methods to Nuclear Applications*, September 9-13, 2001, Salt Lake City, Utah, CD-ROM (ISBN: 0-89448-661-6, ANS Order No. 700286) available from the American Nuclear Society, 555 N. Kensington Avenue, La Grange Park, IL 60525.

[299] Wareing T.A., McGhee J.M., Morel J.E., and Pautz S.D. (2001) "Discontinuous Finite Element S_N Methods on Three-Dimensional Unstructured Grids," *Nucl. Sci. Eng.* **138**, 256.

[300] Warsa J.S., Wareing T.A., and Morel J.E. (2001) "Fully Consistent, Linear Discontinuous Diffusion Synthetic Acceleration on 3D Unstructured Meshes," Proc. ANS Topical Meeting: *International Conference on Mathematical Methods to Nuclear Applications*, September 9-13, 2001, Salt Lake City, Utah, CD-ROM (ISBN: 0-89448-661-6, ANS Order No. 700286) available from the American Nuclear Society, 555 N. Kensington Avenue, La Grange Park, IL 60525.

[301] Zmijarevic I., Sanchez R., and Lamponi, D. (2001) "Diffusion Synthetic Acceleration of SN Linear Nodal Schemes in Weighted Difference Form," Proc. ANS Topical Meeting: *International Conference on Mathematical Methods to Nuclear Applications*, September 9-13, 2001, Salt Lake City, Utah, CD-ROM (ISBN: 0-89448-661-6, ANS Order No. 700286) available from the American Nuclear Society, 555 N. Kensington Avenue, La Grange Park, IL 60525.

APPENDIX A: LIST OF ACRONYMS

The following is a list of acronyms used in this Review, together with their meaning and some pages in which they are used and discussed.

		page(s)
AMG	Algebraic Multigrid	89
ASE	Asymptotic Source Extrapolation	98, 103
BCGSTAB	Bi-Conjugate Gradient Stabilized	98, 112, 113
BLC	Bilinear Continuous	87
BLD	Bilinear Discontinuous	17, 85, 87
BPA	Boundary Projection Acceleration	18, 84, 95, 96
CB	Corner Balance	85
CC	Constant-Constant (nodal method)	99
CG	Conjugate Gradient	18, 107, 140
CMR	Coarse Mesh Rebalance	90, 93, 95, 96
DD	Diamond Difference	48, 98, 137
DFE	Discontinuous Finite Element	17, 86
DSA	Diffusion Synthetic Acceleration	16, 27, 52, 82
FMR	Fine Mesh Rebalance	90, 136
FEM	Finite Element Method	112
FF	First Flux	45
GCB	Generalized Corner Balance	71, 73, 76
GMRES	Generalized Minimum Residual	112, 140
GS	Gauss-Seidel	114, 117
GTA	Grey Transport Acceleration	124
IAEA	International Atomic Energy Agency	95
ICSA	Interface Current Synthetic Acceleration	95
KP	Lebedev Acceleration Schemes	11, 14, 32, 67
LD	Linear Discontinuous	17, 71, 100, 117
LM	Lewis-Miller	21, 37, 63, 77
M4S	Modified 4-Step	74
NLBPA	Nonlinear Boundary Projection Acceleration	96, 98, 113
PI	Power Iteration	127, 132

		page(s)
QD	Quasidiffusion	19, 40, 65, 77
SAAF	Self Adjoint Angular Flux (equation)	47, 68
SF	Second Flux	45
SI	Source Iteration	8, 23, 48
SIMG	Source Iteration Multigrid	99
SPD	Symmetric Positive Definite	109, 111
SPI	Shifted Power Iteration	129, 132
S_2SA	S_2 Synthetic Acceleration	31, 58, 83
S_3SA	S_4 Synthetic Acceleration	84
TG	Two-Grid	116
TSA	Transport Synthetic Acceleration	18, 34, 62, 77
WA	Weighted Alpha	20, 43, 66, 77