# ITERATIVE METHODS FOR NEUTRON AND THERMAL RADIATION TRANSPORT PROBLEMS 

A Dissertation
by

## ANTHONY PETRU BARBU

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Chair of Committee, Marvin L. Adams<br>Committee Members, Jim E. Morel<br>Raytcho Lazarov<br>Jean C. Ragusa<br>Head of Department, Michael Nastasi

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#### Abstract

We develop, analyze, and test iterative methods for three kinds of multigroup transport problems: (1) $k$-eigenvalue neutronics, (2) thermal radiation transport, and (3) problems with "upscattering," in which particles can gain energy from collisions.

For $k$-eigenvalue problems, many widely used methods to accelerate power iteration use "loworder" equations that contain nonlinear functionals of the transport solution. The nonlinear functionals require that the transport discretization produce strictly positive solutions, and the low-order problems are often more difficult to solve than simple diffusion problems. Similar iterative methods have been proposed that avoid nonlinearities and employ simple diffusion operators in their low-order problems. However, due partly to theoretical concerns, such methods have been largely overlooked by the reactor analysis community. To address theoretical questions, we present analyses showing that a power-like iteration process applied to the linear low-order problem (which looks like a $k$-eigenvalue problem with a fixed source) provides rapid acceleration and produces the correct transport eigenvalue and eigenvector. We also provide numerical results that support the existing body of evidence that these methods give rapid iterative convergence, similar to methods that use nonlinear functionals.

Thermal-radiation problems solve for radiation intensity and material temperature using coupled equations that are nonlinear in temperature. Some of the most powerful iterative methods in use today solve the coupled equations using a low-order equation in place of the transport equation, where the low-order equation contains nonlinear functionals of the transport solution. The nonlinear functionals need to be updated only a few times before the system converges. We develop, analyze, and test a new method that works in the same way but employs a simple diffusion low-order operator without nonlinear functionals. Our analysis and results show rapid iterative convergence, comparable to methods that use nonlinear functionals in more complicated low-order equations.

For problems with upscattering, we have investigated the importance of linearly anisotropic scattering for problems dominated by scattering in Graphite. Our results show that the linearly


anisotropic scattering encountered in problems of practical interest does not degrade the effectiveness of the iterative acceleration method. Additionally, we have tested a method devised by Hanuš and Ragusa using the semi-consistent Continuous/Discontinuous Finite Element Method (CDFEM) diffusion discretization we have devised, in place of the Modified Interior Penalty (MIP) discretization they employed. Our results with CDFEM show an increased number of transport iterations compared to MIP when there are cells with high-aspect ratio, but a reduction in overall runtime due to reduced degrees of freedom of the CDFEM operator compared to the MIP operator.

## DEDICATION

To all those in academia who teach because it brings them joy, I thank you for making my time at Texas A\&M a wonderful-albeit long-experience.

To Dr. Adams, for your infinite patience and willingness to teach even a rock how to move, I thank you.

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## 1. INTRODUCTION

In this thesis we discuss systems that have particle transport as one of the physical phenomena, which can be described by a Boltzmann transport equation of the form:

$$
\begin{align*}
& \vec{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, \vec{\Omega}, E)+\mathcal{T}(\vec{r}, E) \psi(\vec{r}, \vec{\Omega}, E) \\
& =\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \Omega^{\prime} \mathcal{X}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, E^{\prime} \rightarrow E\right) \psi\left(\vec{r}, \vec{\Omega}^{\prime}, E^{\prime}\right)+q^{f i x e d}(\vec{r}, \vec{\Omega}, E) . \tag{1.1}
\end{align*}
$$

Here $\psi$ is angular intensity, $\vec{\Omega}$ is a unit vector in the direction of particle motion, $E$ is the energy variable, $\mathcal{T}(\vec{r}, E)$ is the total interaction operator, and $\mathcal{X}\left(\vec{r}, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}, E^{\prime} \rightarrow E\right)$ is a generic transfer operator, and $q^{f i x e d}(\vec{r}, \vec{\Omega}, E)$ is an external fixed source. It is necessary to discretize the problem, and iterative methods are required to solve the discrete system. The iterative methods may have difficulty converging depending on physical properties of the system, and how the transport quantities are coupled to other physics.

Solution methods for linear systems have been widely studied for the transport equation. When discrete ordinates ( $S_{N}$ ) angle discretization and discontinuous finite element (DFEM) spatial discretization are applied, the system is hyperbolic and asymmetric and is typically solved with Richardson iteration or an asymmetric Krylov iterative method such as GMRES.

Richardson iteration converges at a rate of the spectral radius of the discrete iteration operator. Problems with spectral radii close to unity require an impractical amount of time to converge with Richardson iteration alone, and the phenomenon of false convergence can be difficult to address in such problems. [1] Krylov iterations converge at rates that depend on the clustering of eigenvalues and the condition number of the discrete system. Problems with large condition numbers may converge slowly and have iteration errors larger than their residuals. Problems with evenly spaced eigenvalues require a large Krylov subspace to approximate the solution, which implies a large number of iterations to generate that subspace. To hasten convergence of linear solution methods, the community has sought effective preconditioners that reduce the spectral radius, reduce the
condition number, and condense the eigenvalue clustering of the transport operator.
One preconditioning approach for the transport equation is to use a lower-order angle method, such as a diffusion operator, which approximates the angular dependence of the iteration error as linear in angle $(\vec{\Omega})$. This is historically referred to as diffusion synthetic acceleration (DSA), especially when used with Richardson iteration. For this strategy to be effective, the low-order operator must be consistent in some sense [2,1] with the spatial discretization. There are numerous variations of DSA, with varying advantages and disadvantages. Fully-consistent DSA, while rapidly convergent, can require the solution of its own ill-conditioned system of equations with a relatively large number of degrees of freedom, and thus can introduce more expense than is desirable. Inconsistent DSA effectiveness degrades depending on approximations chosen, but may have diffusion-like equations that are significantly easier to solve.

Another preconditioning approach also uses a lower-order angle method, but obtains the actual solution using a nonlinear transport closure that ensures consistency with the transport solution upon convergence. This family of methods, dubbed Projected Discrete Ordinates iterative methods by Larsen in 1986 [3], Nonlinear Projective Iterative (NPI) methods by Anistratov and Gol'din [4], and more well known in the community as High-Order/Low-Order (HOLO) [5] methods, includes methods such as Quasi-Diffusion (QD) [6, 7, 8] and Coarse Mesh Finite Difference (CMFD).[9, 10] In general, this family of methods requires positive solutions at every step of the iteration to prevent division by zero.[3, 11] Additionally, the low-order equations that result may be more difficult to solve than simple elliptic diffusion problems. However, these methods are rapidly convergent for appropriate problems, the choice of low-order system is flexibile since the consistency is maintained by the nonlinear closure, and theoretical stability has been demonstrated. [12, 13, 14, 15]

Some problems that have particle transport as one of the physical phenomena are coupled to other physics nonlinearly. These problems are also solved iteratively, using nonlinear methods such as linearization, Newton's method, Newton Krylov (NK), and inexact formulations of Newton's Method such as Jacobian-Free Newton Krylov (JFNK). In general, nonlinear iteration schemes
can require an initial guess near the global minimum error, are bound by stability criteria that are dependent on mesh and material properties, or make approximations to reduce cost that limit stability. For instance, the Jacobian-Free Newton-Krylov iterative method does not evaluate the Jacobian exactly and as a result degrades in the presence of sharp nonlinear solution structure such as a shock or reaction front [16]. Much like linear iterative methods, nonlinear iterative methods may benefit from acceleration by improving stability or hastening convergence.

Historically, nonlinear problems with a transport phenomena have predominantly been accelerated using HOLO methods, since HOLO methods are inherently nonlinear, the choice of low-order operator is flexible, and it is relatively straightforward to derive and implement. Linear acceleration schemes have been used by the community for some time, but have not had a theoretical basis to show stability and prove uniqueness of the solution.

We focus on three kinds of problems that have transport-driven physics that frequently require preconditioning to solve the inner iteration system and instead apply the preconditioner as a linear correction to the outer iteration: 1) thermal radiative transport, which describes the movement of energy in a system driven by the transport of thermal radiation; 2) $k$-eigenvalue for neutron transport, which solves for the effective multiplication factor (eigenvalue) and fundamental-mode (eigenfunction or eigenvector for discrete systems) of reactors; and 3) thermal upscattering of neutrons, which describes the transport of low-energy neutrons. We propose a novel method for thermal radiative transfer that uses a linear equation for a correction, and investigate a method for $k$-eigenvalue problems that uses a linear equation for a correction.

## 2. LITERATURE REVIEW

### 2.1 Thermal Radiative Transport

The current state of the art of radiative transfer iteration uses a two-level iteration at each time step: an outer modified Newton's method iteration for material temperature, and an inner Krylov iteration for a transport operator to obtain radiation intensity.

For the outer temperature iteration, a modified Newton's method is used in which only the Planckian is included in the Jacobian. The modified Newton's method performs exceptionally well when the starting iterate is close to the solution, and convergence is observed in practice as long as non-physical negativities are prevented. At each step of the modified Newton's method, the inner iteration for radiation intensity is carried through until convergence.

The inner iteration is usually a Krylov or Preconditioned Richardson iterative method to solve a transport equation for the radiation intensity. A one-group (gray) diffusion or transport preconditioner, which is used after each multigroup transport sweep, is usually defined to eliminate the "flat" $(\vec{\lambda}=\overrightarrow{0})$ error mode. Here $\vec{\lambda}$ is the wave number of a given Fourier mode, whose spatial shape is a planar wave in the mode direction: $e^{(i \vec{\lambda} \cdot \vec{r})}$.

The key to an effective preconditioner is a low-order operator that eliminates the slowest converging iteration error modes. Two notable preconditioners that identically eliminate the slowest mode (the flat mode) are Gray Transport Acceleration (GTA) [17] and Linear Multifrequency Gray (LMFG) [18]. The GTA preconditioner is a gray transport preconditioner for multigroup transport, and the LMFG preconditioner is a gray-diffusion preconditioner first proposed for multigroup diffusion. We have previously developed a method, Gray Diffusion Acceleration (GDA), which is a gray diffusion preconditioner for multigroup transport, using the same opacities prescribed by the GTA scheme. The GDA method exhibits multi-group error reduction similar to the GTA preconditioner and degradation for high aspect ratio geometry similar to the semi-consistent DSA method from Wareing [19, 17, 20].

One recent acceleration method for thermal radiative transport was developed by Brunner et al.[21] They eliminate the temperature Jacobian locally and perform updates to the temperature and the emission source using a low-order equation. In their paper, they explicitly cover a method where a multi-group diffusion operator is accelerated by a gray diffusion operator that updates temperature and emission sources. Their work is a generalization of the method initially developed by Nowak that performed local updates to temperature and emission sources. The thermal radiative transport method we have developed is of this family of methods, where a multi-group transport operator is accelerated by a gray diffusion operator that updates temperature and emission sources. In this family of methods, the low-order closure is included as an extra source term. Brunner demonstrates unconditional stability, provided either the high-order or low-order equations are converged fully at each step of the outermost iteration for temperature. [21]

Another family of acceleration methods for thermal radiative transport has been developed by Park et al.[22] Their approach is fundamentally different than the above methods, as their methods instead use a "consistency" term in the low-order operators to close the equations. Many low-order operators have been investigated in this family, including Quasi-Diffusion (QD) and Coarse Mesh Finite Difference (CMFD). The consistency term in QD is included through an Eddington tensor in the operator of the low-order equation. The consistency term in CMFD is included through a transport correction to Fick's law to particle flow at cell boundaries. The HOLO consistency terms act as a drift term in the diffusion operator. Haut et al. have shown conditional stability for predictor/corrector HOLO methods for thermal radiative transfer.[15] Similarly, CMFD has been shown to be conditionally stable depending on the consistency term. [12]

The close relationship between DSA and QD has been known for some time. [1, 3] It has been shown that DSA is equivalent to QD if the solution is linear in angle. Larsen and Kelley [11] have generalized this relationship and have shown that Coarse-Mesh DSA (CMDSA) is equivalent to a linearization of CMFD.

## 2.2 k-Eigenvalue

Iterative methods for general eigenvalue problems have been widely studied. Successful methods include power iteration, nonlinear Arnoldi iteration, and Chebyshev iteration. For neutronic $k$ eigenvalue problems power iteration has often been the method of choice due to simplicity and robustness in finding the largest eigenvalue and its associated eigenvector (the "fundamental" mode). However, the convergence rate of power iteration is dependent on the dominance ratio of eigenvalues, which may be arbitrarily close to one. Thus, acceleration methods for power iteration have been developed to hasten convergence.

The iterative convergence rate of Power Iteration alone can be improved by employing a Krylov method [23, 24], or casting the problem as a nonlinear PDE constraint problem and use a nonlinear solver such as a Newton-like method. However, these improvements are limited if the problem dominated by the convergence rate of the scattering problem and not the dominance ratio of the eigenvalues. [25] For realistic problems, the scattering ratio and dominance ratio are frequently close to one, and it is necessary to also accelerate the scattering problem. This has been accomplished by using low-order methods, usually involving a reduction in angle, in an inner iteration.

The current state of the art is a nested scheme that begins with a high-order solve (transport sweep) to generate parameters for a low-order $k$-eigenvalue problem. The transport sweep is followed by an eigenvalue solution of the low-order eigenvalue problem. The high-order eigenvalue and eigenvector are then updated, either linearly or nonlinearly depending on the formulation of the low-order eigenvalue problem, using the low-order solution.

Nonlinear schemes of this kind can produce true low-order eigenvalue problems. Low-order schemes have been shown to be superior to power iteration alone. Notable low-order schemes include the following: HOLO methods [26, 25], quasi-diffusion [27, 6], and coarse-mesh finitedifference (CMFD) [10, 9].

HOLO methods for k-Eigenvalue problems have been investigated by the community extensively. Willert et al. have a comprehensive comparison of combinations of Power Iteration, JFNK, and NKA when unaccelerated and preconditioned by HOLO methods. [28] They find that the most
efficient algorithm for all problems studied is when the nonlinear solver is used to solve a low-order nonlinear diffusion equation, which they call nonlinear-diffusion nonlinear-criticality acceleration (NDA-NCA).

Another approach investigated by Cornejo and Anistratov uses a hierarchy of coarse energy grids $[29,30]$. They have formulated Low-Order Nonlinear Diffusion Acceleration (LONDA) equations, and Multi-Level Quasi-Diffusion (MLQD) equations, and solved these equations with multiple different multigrid algorithms. They find that more levels shifts more work to the acceleration method and decreases the number of transport iterations required, and note that the optimal choice of solution method is problem dependent.

Recognizing stability issues that might occur for Quasi-diffusion methods, Dodson et al. developed a method that they describe as semi-linear. [31] Instead of a nonlinear closure, it defines a non-invertible diffusion operator that has a finite source term. Then, using the Fredholm Alternative theorem and one solution of an adjoint diffusion operator, they find the solvability condition of the original non-invertible diffusion operator through Rayleigh Quotient power iteration. The additional cost of solving one adjoint problem is amortized over the entire eigenvalue iteration. Alternatively, Prince et al. uses a nonlinear solver, preconditioned JFNK (PJFNK), to solve the low-order eigenvalue equation for $k$ and the correction to the scalar variable. [32]

In contrast, linear low-order schemes produce eigenvalue-like problems with fixed source terms. Although there is yet no compelling theory that explains why the modified eigenvalue problem works, and a cursory look suggests that this system could produce any number for the eigenvalue, in practice the linear low-order modified power iteration scheme accelerates convergence to the correct largest eigenvalue and the corresponding eigenvector of the discrete operator. [33, 34, 35, 32]

### 2.3 Thermal Neutron Upscattering

The current state of the art for thermal neutron scattering is a two-grid method in energy: a Gauss-Seidel iteration for a multi-group transport equation, and a one-group diffusion preconditioner. Gauss-Seidel iteration significantly reduces spatial error modes with small spatial variation,
and the one-group diffusion preconditioner is derived to reduce the spatially flat error modes for all angles and energy groups.

For scattering dominated problems the spatially flat error mode is approximately a thermal Maxwellian in energy and is nearly isotropic in angle [36], with perturbations in the energy and angle variation caused by leakage and absorption. The two-grid preconditioner was derived to eliminate the flat error mode of infinite medium problems exactly, whose spatially flat error mode is also approximately thermal Maxwellian in energy and is nearly isotropic in angle, perturbed only by absorption.

The two-grid method uses the infinite medium eigenfunction of the largest eigenvalue as a weight function for averaging and as an interpolation function for prolongation of the coarse-grid (one-group) error estimate onto the fine-grid (multi-group).

The two-grid method was derived and analyzed specifically for Gauss-Seidel iteration in one and two dimensions for linear discontinuous spatial discretizations [36]. Extension of the two-grid method to arbitrary dimension and spatial discretization requires no modification of the scheme. However, changing the operator splitting, for example from Gauss-Seidel to Jacobi, alters the transfer operator's eigenvalues and eigenfunctions, and thus the behavior of the two-grid scheme.

Because Gauss-Seidel requires successive solution of each group's transfer equation, it is difficult to distribute the computation effort among parallel processors. Jacobi iteration is trivially parallel, but performs poorly for problems dominated by scattering even with preconditioners that eliminate the flat mode, as many of the eigenvalues of other modes are close to one in magnitude. We seek to analyze and test the two-grid method applied to the Jacobi thermal scattering operator to determine its spectral radius, eigenvalue clustering, eigenfunctions, and effectiveness at solving practical problems.

## 3. DISCRETIZATION AND ITERATION METHODS

This chapter describes the discretizations we have used for the neutral particle transport equation, which are the same for each of the equations of interest, and a complete description of the equations and boundary conditions of the low-order equations that arise in our low-order problems. Descriptions of iterative methods used for different problem types are located in the corresponding chapters.

### 3.1 Discretization

In this section, we describe the representation of scattering using a truncated spherical harmonics expansion, the representation of energy dependence using multi-group energy discretization, the representation of angle dependence using discrete ordinates $\left(S_{N}\right)$, and representation of spatial dependence using a discontinuous finite element method (DFEM).

We note that all variables in the upcoming equations have spatial dependence, so we suppress this dependence until the spatial discretization is discussed.

### 3.1.1 Spherical Harmonic Representation of the Scattering Source

The complete scattering matrix describing the incoming source into the angle $\vec{\Omega}$ and energy $E$ from angle $\overrightarrow{\Omega^{\prime}}$ and energy $E^{\prime}$ would be prohibitive and unnecessary to store. Instead, the angle dependence of the scattering matrix is projected onto a basis of Legendre polynomials of the cosine of the scattering angle:

$$
\begin{equation*}
\mathcal{X}\left(\overrightarrow{\Omega^{\prime}} \cdot \vec{\Omega}, E^{\prime} \rightarrow E\right) \approx \sum_{\breve{l}=0}^{L} \frac{2 \breve{l}+1}{4 \pi} \sigma_{s, \breve{l}}\left(E^{\prime} \rightarrow E\right) P_{\breve{l}}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right), \tag{3.1}
\end{equation*}
$$

Similarly we expand $\psi\left(\vec{\Omega}^{\prime}, E^{\prime}\right)$ in terms of spherical harmonic functions:

$$
\begin{equation*}
\psi\left(\vec{\Omega}^{\prime}, E^{\prime}\right)=\sum_{l=0}^{\infty} \sum_{n=-l}^{l} \frac{2 l+1}{4 \pi} \phi_{l, n}\left(E^{\prime}\right) Y_{l}^{n}\left(\vec{\Omega}^{\prime}\right) \tag{3.2}
\end{equation*}
$$

where,

$$
\begin{equation*}
\phi_{l, n}\left(E^{\prime}\right)=\int_{4 \pi} d \Omega^{\prime} \psi\left(\vec{\Omega}^{\prime}, E^{\prime}\right)\left(Y_{l}^{n}\left(\vec{\Omega}^{\prime}\right)\right)^{*} \tag{3.3}
\end{equation*}
$$

We recognize the spherical harmonic addition theorem,

$$
\begin{equation*}
P_{\breve{l}}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)=\frac{4 \pi}{2 \breve{l}+1} \sum_{\breve{m}=-\breve{l}}^{\breve{l}} Y_{\breve{l}}^{\breve{m}}(\vec{\Omega})\left(Y_{\breve{l}}^{\breve{m}}\left(\vec{\Omega}^{\prime}\right)\right)^{*} \tag{3.4}
\end{equation*}
$$

where $\breve{l}$ and $\breve{m}$ are the indices of the degree and order of the spherical harmonic function $Y_{\breve{l}}^{\breve{m}}(\vec{\Omega})$, and $*$ denotes the complex conjugate. The spherical harmonic functions are defined as:

$$
\begin{equation*}
Y_{\breve{l}}^{\breve{m}}(\vec{\Omega})=(-1)^{\breve{m}} \sqrt{\frac{2 \breve{l}+1}{4 \pi} \frac{(\breve{l}-\breve{m})!}{(\breve{l}+\breve{m})!} P_{l}^{\breve{m}}(\cos (\breve{\theta})) e^{\mathrm{i} \breve{m} \breve{\varphi}}, ., \text {. }} \tag{3.5}
\end{equation*}
$$

where $\breve{\theta}$ and $\breve{\varphi}$ are the azimuthal and polar angles of $\vec{\Omega}$ respectively, and $P_{\breve{l}}^{\breve{m}}(\cos (\breve{\theta}))$ are associated Legendre polynomials. The first few associated Legendre polynomials are, where $\mu=\cos (\breve{\theta})$ :

$$
\begin{gather*}
P_{0}^{0}(\mu)=1,  \tag{3.6}\\
P_{1}^{0}(\mu)=\mu,  \tag{3.7}\\
P_{1}^{1}(\mu)=-\left(1-\mu^{2}\right)^{1 / 2},  \tag{3.8}\\
P_{1}^{-1}(\mu)=\frac{1}{2}\left(1-\mu^{2}\right)^{1 / 2}, \tag{3.9}
\end{gather*}
$$

We insert these expansions into the angle integral in Eq. (1.1):

$$
\begin{align*}
& \int_{4 \pi} d \Omega^{\prime} \mathcal{X}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, E^{\prime} \rightarrow E\right) \psi\left(\vec{r}, \vec{\Omega}^{\prime}, E^{\prime}\right)=\sum_{\breve{l}=0}^{L} \frac{2 \breve{l}+1}{4 \pi} \sigma_{s, \breve{l}}\left(E^{\prime} \rightarrow E\right)  \tag{3.10}\\
& \times \int_{4 \pi} d \Omega^{\prime} \frac{4 \pi}{2 \breve{l}+1} \sum_{\breve{m}=-\breve{l}}^{\breve{l}} Y_{\breve{l}}^{\breve{m}}(\vec{\Omega})\left(Y_{l}^{\breve{m}}\left(\vec{\Omega}^{\prime}\right)\right)^{*} \sum_{l=0}^{\infty} \sum_{n=-l}^{l} \frac{2 \breve{l}+1}{4 \pi} \phi_{l, n}\left(E^{\prime}\right) Y_{l}^{n}\left(\vec{\Omega}^{\prime}\right)
\end{align*}
$$

From orthogonality of spherical harmonics, the only non-zero integrals over $\vec{\Omega}^{\prime}$ are when $l=\breve{l}$ and $n=\breve{m}$ :

$$
\begin{equation*}
\int_{4 \pi} d \Omega^{\prime} \mathcal{X}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, E^{\prime} \rightarrow E\right) \psi\left(\vec{r}, \vec{\Omega}^{\prime}, E^{\prime}\right)=\sum_{l=0}^{L} \frac{2 l+1}{4 \pi} \sigma_{s, l}\left(E^{\prime} \rightarrow E\right) \sum_{n=-l}^{l} Y_{l}^{n}(\vec{\Omega}) \phi_{l, n}\left(E^{\prime}\right) \tag{3.11}
\end{equation*}
$$

### 3.1.2 Multigroup Energy Discretization

The energy dependence is resolved using a multi-group discretization, which solves the transport equation in an integral sense, with integrals over energy in $G$ discrete ranges (groups). In general these integrals should include the spatial variation of the intensity function, but in practice are often evaluated at an asymptotic distribution or at element-averaged intensities; thus, we spatial dependence of radiation intensity in the following definitions. If we number the energy boundaries in descending order, we define a group angular intensity:

$$
\begin{equation*}
\psi_{g}(\vec{\Omega})=\int_{E_{g}}^{E_{g-1}} \psi(\vec{\Omega}, E) \tag{3.12}
\end{equation*}
$$

We define a total group interaction probability:

$$
\begin{equation*}
\sigma_{t, g}=\frac{\int_{E_{g}}^{E_{g-1}} \mathcal{T}(E) \psi(\vec{\Omega}, E)}{\int_{E_{g}}^{E_{g-1}} \psi(\vec{\Omega}, E)} . \tag{3.13}
\end{equation*}
$$

We define scattering moments:

$$
\begin{equation*}
\phi_{l, n, g}=\int_{E_{g}}^{E_{g-1}} d E \phi_{l, n}(E) \tag{3.14}
\end{equation*}
$$

and a group-to-group scattering cross section for each of the scattering moments:

$$
\begin{equation*}
\sigma_{s, g^{\prime}, g, l}=\frac{\int_{E_{g}^{\prime}}^{E_{g^{\prime}-1}} d E^{\prime} \int_{E_{g}}^{E_{g-1}} d E \sigma_{s, l}\left(E^{\prime} \rightarrow E\right) \sum_{n=-l}^{l} Y_{l}^{n}(\vec{\Omega}) \phi_{l, n}\left(E^{\prime}\right)}{\int_{E_{g}^{\prime}}^{E_{g^{\prime}-1}} d E^{\prime} \sum_{n=-l}^{l} Y_{l}^{n}(\vec{\Omega}) \phi_{l, n}\left(E^{\prime}\right)}, \tag{3.15}
\end{equation*}
$$

such that:

$$
\begin{equation*}
\sigma_{s, g^{\prime}, g, l} \sum_{n=-l}^{l} Y_{l}^{n} \phi_{l, n, g}=\int_{E_{g}^{\prime}}^{E_{g^{\prime}-1}} d E^{\prime} \int_{E_{g}}^{E_{g-1}} d E \sigma_{s, l}\left(E^{\prime} \rightarrow E\right) \sum_{n=-l}^{l} Y_{l}^{n}(\vec{\Omega}) \phi_{l, n}\left(E^{\prime}\right) \tag{3.16}
\end{equation*}
$$

An external source contributes a quantity that is the integral over the group range:

$$
\begin{equation*}
q_{g}^{f i x e d}(\vec{\Omega})=\int_{E_{g}}^{E_{g-1}} d E q^{f i x e d}(\vec{\Omega}, E) . \tag{3.17}
\end{equation*}
$$

To summarize the discretizations thus far, we write the transport equation in block matrix form, where capital letters signify matrices and vectors in energy groups:

$$
\begin{equation*}
\vec{\Omega} \cdot \vec{\nabla} \Psi(\vec{\Omega})+T \Psi(\vec{\Omega})=\sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l} \sum_{n=-l}^{l} Y_{l}^{n}(\vec{\Omega}) \Phi_{l, n}+Q^{f i x e d}(\vec{\Omega}) \tag{3.18}
\end{equation*}
$$

The integrals in this section contain the energy-dependence of $\psi(\vec{\Omega}, E)$ and $\phi_{l, n}(E)$, which are not known during the current solution. In practice, the cross sections are calculated using an approximate spectrum in their places.

### 3.1.3 Discrete Ordinates Angular Discretization

Since the choice of angular discretization affects the spatial discretization due to upwinding, we describe the angular discretization first. We choose the method of discrete-ordinates $\left(S_{n}\right)$, where the radiative transfer equations are discretized in angle and solved along the direction of particle travel. In the discrete-ordinates method, integrals over solid angle become become quadrature sums over all $M$ discrete angles, e.g. the angular intensity integral becomes:

$$
\begin{equation*}
\int_{4 \pi} d \Omega^{\prime} \psi(\vec{\Omega}) \approx \sum_{m=0}^{M} w_{m} \Psi\left(\vec{\Omega}_{m}\right)=\sum_{m=0}^{M} w_{m} \Psi_{m} \tag{3.19}
\end{equation*}
$$

where $w_{m}$ is the quadrature weight associated with the discrete angle $\vec{\Omega}_{m}$, and quantities dependent on $\vec{\Omega}_{m}$ are denoted with a subscript $m$. The transport equation with discrete-ordinates discretization is:

$$
\begin{equation*}
\vec{\Omega}_{m} \cdot \vec{\nabla} \psi_{m, g}+T \Psi_{m}=\sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right) \Phi_{l, n}+\frac{1}{4 \pi} Q_{m}^{f i x e d} \tag{3.20}
\end{equation*}
$$

We also define several commonly used moments of the angular intensity:

$$
\begin{gather*}
\sum_{m=0}^{M} w_{m} \Psi_{m}=\Phi,  \tag{3.21}\\
\sum_{m=0}^{M} w_{m} \vec{\Omega}_{m} \Psi_{m}=\vec{J},  \tag{3.22}\\
\sum_{m=0}^{M} w_{m} \vec{\Omega}_{m} \vec{\Omega}_{m} \Psi_{m}=\overrightarrow{\vec{P}} . \tag{3.23}
\end{gather*}
$$

The transport operator with spherical harmonic scattering, multi-group energy discretization, and discrete ordinates angle discretization is:

$$
\begin{equation*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) \Psi_{m}=\sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right) \Phi_{l, n}+\frac{1}{4 \pi} Q_{m}^{f i x e d} . \tag{3.24}
\end{equation*}
$$

### 3.1.4 Discontinuous Finite Element Method Spatial Discretization

We discretize the spatial dependence of the transport solution using a discontinuous Galerkin finite element method. The discontinuous Galerkin method uses the same basis functions with local support to an individual element of the mesh to represent the test function and solution function in the weak bilinear form. Galerkin methods are a common choice as this guarantees the discrete system is well-posed. Having the test and solution functions equal will also be important when deriving the low-order equation, as we perform integration by parts on the leakage operator. Using basis functions that are discontinuous allow upwinding schemes that are important physically, where it is important to capture the forward travel of particles, and mathematically, to obtain fully implicit spatial dependencies that do not require prohibitively large number of degrees of freedom to satisfy stability criteria.

We discretize the solution function by expressing it as a vector of coefficients multiplying a vector of piecewise polynomial discontinuous basis functions. The discontinuous functions we choose have local support (are only non-zero) within a spatial element ( $\tau$ ) that they represent. Because of the discontinuous basis functions, it is useful to express the solution discretization as a sum of all elements in the global domain, $\Gamma$ :

$$
\begin{gather*}
\Psi_{m}(\vec{r})=\sum_{\tau \in \Gamma} \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau} .  \tag{3.25}\\
\Phi_{l, n}(\vec{r})=\sum_{\tau \in \Gamma} \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Phi}_{\tau} \tag{3.26}
\end{gather*}
$$

To simplify the following derivation, we assume constant spatial dependence of interaction probabilities within an individual element.

We obtain the discontinuous Galerkin weak bilinear equations by taking the inner product of the vector of basis functions we used to discretize the solution and the discrete equation itself. The local nature of the basis functions produces many systems of local equations where the inner products are only nonzero within the element the basis functions have support; we look at one of
these local systems of equations now:

$$
\begin{align*}
& \vec{\Omega}_{m} \cdot \int_{\tau} d V \underline{b}_{\tau}(\vec{r}) \vec{\nabla} \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau}+T_{\tau} \int_{\tau} d V \underline{b}_{\tau}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau} \\
& \quad=\sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right) \int_{\tau} d V \underline{b}_{\tau}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r}) \Phi_{l, n, \tau}+\int_{\tau} d V \underline{b}_{\tau}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r}) \underline{Q}_{m, \tau}^{f i x e d} \tag{3.27}
\end{align*}
$$

We use integration by parts on the left hand side gradient term, introducing discontinuous surface quantities on each of the boundary faces $\left(\partial \tau_{k}\right)$ of the element:

$$
\begin{equation*}
\int_{\tau} d V \underline{b}_{\tau}(\vec{r}) \vec{\Omega}_{m} \cdot \vec{\nabla} \underline{\underline{b}}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau}=\sum_{k \in \partial \tau} \int_{\partial \tau_{k}} d S \vec{\Omega}_{m} \cdot \vec{n}_{k} \underline{b}_{\tau}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau, k}-\int_{\tau} d V \vec{\nabla}_{\underline{b}}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau} \tag{3.28}
\end{equation*}
$$

At the interfaces between neighbors, we "upwind" the surface quantities by choosing "upstream" of the direction of flow.

$$
\underline{\Psi}_{m, \tau, k}=\left\{\begin{array}{l}
\underline{\Psi}_{m, \tau}, \vec{\Omega}_{m} \cdot \vec{n}_{k}>0  \tag{3.29}\\
\underline{\Psi}_{m, \tau, k+}, \vec{\Omega}_{m} \cdot \vec{n}_{k}<0
\end{array}\right.
$$

where $\vec{n}_{k}$ is the outward unit normal averaged across the given face, and $\underline{\Psi}_{m, \tau, k+}$ are the upwind unknowns in the neighboring element with shared face $k$. This forms a closure that couples neighboring cells across discontinuities.

In order to "lump" the mass matrix, an operation that diagonalizes the mass matrix and surface matrices, we perform an additional step. Without this step, lumping the surface matrix in the above equation would effectively modify the leakage operator. Instead, we add and subtract a surface term:

$$
\begin{align*}
\int_{\tau} d V \underline{b}_{\tau}(\vec{r}) \vec{\nabla} \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau} & =\sum_{k \in \partial \tau} \int_{\partial \tau_{k}} d S \vec{n}_{k} \underline{b}_{\tau}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau, k}-\sum_{k \in \partial \tau} \int_{\partial \tau_{k}} d S \vec{n}_{k} \underline{b}_{\tau}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau} \\
& +\sum_{k \in \partial \tau} \int_{\partial \tau_{k}} d S \vec{n}_{k} \underline{b}_{\tau}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau}-\int_{\tau} d V \vec{\nabla}_{b_{\tau}}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau} \tag{3.30}
\end{align*}
$$

and reverse integration by parts of terms that only include within cell quantities:

$$
\begin{align*}
\int_{\tau} d V \underline{b}_{\tau}(\vec{r}) \vec{\nabla} \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau} & =\sum_{k \in \partial \tau} \int_{\partial \tau_{k}} d S \vec{n}_{k} \underline{b}_{\tau}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r})\left[\underline{\Psi}_{m, \tau, k}-\underline{\Psi}_{m, \tau}\right]  \tag{3.31}\\
& +\int_{\tau} d V \underline{b}_{\tau}(\vec{r}) \vec{\nabla} \underline{b}_{\tau}^{T}(\vec{r}) \underline{\Psi}_{m, \tau}
\end{align*}
$$

We define a system of naming matrices. $\underline{\underline{A}}$ denotes a finite element matrix with one underline per extent (row, column) of the matrix. A pair of numbers in the superscript denote the gradients of the test function and solution function respectively, which for our equation is only either 0 or 1 . An arrow over the matrix denotes a spatial vector of matrices. The subscript denotes the range of the integral (surface, volume).

$$
\begin{align*}
& \int_{\tau} d V \underline{b}_{\tau}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r})=\underline{\underline{A}}_{\tau}^{00},  \tag{3.32}\\
& \int_{\partial \tau_{k}} d S \underline{b}_{\tau}(\vec{r}) \underline{b}_{\tau}^{T}(\vec{r})=\underline{\underline{A}}_{\partial \tau_{k}}^{00},  \tag{3.33}\\
& \int_{\tau} d V \underline{b}_{\tau}(\vec{r}) \vec{\nabla} \underline{b}_{\tau}^{T}(\vec{r})=\underline{\underline{A}}_{\tau}^{01} . \tag{3.34}
\end{align*}
$$

Then we have matrix of equations for the weak bilinear form of the transport equation for the element $\tau$ :

$$
\begin{align*}
& \vec{\Omega}_{m} \cdot \sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\underline{\Psi}_{m, \tau, k}-\underline{\Psi}_{m, \tau}\right] \\
+ & \vec{\Omega}_{m} \cdot \underline{\underline{A}}_{\tau}^{01} \underline{\Psi}_{m, \tau}+T_{\tau} \underline{\underline{A}}_{\tau}^{00} \underline{\Psi}_{m, \tau}=\sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right) \underline{\underline{A}}_{\tau}^{00} \Phi_{l, n, \tau}+\frac{1}{4 \pi} \underline{\underline{A}}_{\tau}^{00} \underline{Q}_{m, \tau}^{f i x e d} \tag{3.35}
\end{align*}
$$

The global discontinuous finite element matrix is the sum of all of the individual element matrices, which are coupled through the upwinding scheme. In practice, the global system is never explicitly formed as doing so is computationally prohibitive, and instead each element's local matrix is used during calculation. In the subsequent sections, we will also derive low-order operators from the local element matrices.

### 3.2 Source Iteration Scheme

Equation (3.35) is difficult to solve because of coupling across all angles through the scattering term. The source iteration scheme lags some component of the scattering term to a previous iteration to solves a simpler fixed source problem. Here we describe the source iteration scheme, where the down-scattering from groups that are fully determined are at iteration index $i+1$, up-scattering between groups is calculated in an outer iteration and are at index $i$, and the within-group scattering is calculated in an inner iteration at index $l$ :

$$
\begin{align*}
& \vec{\Omega}_{m} \cdot \sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\underline{\Psi}_{m, \tau, k}^{(l+1 / 2)}-\underline{\Psi}_{m, \tau}^{(l+1 / 2)}\right] \\
+ & \vec{\Omega}_{m} \cdot \underline{\underline{\vec{A}}}_{\tau}^{01} \underline{\Psi}_{m, \tau}^{(l+1 / 2)}+T_{\tau} \underline{\underline{A}}_{\tau}^{00} \underline{\Psi}_{m, \tau}^{(l+1 / 2)} \\
= & \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l, D} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right) \underline{\underline{A}}_{\tau}^{00} \Phi_{l, n, \tau}^{(l)}  \tag{3.36}\\
+ & \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l, L} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right) \underline{\underline{A}}_{\tau}^{00} \Phi_{l, n, \tau}^{(i+1)} \\
+ & \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l, U} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right) \underline{\underline{A}}_{\tau}^{00} \Phi_{l, n, \tau}^{(i)}+\frac{1}{4 \pi} \underline{\underline{A}}_{\tau}^{00} \underline{Q}_{m, \tau}^{f i x e d}
\end{align*} .
$$

The next moments are found with a discrete to moment operator, $W$ :

$$
\begin{equation*}
\underline{\Phi}_{\tau}^{(l+1 / 2)}=W \underline{\Psi}_{m, \tau}^{(l+1 / 2)} \tag{3.37}
\end{equation*}
$$

If no moments are accelerated, the moments of the next iterate are set to the current best solution:

$$
\begin{equation*}
\underline{\Phi}_{\tau}^{(i+1)}=\underline{\Phi}_{\tau}^{(l+1 / 2)} . \tag{3.38}
\end{equation*}
$$

The source iteration scheme can be arbitrarily slow to converge based on the scattering ratio of the problem. Krylov iterative algorithms may have better convergence properties, but may still have difficulty converging problems with high effective scattering media. It is best to combine an advanced iterative method with an acceleration method using a low-order operator that is derived from physical intuition of the system and is consistent with the discretization of the original equation. [2, 1]

### 3.2.1 Fourier Analysis of a Gray Source Iteration Scheme

We now derive the behavior of source iteration when no discretization is introduced; the behavior that results demonstrates the error reduction purely of source iteration without contamination from discretization errors. For simplicity we only consider isotropic scattering (first degree spherical harmonic scattering sources are addressed in chapter 6), a homogeneous problem domain, and do not consider energy dependence of the system (gray). We begin with the gray homogeneous transport problem definition, which the converged solution (index $C$ ) satisfies:

$$
\begin{array}{r}
\vec{\Omega} \cdot \vec{\nabla} \psi^{(C)}(\vec{r}, \vec{\Omega})+\sigma_{t} \psi^{(C)}(\vec{r}, \vec{\Omega}) \\
=\int_{4 \pi} d \Omega^{\prime} \sigma_{s} \psi^{(C)}\left(\vec{r}, \overrightarrow{\Omega^{\prime}}\right)+Q^{f i x e d}(\vec{r}, \vec{\Omega}), \tag{3.39}
\end{array}
$$

and the Source Iteration scheme applied to this problem:

$$
\begin{align*}
& \vec{\Omega} \cdot \vec{\nabla} \psi^{(l+1 / 2)}(\vec{r}, \vec{\Omega})+\sigma_{t} \psi^{(l+1 / 2)}(\vec{r}, \vec{\Omega}) \\
= & \int_{4 \pi} d \Omega^{\prime} \sigma_{s} \psi^{(l)}\left(\vec{r}, \vec{\Omega}^{\prime}\right)+\frac{1}{4 \pi} Q^{f i x e d}(\vec{r}, \vec{\Omega}) \tag{3.40}
\end{align*}
$$

We define an equation for the iteration error by subtracting source iteration scheme from the converged equation that satisfies the initial problem:

$$
\begin{equation*}
\vec{\Omega} \cdot \vec{\nabla} \psi_{\dagger}^{(l+1 / 2)}(\vec{r}, \vec{\Omega})+\sigma_{t} \psi_{\dagger}^{(l+1 / 2)}(\vec{r}, \vec{\Omega})=\sigma_{s} \phi_{\dagger}^{(l)}(\vec{r}) \tag{3.41}
\end{equation*}
$$

Here terms denoted by $\dagger$ are errors to their respective transport quantities, which are defined as:

$$
\begin{gather*}
\phi_{\dagger}^{(l)}(\vec{r})=\phi^{(C)}-\phi^{(l)}(\vec{r})  \tag{3.42}\\
\psi_{\dagger}^{(l+1 / 2)}(\vec{r}, \vec{\Omega})=\psi^{(C)}(\vec{\Omega})-\psi^{(l+1 / 2)}(\vec{r}, \vec{\Omega}),  \tag{3.43}\\
\phi_{\dagger}^{(l+1)}(\vec{r})=\phi^{(C)}-\phi^{(l+1)}(\vec{r}) \tag{3.44}
\end{gather*}
$$

We expand transport errors into infinite Fourier modes:

$$
\begin{gather*}
\phi_{\dagger}^{(l)}(\vec{r})=\iiint_{0}^{\infty} d^{3} \lambda a(\vec{\lambda}) \omega^{l} e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}},  \tag{3.45}\\
\psi_{\dagger}^{(l+1 / 2)}(\vec{r}, \vec{\Omega})=\iiint_{0}^{\infty} d^{3} \lambda b(\vec{\Omega}, \vec{\lambda}) \omega^{l} e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}},  \tag{3.46}\\
\phi_{\dagger}^{(l+1)}(\vec{r})  \tag{3.47}\\
=\iiint_{0}^{\infty} d^{3} \lambda a(\vec{\lambda}) \omega^{l+1} e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}},
\end{gather*}
$$

and use the fact that each of these modes is orthogonal to obtain an equation that each of the modes
must independently satisfy:

$$
\begin{equation*}
\left(\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{\Omega}+\sigma_{t}\right) b(\vec{\Omega}, \vec{\lambda}) \omega^{l} e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}}=\frac{1}{4 \pi} \sigma_{s} a(\vec{\lambda}) \omega^{l} e^{i \vec{\lambda} \cdot \vec{r}} . \tag{3.48}
\end{equation*}
$$

We solve for $b(\vec{\Omega}, \vec{\lambda})$ :

$$
\begin{equation*}
b(\vec{\Omega}, \vec{\lambda})=\frac{1}{4 \pi} \frac{1}{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{\Omega}+\sigma_{t}} \sigma_{t} a(\vec{\lambda}) \tag{3.49}
\end{equation*}
$$

After we multiply and divide by $\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{\Omega}-\sigma_{t}$ :

$$
\begin{equation*}
b(\vec{\Omega}, \vec{\lambda})=\frac{1}{4 \pi} \frac{1-\mathbf{i} \vec{\lambda} \cdot \vec{\Omega}}{1+(\vec{\lambda} \cdot \vec{\Omega})^{2}} \frac{\sigma_{s}}{\sigma_{t}} a(\vec{\lambda}) \tag{3.50}
\end{equation*}
$$

Then $\phi_{\dagger}^{(l+1 / 2)}$ is the integral of $\psi_{\dagger}(\vec{\Omega})$ :

$$
\begin{align*}
\phi_{\dagger}^{(l+1 / 2)} & =\int_{4 \pi} d \Omega \omega^{l} e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}} \frac{1}{4 \pi} \frac{1-\mathbf{i} \vec{\lambda} \cdot \vec{\Omega}}{1+(\vec{\lambda} \cdot \vec{\Omega})^{2}} \frac{\sigma_{s}}{\sigma_{t}} a(\vec{\lambda}),  \tag{3.51}\\
& =\frac{\tan ^{-1}(\vec{\lambda})}{\vec{\lambda}} \omega^{l} e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}} \frac{\sigma_{s}}{\sigma_{t}} a(\vec{\lambda}) .
\end{align*}
$$

We use the update equation to solve for the iteration error reduction per iteration, $\omega_{S I}$ :

$$
\begin{equation*}
\omega_{S I}=\int_{4 \pi} d \Omega \frac{1}{4 \pi} \frac{1}{1+(\vec{\lambda} \cdot \vec{\Omega})^{2}} \frac{\sigma_{s}}{\sigma_{t}}=\frac{\tan ^{-1}(|\vec{\lambda}|)}{|\vec{\lambda}|} \frac{\sigma_{s}}{\sigma_{t}} . \tag{3.52}
\end{equation*}
$$

The slowest error reduction occurs when $\vec{\lambda}=0$ :

$$
\begin{equation*}
\max \left(\omega_{S I}\right)=\frac{\sigma_{s}}{\sigma_{t}} . \tag{3.53}
\end{equation*}
$$

### 3.2 2 Fourier Analysis of Diffusion Acceleration for a One Group Source Iteration Scheme

We obtain an equation for a correction defined by:

$$
\begin{equation*}
f^{(l+1 / 2)}(\vec{r}, \vec{\Omega})=\psi^{(C)}(\vec{r}, \vec{\Omega})-\psi^{(l+1 / 2)}(\vec{r}, \vec{\Omega}) \tag{3.54}
\end{equation*}
$$

by subtracting the the source iteration equation from the converged transport equation:

$$
\begin{equation*}
\vec{\Omega} \cdot \vec{\nabla} f^{(l+1 / 2)}(\vec{r}, \vec{\Omega})+\sigma_{t} f^{(l+1 / 2)}(\vec{r}, \vec{\Omega})=\sigma_{s} \int_{4 \pi} d \Omega \psi^{(C)}(\vec{r}, \vec{\Omega})-\sigma_{s} \phi^{(l)}(\vec{r}) \tag{3.55}
\end{equation*}
$$

We add and subtract $\sigma_{s} \int_{4 \pi} d \Omega \psi^{(l+1 / 2)}(\vec{r}, \vec{\Omega})$ on the right hand side:

$$
\begin{equation*}
\vec{\Omega} \cdot \vec{\nabla} f^{(l+1 / 2)}(\vec{r}, \vec{\Omega})+\sigma_{t} f^{(l+1 / 2)}(\vec{r}, \vec{\Omega})=\sigma_{s} \int_{4 \pi} d \Omega f^{(l+1 / 2)}(\vec{\Omega})+\sigma_{s} \phi^{(l+1 / 2)}(\vec{r})-\sigma_{s} \phi^{(l)}(\vec{r}) . \tag{3.56}
\end{equation*}
$$

To generate a simpler equation for an approximate correction, we make the approximation that the correction, $f^{(l+1 / 2)}(\vec{r}, \vec{\Omega})$, is linear in angle:

$$
\begin{equation*}
f^{(l+1 / 2)}(\vec{r}, \vec{\Omega}) \approx \frac{1}{4 \pi}\left(F^{(l+1 / 2)}(\vec{r})+3 \vec{\Omega} \cdot \vec{G}^{(l+1 / 2)}(\vec{r})\right) \tag{3.57}
\end{equation*}
$$

and take 0th and 1st angular moments of the error equation:

$$
\begin{gather*}
\vec{\nabla} \cdot \vec{G}^{(l+1 / 2)}(\vec{r})+\left(\sigma_{t}-\sigma_{s}\right) F^{(l+1 / 2)}(\vec{r})=\sigma_{s} \phi^{(l+1 / 2)}-\sigma_{s} \phi^{(l)}(\vec{r}),  \tag{3.58}\\
\frac{1}{3} \vec{\nabla} F^{(l+1 / 2)}(\vec{r})+\sigma_{t} \vec{G}^{(l+1 / 2)}(\vec{r})=0 . \tag{3.59}
\end{gather*}
$$

We eliminate $\vec{G}^{(l+1 / 2)}(\vec{r})$ using the 1 st moment and obtain a one group diffusion equation for a scalar correction:

$$
\begin{equation*}
-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2} F^{(l+1 / 2)}(\vec{r})+\left(\sigma_{t}-\sigma_{s}\right) F^{(l+1 / 2)}(\vec{r})=\sigma_{s} \phi^{(l+1 / 2)}(\vec{r})-\sigma_{s} \phi^{(l)}(\vec{r}) \tag{3.60}
\end{equation*}
$$

Instead of the simple update equation used before, we use a linear combination of the highorder iterate and low-order correction:

$$
\begin{equation*}
\phi^{(l+1)}(\vec{r})=\phi^{(l+1 / 2)}(\vec{r})+F^{(l+1 / 2)}(\vec{r}) . \tag{3.61}
\end{equation*}
$$

Following the same steps for the error in the scalar correction and the corresponding update obtains similar equations:

$$
\begin{gather*}
-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2} F_{\dagger}^{(l+1 / 2)}(\vec{r})+\left(\sigma_{t}-\sigma_{s}\right) F_{\dagger}^{(l+1 / 2)}(\vec{r})=\sigma_{s} \phi_{\dagger}^{(l+1 / 2)}(\vec{r})-\sigma_{s} \phi_{\dagger}^{(l)}(\vec{r}),  \tag{3.62}\\
\phi_{\dagger}^{(l+1)}(\vec{r})=\phi_{\dagger}^{(l+1 / 2)}(\vec{r})+F_{\dagger}^{(l+1 / 2)}(\vec{r}) . \tag{3.63}
\end{gather*}
$$

We expand the diffusion correction error in infinite Fourier modes:

$$
\begin{equation*}
F_{\dagger}^{(l+1 / 2)}(\vec{r})=\iiint_{0}^{\infty} d^{3} \lambda d \lambda c(\vec{\lambda}) \omega^{l} h(\vec{\lambda}) e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}} \tag{3.64}
\end{equation*}
$$

The following equation must be satisfied mode by mode, where we have already determined $\phi_{\dagger}^{(l+1 / 2)}(\vec{r})$ in the previous subsection:

$$
\begin{equation*}
\frac{1}{3} \sigma_{t}|\vec{\lambda}|^{2} \omega^{l} h(\vec{\lambda})+\left(\sigma_{t}-\sigma_{s}\right) h(\vec{\lambda})=\sigma_{s} \phi_{\dagger}^{(l+1 / 2)}(\vec{r})-\sigma_{s} \phi_{\dagger}^{(l)}(\vec{r}) . \tag{3.65}
\end{equation*}
$$

We solve for $h(\vec{\lambda})$ :

$$
\begin{equation*}
h(\vec{\lambda})=\frac{1}{\left(\frac{1}{3}|\vec{\lambda}|^{2}+\left(1-\frac{\sigma_{s}}{\sigma_{t}}\right)\right)} \frac{\sigma_{s}}{\sigma_{t}}\left(\frac{\sigma_{s}}{\sigma_{t}} \frac{\tan ^{-1}(|\vec{\lambda}|)}{|\vec{\lambda}|}-1\right) a(\vec{\lambda}) \tag{3.66}
\end{equation*}
$$

and we use the update equation to solve for $\omega_{D S A}$ :

$$
\begin{equation*}
\omega_{D S A}=\frac{\sigma_{s}}{\sigma_{t}} \frac{\tan ^{-1}(|\vec{\lambda}|)}{|\vec{\lambda}|}+\frac{1}{\left(\frac{1}{3}|\vec{\lambda}|^{2}+\left(1-\frac{\sigma_{s}}{\sigma_{t}}\right)\right)} \frac{\sigma_{s}}{\sigma_{t}}\left(\frac{\sigma_{s}}{\sigma_{t}} \frac{\tan ^{-1}(|\vec{\lambda}|)}{|\vec{\lambda}|}-1\right) . \tag{3.67}
\end{equation*}
$$

We compare the error reduction per mode for Source Iteration and DSA for Source Iteration in Figure 3.1.


Figure 3.1: Error reduction per mode for Source Iteration with and without DSA.

### 3.3 Discretization of Low-Order Acceleration Equations

We describe a particular low-order operator we have developed and implemented that uses a continuous-diffusion operator to approximate surface quantities in the fully-consistent diffusion operator. Included in this section is a derivation of the fully-consistent operator, the continuousdiffusion operator, the surface-approximated diffusion operator, with vacuum, reflecting, and opposed reflecting boundary conditions for each operator.

From the discrete transport source iteration scheme in Eq. (3.36), we make several notable changes. First, we eschew the angular discretization to determine angular moments that arise analytically. While the angular moments can be calculated using the discrete quadrature, it is useful to determine them analytically. In addition, we have found from previous work that the analytic terms do not cause sufficient inconsistency to cause the method to degrade.[19] Because we derive the equation for each energy group and spatial mesh as an independent set of equations, we make omit the indices $g$ and $\tau$ from all of the variables and treat any source from other groups as an external source for the current iteration. Finally, we only consider isotropic scattering because we are only considering acceleration of the scalar intensity.

$$
\begin{align*}
& \vec{\Omega} \cdot \sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\underline{\psi}_{k}^{(l+1 / 2)}(\vec{\Omega})-\underline{\psi}^{(l+1 / 2)}(\vec{\Omega})\right]  \tag{3.68}\\
+ & \vec{\Omega} \cdot \overrightarrow{\underline{A}}_{\tau}^{01} \underline{\Psi}^{(l+1 / 2)}(\vec{\Omega})+\sigma_{t} \underline{\underline{A}}_{\tau}^{00} \underline{\Psi}^{(l+1 / 2)}(\vec{\Omega})=\sigma_{s} \phi^{(l)}+\underline{Q}^{f i x e d}(\vec{\Omega})
\end{align*}
$$

where the external source is determined from terms not in the inner iteration:

$$
\begin{equation*}
\underline{Q}^{f i x e d}(\vec{\Omega})=\sum_{g^{\prime}=g+1}^{G} \sigma_{s, g^{\prime}, g, \tau}(\vec{\Omega}) \phi_{g^{\prime}, \tau}^{(i+1)}+\sum_{g^{\prime}=1}^{g-1} \sigma_{s, g^{\prime}, g, \tau}(\vec{\Omega}) \phi_{g^{\prime}, \tau}^{(i)}+\underline{Q}^{\text {fixed }}(\vec{\Omega}) \text {. } \tag{3.69}
\end{equation*}
$$

As in the Fourier analysis above, we define a correction to the converged solution:

$$
\begin{equation*}
\underline{f}^{(l+1 / 2)}(\vec{\Omega})=\underline{\psi}^{(C)}(\vec{\Omega})-\underline{\psi}^{(l+1 / 2)}(\vec{\Omega}) . \tag{3.70}
\end{equation*}
$$

We subtract the iteration equation from the converged equation to obtain an equation for a correction. Note that this equation has only one surface sum that depends on the "upwind" correction:

$$
\begin{align*}
& \sum_{k \in \partial \tau} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega}) \\
- & \vec{\Omega} \cdot\left[-\sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}+\underline{\underline{A}}_{\tau}^{01}\right] \underline{f}^{(l+1 / 2)}(\vec{\Omega})+\sigma_{t} \underline{\underline{A}}_{\tau}^{00} \underline{f}^{(l+1 / 2)}(\vec{\Omega})  \tag{3.71}\\
= & \frac{\sigma_{s}}{4 \pi} \underline{\underline{A}}_{\tau}^{00} \int_{4 \pi} d \Omega^{\prime} \underline{f}^{(l+1 / 2)}\left(\vec{\Omega}^{\prime}\right)+\underline{\psi}^{(l+1 / 2)}\left(\vec{\Omega}^{\prime}\right)-\underline{\psi}^{(l)}\left(\vec{\Omega}^{\prime}\right)
\end{align*}
$$

At this point we make an approximation, since this equation is as difficult to solve as the original transport equation. Alcouffe showed that the low-order equation must be "consistent" in some sense with the discrete transport equation to effectively accelerate scattering iteration. [2] Next we obtain the fully consistent DFEM DSA method using a four step procedure developed by Larsen. [37, 38, 1]

### 3.3.1 Fully Consistent Discontinuous Finite Element Method Diffusion Synthetic Acceleration

We obtain a fully consistent diffusion-like set of equations by approximating the correction as linear varying in angle, the $P_{1}$ approximation:

$$
\begin{equation*}
\underline{f}^{(l+1 / 2)}(\vec{\Omega}) \approx \frac{1}{4 \pi}(\underline{F}+3 \vec{\Omega} \cdot \underline{\vec{G}}) . \tag{3.72}
\end{equation*}
$$

We then find the zeroth angular moment:

$$
\begin{align*}
& \int_{4 \pi} d \Omega \sum_{k \in \partial \tau} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega}) \\
- & {\left[-\sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}+\underline{\underline{\vec{A}}}_{\tau}^{01}\right] \cdot \underline{\vec{G}}+\sigma_{a} \underline{\underline{A}}_{\tau}^{00} \underline{F}, }  \tag{3.73}\\
= & \sigma_{s} \underline{\underline{A}}_{\tau}^{00}\left(\underline{\phi}^{(l+1 / 2)}-\underline{\phi}^{(l)}\right)
\end{align*}
$$

and the first angular moment:

$$
\begin{align*}
& \int_{4 \pi} d \Omega \vec{\Omega} \sum_{k \in \partial \tau} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} f_{k}^{(l+1 / 2)}(\vec{\Omega}) \\
- & \frac{1}{3}\left[-\sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}+\underline{\underline{A}}_{\tau}^{01}\right] \underline{F}+\sigma_{t} \underline{\underline{A}}_{\tau}^{00} \underline{\vec{G}} .  \tag{3.74}\\
= & 0
\end{align*}
$$

The update equation for the next iterate when only the scalar intensity is corrected:

$$
\begin{equation*}
\underline{\phi}^{(l+1)}=\underline{\phi}^{(l+1 / 2)}+\underline{F}^{(l+1 / 2)} . \tag{3.75}
\end{equation*}
$$

We note that while it is possible to reverse integration by parts (again) to make fewer sums over faces; however, doing so creates errors that must be accounted for if the surface matrix is lumped. These equations form a coupled system of equations through the upstream face quantities that must be solved globally. Evaluation of the integrals of the surface quantities requires that we input the upwinding scheme we have chosen, and depends on the boundary condition for that surface. In the following sections, we devise the exact form of the boundary term for some boundaries we encounter in common problems: interior face boundaries, vacuum boundaries, reflecting boundaries, and opposing reflected boundaries.

### 3.3.1.1 Interior Boundaries

In the 0th moment equation, the interior boundary term is expressed as:

$$
\begin{align*}
\int_{4 \pi} d \Omega & \sum_{k \in \text { Interior }} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega}) \\
& =\sum_{k \in \text { Interior }} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\alpha_{\text {inc }}^{F 0} \underline{F}_{k+}+\alpha_{o u t}^{F 0} \underline{F}+\vec{\alpha}_{\text {inc }, k}^{G 0} \cdot \underline{\vec{G}}_{k+}+\vec{\alpha}_{o u t, k}^{G 0} \cdot \underline{\vec{G}}\right], \tag{3.76}
\end{align*}
$$

where the $\alpha$ constants are defined by the half range continuous angle integrals:

$$
\begin{align*}
& \alpha_{o u t}^{F 0}=\frac{1}{4 \pi} \int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{\Omega} \cdot \vec{n}_{k}=\frac{1}{4}, \\
& \alpha_{i n c}^{F 0}=\frac{1}{4 \pi} \int_{\vec{n}_{k} \cdot \vec{\Omega}<0} d \Omega \vec{\Omega} \cdot \vec{n}_{k}=-\frac{1}{4},  \tag{3.77}\\
& \vec{\alpha}_{o u t, k}^{G 0}=\frac{3}{4 \pi} \int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k}=\frac{1}{2} \vec{n}_{k}, \\
& \vec{\alpha}_{\text {inc,k}}^{G 0}=\frac{3}{4 \pi} \int_{\vec{n}_{k} \cdot \vec{\Omega}<0} d \Omega \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k}=\frac{1}{2} \vec{n}_{k} .
\end{align*}
$$

In the $1^{\text {st }}$ moment equation, the interior boundary term is:

$$
\begin{align*}
\int_{4 \pi} d \Omega & \sum_{k \in \text { Interior }} \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega}) \\
& =\sum_{k \in \text { Interior }} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\vec{\alpha}_{i n c, k}^{F 1} \underline{F}_{k+}+\vec{\alpha}_{o u t, k}^{F 1} \underline{F}+\overrightarrow{\hat{\alpha}}_{\text {inc }}^{G 1} \underline{\vec{G}_{k+}}+\overrightarrow{\vec{\alpha}}_{\text {out }}^{G 1} \underline{\vec{G}}\right] \tag{3.78}
\end{align*}
$$

where,

$$
\begin{align*}
& \vec{\alpha}_{i n c, k}^{F 1}=\frac{1}{4 \pi} \int_{\vec{n}_{k} \cdot \vec{\Omega}<0} d \Omega \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k}=\frac{1}{6} \vec{n}_{k},  \tag{3.79}\\
& \vec{\alpha}_{o u t, k}^{F 1}=\frac{1}{4 \pi} \int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k}=\frac{1}{6} \vec{n}_{k} .
\end{align*}
$$

We evaluate the remaining coefficient more carefully. To evaluate the resulting 2D tensor of $\vec{\Omega} \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k}$, we choose substitutions:

$$
\begin{gather*}
\vec{\Omega} \cdot \vec{n}_{k}=\mu  \tag{3.80}\\
\vec{\Omega}=\left[\mu \vec{n}_{k}+\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{1}+\left(1-\mu^{2}\right)^{1 / 2} \sin (\gamma) \vec{e}_{2}\right], \tag{3.81}
\end{gather*}
$$

where $\vec{e}_{1}, \vec{e}_{2}$ are unit vectors orthogonal to $\vec{n}_{k}$ and themselves, and $\gamma$ is the azimuthal angle about $\vec{n}_{k}$. We insert the substitutions into the interior boundary outgoing half-range integral:

$$
\begin{align*}
\overrightarrow{\vec{\alpha}}_{\text {out }}^{G 1} & =\frac{3}{4 \pi} \int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{\Omega} \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k}, \\
& =\frac{3}{4 \pi} \int_{\mu>0} d \mu \int_{2 \pi} d \gamma\left(\begin{array}{l}
\mu \\
\times\left[\mu \vec{n}_{k}+\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{1}+\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{2}\right] \\
\\
\times\left[\mu \vec{n}_{k}+\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{1}+\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{2}\right]
\end{array}\right) \tag{3.82}
\end{align*}
$$

First we evaluate the integral of $\gamma$. We note that terms that are linear in either $\cos (\gamma), \sin (\gamma)$, or both are identically zero:

$$
\overrightarrow{\vec{\alpha}}_{o u t}^{G 1}=\frac{3}{4 \pi} \int_{\mu>0} d \mu 2 \pi\left[\begin{array}{l}
\mu^{3} \vec{n}_{k} \vec{n}_{k}+\left(\mu-\mu^{3}\right) \vec{e}_{1} \vec{e}_{1}+\left(\mu-\mu^{3}\right) \vec{e}_{2} \vec{e}_{2}  \tag{3.83}\\
+0 \times\left(\vec{n}_{k} \vec{e}_{1}+\vec{n}_{k} \vec{e}_{2}+\vec{e}_{1} \vec{n}_{k}+\vec{e}_{1} \vec{e}_{2}+\vec{e}_{2} \vec{n}_{k}+\vec{e}_{2} \vec{e}_{1}\right)
\end{array}\right]
$$

After we evaluate the integral of $\mu$, we have:

$$
\begin{align*}
\overrightarrow{\vec{\alpha}}_{o u t}^{G 1} & =\frac{3}{2}\left[\frac{1}{4} \vec{n}_{k} \vec{n}_{k}+\frac{1}{8} \vec{e}_{1} \vec{e}_{1}+\frac{1}{8} \vec{e}_{2} \vec{e}_{2}\right]  \tag{3.84}\\
& =\frac{3}{16} \overrightarrow{\vec{I}}_{\vec{n}_{k}}+\frac{3}{16} \vec{n}_{k} \vec{n}_{k}
\end{align*}
$$

where $\overrightarrow{\vec{I}}_{\vec{n}_{k}}$ is the identity tensor corresponding to $\left\langle\vec{n}_{k}, \vec{e}_{1}, \vec{e}_{2}\right\rangle$. The incoming coefficient is found similarly, except the integral of $\mu$ results in negative values:

$$
\begin{align*}
\overrightarrow{\vec{\alpha}}_{i n c}^{G 1} & =\frac{3}{4 \pi} \int_{\vec{n}_{k} \cdot \vec{\Omega}<0} d \Omega \vec{\Omega} \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k} \\
& =-\frac{3}{2}\left[\frac{1}{4} \vec{n}_{k} \vec{n}_{k}+\frac{1}{8} \vec{e}_{1} \vec{e}_{1}+\frac{1}{8} \vec{e}_{2} \vec{e}_{2}\right]  \tag{3.85}\\
& =-\frac{3}{16} \overrightarrow{\bar{I}}_{\vec{n}_{k}}-\frac{3}{16} \vec{n}_{k} \vec{n}_{k}
\end{align*}
$$

It is of interest, though not quantified in this work, how important the terms in the first moment equation are to the consistency of the low-order operator. During previous research, we implemented and tested this method with a slightly different value of $\overrightarrow{\vec{\alpha}}_{o u t}^{G 1}$ and $\overrightarrow{\vec{\alpha}}_{i n c}^{G 1}$, and obtained an
operator that was an effective preconditioner to Source Iteration for transport. [19] In that previous work, we approximated the 1st moment surface terms as:

$$
\begin{align*}
& \overrightarrow{\vec{\alpha}}_{o u t}^{G 1} \approx \frac{3}{8} \vec{n}_{k} \vec{n}_{k},  \tag{3.86}\\
& \overrightarrow{\vec{\alpha}}_{\text {inc }}^{G 1} \approx-\frac{3}{8} \vec{n}_{k} \vec{n}_{k}
\end{align*}
$$

### 3.3.1.2 Boundary Conditions: Vacuum

On vacuum boundaries, the upstream incoming angular flux and correction are zero:

$$
\begin{align*}
& \underline{\psi}_{k+}^{(l+1 / 2)}(\vec{\Omega})=0,  \tag{3.87}\\
& \underline{f}_{k+}^{(l+1 / 2)}(\vec{\Omega})=0 . \tag{3.88}
\end{align*}
$$

Having already defined the outgoing integrals of $\vec{\Omega}$, the 0th moment of the upstream surface quantity with vacuum boundary is:

$$
\begin{align*}
\int_{4 \pi} d \Omega \sum_{k \in \text { Vacuum }} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega}) & =\sum_{k \in \text { Vacuum }} \int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}^{(l+1 / 2)}(\vec{\Omega}),  \tag{3.89}\\
& =\sum_{k \in \text { Vacuum }} \underline{A}_{\partial \tau_{k}}^{00}\left[\alpha_{\text {out }}^{F 0} \underline{F}+\vec{\alpha}_{o u t, k}^{G 0} \cdot \underline{\vec{G}}\right],
\end{align*}
$$

and the 1 st moment of the upstream surface quantity with vacuum boundary is:

$$
\begin{align*}
\int_{4 \pi} d \Omega \sum_{k \in \text { Vacuum }} \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} f_{k}^{(l+1 / 2)}(\vec{\Omega}) & =\sum_{k \in \text { Vacuum }} \int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}^{(l+1 / 2)}(\vec{\Omega}), \\
& =\sum_{k \in \text { Vacuum }} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\vec{\alpha}_{o u t, k}^{F 1} \underline{F}+\vec{\alpha}_{o u t}^{G 1} \cdot \underline{\vec{G}}\right] . \tag{3.90}
\end{align*}
$$

### 3.3.1.3 Boundary Conditions: Reflecting

The upstream angular flux and incoming angular correction on a reflected surface is the equal to the corresponding downstream quantity in the reflected direction:

$$
\begin{align*}
& \underline{\psi}_{k+}^{(l+1 / 2)}(\vec{\Omega})=\underline{\psi}^{(l+1 / 2)}\left(\vec{\Omega}_{R e f}\right), \vec{\Omega} \cdot \vec{n}_{k}<0,  \tag{3.91}\\
& \underline{f}_{k+}^{(l+1 / 2)}(\vec{\Omega})=\underline{f}^{(l+1 / 2)}\left(\vec{\Omega}_{R e f}\right), \vec{\Omega} \cdot \vec{n}_{k}<0 . \tag{3.92}
\end{align*}
$$

Using the terminology in Eq. (3.81), the angle that is reflected about the plane with normal $\vec{n}_{k}$ is:

$$
\begin{equation*}
\vec{\Omega}_{R e f}=\left[-\mu \vec{n}_{k}+\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{1}+\left(1-\mu^{2}\right)^{1 / 2} \sin (\gamma) \vec{e}_{2}\right] \tag{3.93}
\end{equation*}
$$

We evaluate the integral on the boundary in the 0th moment after substituting the upstream angular correction and the expression for the reflected direction:

$$
\begin{align*}
& \int_{4 \pi} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega})= \int_{\vec{n}_{k} \cdot \vec{\Omega}<0} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \underline{f}_{k+}^{(l+1 / 2)}(\vec{\Omega})+\int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \underline{f}^{(l+1 / 2)}(\vec{\Omega}) \\
&= \int_{\vec{n}_{k} \cdot \vec{\Omega}<0} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \frac{1}{4 \pi}\left[\underline{F}+3 \vec{\Omega}_{R e f} \cdot \underline{\vec{G}}\right]+\int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \frac{1}{4 \pi}[\underline{F}+3 \vec{\Omega} \cdot \vec{G}] \\
& \frac{1}{4 \pi} \int_{0}^{2 \pi} d \gamma \int_{-1}^{0} d \mu\left(\mu\left[\underline{F}+3\left(\begin{array}{l}
-\mu \vec{n}_{k} \\
= \\
+\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{1} \\
+\left(1-\mu^{2}\right)^{1 / 2} \sin (\gamma) \vec{e}_{2}
\end{array}\right) \cdot \underline{\vec{G}}\right]\right) \\
& \quad+\frac{1}{4 \pi} \int_{0}^{2 \pi} d \gamma \int_{0}^{1} d \mu\left(\mu\left(\underline{F}+3\left(\begin{array}{l}
\mu \vec{n}_{k} \\
+\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{1} \\
+\left(1-\mu^{2}\right)^{1 / 2} \sin (\gamma) \vec{e}_{2}
\end{array}\right) \cdot \underline{\vec{G}}\right]\right) \tag{3.94}
\end{align*}
$$

We can quickly see that each integral evaluates to zero. All terms that are linear in either $\cos (\gamma), \sin (\gamma)$, or both are zero; in addition, we may combine integrals to obtain functions that are
odd powers of $\mu$, whose integrals also evaluate to zero; finally, the integrals of $\vec{n}_{k} \cdot \underline{G}$ cancel each other due to the minus sign from the reflected angle cosine:

$$
\begin{align*}
& \int_{4 \pi} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega})= \\
& \frac{1}{4 \pi} \int_{0}^{2 \pi} d \gamma\left[\int_{-1}^{0} d \mu \mu+\int_{0}^{1} d \mu \mu\right]_{-}^{T} \\
& +\frac{1}{4 \pi}\left[\int_{-1}^{0} d \mu \mu\left(1-\mu^{2}\right)^{1 / 2}+\int_{0}^{1} d \mu \mu\left(1-\mu^{2}\right)^{1 / 2}\right]\left(\int_{Q}^{2 \pi} d \gamma \operatorname{los}(\gamma) \vec{e}_{1}+\int_{Q}^{0} d \gamma \sin (\gamma) \vec{e}_{2}\right) \cdot \underline{\vec{G}} \\
& +\frac{1}{4 \pi} \int_{0}^{2 \pi} d \gamma\left[\int_{0}^{0} d \mu\left(-\mu^{2}\right)+\int_{-1}^{1} d \mu\left(\mu^{2}\right)\right] \vec{n}_{k} \cdot \underline{\vec{G}} \\
& \quad=0 . \tag{3.95}
\end{align*}
$$

We follow similar steps to evaluate the integral on the boundary in the $1^{\text {st }}$ moment. After substituting the expression for the upstream angular correction and the reflected direction, we evaluate the following integrals:

$$
\begin{align*}
& \int_{4 \pi} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \vec{\Omega} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega}) \\
& =\int_{\vec{n}_{k} \cdot \vec{\Omega}<0} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \vec{\Omega} \underline{f}_{k+}^{(l+1 / 2)}(\vec{\Omega})+\int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \vec{\Omega} \underline{f}^{(l+1 / 2)}(\vec{\Omega}) \\
& =\int_{\vec{n}_{k} \cdot \vec{\Omega}<0} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \vec{\Omega} \frac{1}{4 \pi}\left[\underline{F}+3 \vec{\Omega}_{R e f} \cdot \underline{\vec{G}}\right]+\int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \vec{\Omega} \frac{1}{4 \pi}[\underline{F}+3 \vec{\Omega} \cdot \underline{\vec{G}}] \\
& =\frac{1}{4 \pi} \int_{0}^{2 \pi} d \gamma \int_{-1}^{0} d \mu\left(\mu\left(\begin{array}{r}
\mu \vec{n}_{k} \\
\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{1} \\
\left(1-\mu^{2}\right)^{1 / 2} \sin (\gamma) \vec{e}_{2}
\end{array}\right)\left[\underline{F}+3\left(\begin{array}{r}
-\mu \vec{n}_{k} \\
\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{1} \\
\left(1-\mu^{2}\right)^{1 / 2} \sin (\gamma) \vec{e}_{2}
\end{array}\right) \cdot \underline{\underline{G}}\right]\right) . \\
& \begin{aligned}
&=+\frac{1}{4 \pi} \int_{0}^{2 \pi} d \gamma \\
& 0
\end{aligned} \int_{0}^{1} d \mu\left(\mu\left(\vec{n}_{k}\right)\left[\begin{array}{r}
\mu \vec{n}_{k} \\
\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{1} \\
\left(1-\mu^{2}\right)^{1 / 2} \sin (\gamma) \vec{e}_{2}
\end{array}\right)\left[\underline{F}+3\left(\begin{array}{r} 
\\
\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{1} \\
\left(1-\mu^{2}\right)^{1 / 2} \sin (\gamma) \vec{e}_{2}
\end{array}\right) \cdot \underline{\vec{G}}\right]\right) \tag{3.96}
\end{align*}
$$

We eliminate integrals with $\underline{F}$ that are not in direction $\vec{n}_{k}$ because they are linear functions of $\cos (\gamma)$ or $\sin (\gamma)$. We also eliminate all off-diagonal terms of the resulting tensor multiplying $\underline{\vec{G}}$ that are linear functions of $\cos (\gamma), \sin (\gamma)$, or both. After we eliminate integrals over the full range of odd fuctions of $\mu$, the remaining integrals are as follows:

$$
\begin{align*}
\int_{4 \pi} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \vec{\Omega} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega})= & \frac{1}{4 \pi} \int_{0}^{2 \pi} d \gamma\left(\int_{-1}^{0} d \mu\left[\mu^{2}\right]+\int_{0}^{1} d \mu\left[\mu^{2}\right]\right) \vec{n}_{k} \underline{F}  \tag{3.97}\\
& +\frac{3}{4 \pi} \int_{0}^{2 \pi} d \gamma\left(\int_{-1}^{0} d \mu\left[-\mu^{3}\right]+\int_{0}^{1} d \mu\left[\mu^{3}\right]\right) \vec{n}_{k} \vec{n}_{k} \cdot \underline{\vec{G}}
\end{align*}
$$

We evaluate these integrals to find the upstream surface quantity on reflecting boundaries expressed in terms of only within-cell quantities:

$$
\begin{equation*}
\int_{4 \pi} d \Omega \vec{n}_{k} \cdot \vec{\Omega} \vec{\Omega} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega})=\frac{1}{3} \vec{n}_{k} \underline{F}+\frac{3}{4} \vec{n}_{k} \vec{n}_{k} \cdot \underline{\vec{G}} . \tag{3.98}
\end{equation*}
$$

### 3.3.1.4 Fully Consistent Discontinuous Finite Element Method Diffusion Synthetic Acceleration

## Equations with Boundary Conditions

The resulting system of equations for one element is coupled to all other elements through boundary terms. As a reference, we show the equations with all boundary conditions considered:

$$
\begin{align*}
& \sum_{k \in \text { Interior }} \underline{A}_{\partial \tau_{k}}^{00}\left[\alpha_{\text {inc }}^{F 0} \underline{F}_{k+}+\alpha_{\text {out }}^{F 0} \underline{F}+\vec{\alpha}_{\text {inc, } k}^{G 0} \cdot \underline{\vec{G}}_{k+}+\vec{\alpha}_{\text {out }, k}^{G 0} \cdot \underline{\vec{G}}\right] \\
& +\sum_{k \in \text { Vacuum }} \underline{\underline{A}}_{=\tau_{k}}^{00}\left[\alpha_{\text {out }}^{F 0} \underline{F}+\vec{\alpha}_{\text {out }, k}^{G 0} \cdot \underline{\vec{G}}\right] \\
& +\sum_{k \in \text { Reflect }} 0  \tag{3.99}\\
& +\left[-\sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}+\underline{\underline{\vec{A}}}_{\tau}^{01}\right] \cdot \underline{\underline{G}}+\sigma_{a} \underline{\underline{A}}_{\tau}^{00} \underline{F} \\
& =\sigma_{s} \underline{\underline{A}}_{\tau}^{00}\left(\underline{\phi}^{(l+1 / 2)}-\underline{\phi}^{(l)}\right) \text {, } \\
& \sum_{k \in \text { Interior }} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\vec{\alpha}_{i n c, k}^{F 1} \underline{F}_{k+}+\vec{\alpha}_{o u t, k}^{F 1} \underline{F}+\overrightarrow{\vec{\alpha}}_{i n c}^{G 1} \cdot \underline{\vec{G}}_{k+}+\overrightarrow{\vec{\alpha}}_{o u t}^{G 1} \cdot \underline{\vec{G}}\right] \\
& +\sum_{k \in \text { Vacuum }} \underline{A}_{\partial \tau_{k}}^{00}\left[\vec{\alpha}_{\text {out }, k}^{F 1} \underline{F}+\overrightarrow{\vec{\alpha}}_{\text {out }}^{G 1} \cdot \underline{\vec{G}}\right] \\
& +\sum_{k \in \text { Reflect }} \underline{A}_{\partial \tau_{k}}^{00}\left[\frac{1}{3} \vec{n}_{k} \underline{F}+\frac{3}{4} \vec{n}_{k} \vec{n}_{k} \cdot \underline{\vec{G}}\right]  \tag{3.100}\\
& +\frac{1}{3}\left[-\sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}+\underline{\underline{\vec{A}}}_{\tau}^{01}\right] \underline{F}+\sigma_{t} \underline{\underline{A}}_{\tau}^{00} \underline{\vec{G}}=0, \\
& \underline{\phi}^{(l+1)}=\underline{\phi}^{(l+1 / 2)}+\underline{F}^{(l+1 / 2)} . \tag{3.101}
\end{align*}
$$

This system has been shown to be difficult to solve.[23] To accelerate only the scalar intensity for one energy group, the fully consistent method has a solution size ( $N_{F C}$ ) equal to:

$$
\begin{equation*}
N_{F C}=N_{\text {SpatialDoF }} \times\left(N_{\text {dimensions }}+1\right) \tag{3.102}
\end{equation*}
$$

In general, the coupling to the first moment equations cause the global matrix to be asymmet-
ric. Another source of asymmetry arises when interaction probabilities are not constant within an element. The equations are often ill-conditioned, as the strength of coupling can vary dramatically between the 0th and 1st moment equations.

### 3.3.2 Continuous Finite Element Method Diffusion Synthetic Acceleration

To address the difficulty solving the fully consistent discontinuous method, we devise a continuous finite element method in the most consistent way we know. We map the local operators for each element of the fully consistent method discontinuous finite element space using a mapping operator $\underline{\underline{H}}_{\tau}$ to a continuous space that has continuity between unknowns that share interior neighboring faces (no jump condition). We have returned the subscripts $\tau$ to denote which quantities are from the discontinuous elements and add subscript $C$ to denote a vectors in the global continuous finite element space. For each element we determine the zeroth moment equation:

$$
\begin{align*}
& \underline{\underline{H}}_{\tau} \int_{4 \pi} d \Omega \sum_{k \in \partial \tau} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{\underline{H}}_{\tau}^{T} \underline{f}_{k, C}^{(l+1 / 2)}(\vec{\Omega}) \\
- & \underline{\underline{H}}_{\tau}\left[-\sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}+\underline{\underline{\vec{A}}}_{\tau}^{01}\right] \cdot \underline{\underline{H}}_{\tau}^{T} \underline{\vec{G}}_{C}^{(l+1 / 2)}+\underline{\underline{H}}_{\tau} \sigma_{a, \tau} \underline{\underline{A}}_{\tau}^{00} \underline{\underline{H}}_{\tau}^{T} \underline{\underline{F}}_{C}^{(l+1 / 2)}  \tag{3.103}\\
= & \underline{\underline{H}}_{\tau} \sigma_{s, \tau} \underline{\underline{A}}_{\tau}^{00}\left(\underline{\phi}_{\tau}^{(l+1 / 2)}-\underline{\phi}_{\tau}^{(l)}\right)
\end{align*}
$$

and the first moment equation:

$$
\begin{aligned}
& \underline{\underline{H}}_{\tau} \int_{4 \pi} d \Omega \vec{\Omega} \sum_{k \in \partial \tau} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{\underline{H}}_{\tau}^{T} \underline{\underline{f}}_{k, C}^{(l+1 / 2)}(\vec{\Omega}) \\
- & \underline{\underline{H}}_{\tau} \frac{1}{3}\left[-\sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}+\underline{\underline{A}}_{\tau}^{01}\right] \underline{\underline{H}}_{\tau}^{T} \underline{F}_{C}^{(l+1 / 2)}+\underline{\underline{H}}_{\tau} \sigma_{t, \tau} \underline{\underline{A}}_{\tau}^{00} \underline{\underline{H}}_{\tau}^{T} \overrightarrow{\vec{G}}_{C}^{(l+1 / 2)} \\
= & 0
\end{aligned}
$$

Element by element, the continuous correction is mapped back to the discontinuous space to update the scalar intensity:

$$
\begin{equation*}
\underline{\phi}^{(l+1)}=\underline{\phi}^{(l+1 / 2)}+\underline{\underline{H}}_{\tau}^{T} \underline{F}_{C}^{(l+1 / 2)} . \tag{3.105}
\end{equation*}
$$

### 3.3.2.1 Interior Boundaries

To enforce the continuity of the basis functions, we set the continuous angular correction to be equal on interior surfaces:

$$
\begin{equation*}
\underline{f}_{k+, C}^{(l+1 / 2)}=\underline{f}_{C}^{(l+1 / 2)}, \tag{3.106}
\end{equation*}
$$

and thus:

$$
\begin{align*}
& \underline{F}_{k+C}^{(l+1 / 2)}=\underline{F}_{C}^{(l+1 / 2)}  \tag{3.107}\\
& \underline{\vec{G}}_{k+, C}^{(l+1 / 2)}=\overrightarrow{\underline{G}}_{C}^{(l+1 / 2)} \tag{3.108}
\end{align*}
$$

We enforce continuity into the expression for the 0th moment fully consistent interior boundary, where integrals of linear functions of $\vec{\Omega}$ are zero:

$$
\begin{align*}
\underline{\underline{H}}_{\tau} \int_{4 \pi} d \Omega & \sum_{k \in \text { Interior }} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{\underline{H}}_{\tau}^{T} \underline{f}_{k, C}^{(l+1 / 2)}(\vec{\Omega}) \\
& =\underline{\underline{H}}_{\tau} \sum_{k \in \text { Interior }} \int_{4 \pi} d \Omega \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{\underline{H}}_{\tau}^{T} \frac{1}{4 \pi}\left(\underline{F}_{C}^{(l+1 / 2)}+3 \vec{\Omega} \cdot \vec{G}_{C}^{(l+1 / 2)}\right)  \tag{3.109}\\
& =\underline{\underline{H}}_{\tau} \sum_{k \in \text { Interior }} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{\underline{H}}_{\tau}^{T} \underline{\vec{G}}_{C}^{(l+1 / 2)}
\end{align*}
$$

Similarly, the 1st moment with continuous interior boundaries is:

$$
\begin{align*}
& \underline{\underline{H}} \int_{4 \pi} d \Omega \vec{\Omega} \sum_{k \in \text { Interior }} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{k, C}^{(l+1 / 2)}(\vec{\Omega}) \\
& =\underline{\underline{H}}_{\tau} \sum_{k \in \text { Interior }} \int_{4 \pi} d \Omega \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \frac{1}{4 \pi}\left(\underline{F}_{C}^{(l+1 / 2)}+3 \vec{\Omega} \cdot \underline{\vec{G}}_{C}^{(l+1 / 2)}\right)  \tag{3.110}\\
& =\underline{\underline{H}}_{\tau} \sum_{k \in \text { Interior }} \frac{1}{3} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{F}_{C}^{(l+1 / 2)}
\end{align*}
$$

We note that when all elements are added to the global operator, the contributions from neigh-
boring interior faces operator cancel because of equal and opposite surface normals.

### 3.3.2.2 Boundary Conditions: Vacuum

As in the fully consistent method, on vacuum boundaries the upstream incoming angular correction is zero:

$$
\begin{equation*}
\underline{f}_{k+, C}^{(l+1 / 2)}(\vec{\Omega})=0 . \tag{3.111}
\end{equation*}
$$

The surface term for a vacuum boundary in the zeroth moment is:

$$
\begin{align*}
\int_{4 \pi} d \Omega \sum_{k \in \text { Vacuum }} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{k, C}^{(l+1 / 2)}(\vec{\Omega}) & =\sum_{k \in \text { Vacuum }} \int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{C}^{(l+1 / 2)}(\vec{\Omega}) \\
& =\sum_{k \in \text { Vacuum }} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\alpha_{o u t}^{F 0} \underline{F}_{C}^{(l+1 / 2)}+\vec{\alpha}_{o u t, k}^{G 0} \cdot \underline{G}_{C}^{(l+1 / 2)}\right], \tag{3.112}
\end{align*}
$$

and in the first moment is:

$$
\begin{align*}
\int_{4 \pi} d \Omega \sum_{k \in \text { Vacuum }} \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} f_{k, C}^{(l+1 / 2)}(\vec{\Omega}) & =\sum_{k \in \text { Vacuum }} \int_{\vec{n}_{k} \cdot \vec{\Omega}>0} d \Omega \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{C}^{(l+1 / 2)}(\vec{\Omega}) \\
& =\sum_{k \in \text { Vacuum }} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\vec{\alpha}_{\text {out }, k}^{F 1} \underline{F}_{C}^{(l+1 / 2)}+\overrightarrow{\vec{\alpha}}_{\text {out }}^{G 1} \cdot \underline{\vec{G}}_{C}^{(l+1 / 2)}\right] . \tag{3.113}
\end{align*}
$$

### 3.3.2.3 Boundary Conditions: Reflecting

From the fully consistent method on reflecting boundaries, the reflecting boundary in the 0th moment is:

$$
\begin{equation*}
\int_{4 \pi} d \Omega \sum_{k \in \text { Reflect }} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} f_{k}^{(l+1 / 2)}(\vec{\Omega})=0, \tag{3.114}
\end{equation*}
$$

and the reflecting boundary in the 1 st moment is:

$$
\begin{equation*}
\int_{4 \pi} d \Omega \sum_{k \in \text { Reflect }} \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{\underline{H}}_{\tau} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega})=\sum_{k \in \text { Reflect }} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{\underline{H}}_{\tau}\left[\frac{1}{3} \vec{n}_{k} \underline{F}_{C}^{(l+1 / 2)}+\frac{3}{4} \vec{n}_{k} \vec{n}_{k} \cdot \overrightarrow{\underline{G}}_{C}^{(l+1 / 2)}\right] \tag{3.115}
\end{equation*}
$$

### 3.3.2.4 Continuous Finite Element Method Diffusion Synthetic Acceleration with Boundary Con-

 ditionsThe zeroth moment equations with boundary conditions:

$$
\begin{align*}
& \underline{\underline{H}}_{\tau} \sum_{k \in \text { Interior }} 0 \\
&+\underline{\underline{H}}_{\tau} \sum_{k \in \text { Vacuum }} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{\underline{H}}_{\tau}^{T}\left[\alpha_{o u t}^{F 0} \underline{\underline{F}}_{C}^{(l+1 / 2)}+\vec{\alpha}_{o u t, k}^{G 0} \cdot \underline{\vec{G}}_{C}^{(l+1 / 2)}\right] \\
&+\underline{\underline{H}}_{\tau} \sum_{k \in \text { Reflect }} 0  \tag{3.116}\\
&- \underline{\underline{H}}_{\tau}\left[-\sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}+\underline{\underline{\vec{A}}}_{\tau}^{01}\right] \cdot \underline{\underline{H}}_{\tau}^{T} \underline{\vec{G}}_{C}^{(l+1 / 2)}+\underline{\underline{H}}_{\tau} \sigma_{a} \underline{\underline{A}}_{\tau}^{00} \underline{F}_{C}^{(l+1 / 2)} \\
&= \underline{\underline{H}}_{\tau} \sigma_{s} \underline{\underline{A}}_{\tau}^{00}\left(\underline{\phi}^{(l+1 / 2)}-\underline{\phi}^{(l)}\right)
\end{align*}
$$

and the first moment equations with boundary conditions:

$$
\begin{align*}
& \sum_{k \in \text { Interior }} \frac{1}{3}_{3} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{\underline{F}}_{C}^{(l+1 / 2)} \\
+ & \sum_{k \in \text { Vacuum }} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{\underline{H}}_{\tau}^{T}\left[\vec{\alpha}_{o u t, k}^{F 1} \underline{F}_{C}^{(l+1 / 2)}+\overrightarrow{\hat{\alpha}}_{\text {out }}^{G 1} \underline{\vec{G}}_{C}^{(l+1 / 2)}\right] \\
+ & \sum_{k \in \text { Reflect }} \underline{\underline{A}}_{=2 \tau_{k}}^{00} \underline{\underline{H}}_{\tau}^{T}\left[\frac{1}{3} \vec{n}_{k} \underline{\underline{F}}_{C}^{(l+1 / 2)}+\frac{3}{4} \vec{n}_{k} \vec{n}_{k} \cdot \underline{\vec{G}}_{C}^{(l+1 / 2)}\right],  \tag{3.117}\\
+ & \sum_{k \in \text { OpposedReflect }} \frac{1}{3} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{F}_{C}^{(l+1 / 2)} \\
- & \frac{1}{3}\left[-\sum_{k \in \partial \tau} \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00}+\underline{\underline{A}}_{\tau}^{01}\right] \underline{F}_{C}^{(l+1 / 2)}+\sigma_{t} \underline{\underline{A}}_{\tau}^{00} \underline{\vec{G}}^{(l+1 / 2)} \\
= & 0
\end{align*}
$$

form a coupled system of equations for the additive correction $\underline{F}_{C}$, with update equation:

$$
\begin{equation*}
\underline{\phi}^{(l+1)}=\underline{\phi}^{(l+1 / 2)}+\underline{\underline{H}}_{\tau}^{T} \underline{F}_{C}^{(l+1 / 2)} . \tag{3.118}
\end{equation*}
$$

The 0th moment equation is coupled globally through the leakage term. However, if a lumped mass and surface matrix are employed, then the 1st moment forms a purely diagonal matrix for $\underline{G}_{C}$ that may be inverted analytically for each entry, obtaining an expression that is similar to a Fick's law, and 0th moment matrix that is similar to the stiffness matrix that results from application of a finite element method to the Laplacian operator.

While this low-order operator has the benefit of being formed directly from finite element matrices used in the transport discretization, doing this can be a source of asymmetry of the system if the interaction probabilities are allowed to be varied in the cell. Thus, we also investigate the necessity to keep the continuous finite element method semi-consistent, and instead use a stiffness matrix in the 0th moment equation and eschew the 1st moment equations entirely.

The continuous finite element discretization greatly reduces the number of spatial degrees of freedom, but produces an ineffective acceleration method, as shown in numerical results here in the following chapters, and in previous work. [19] To improve effectiveness, we employ an additional smoothing step during the prolongation of the continuous correction from the continuous space to the discontinuous space. This smoothing step uses the continuous correction as boundary conditions for each element of the fully-consistent method to form locally invertible equations.

### 3.3.3 Discontinuous Update Equation (CDFEM)

In this section we describe changes to interior face boundary conditions of the fully consistent method that make locally invertible equations. We refer to this method as a Continuous and Discontinuous Finite Element Method (CDFEM). From the fully consistent system of equations, we use the continuous finite element correction to approximate the upstream scalar correction:

$$
\begin{equation*}
\underline{F}_{k+}=2 \underline{\underline{H}}_{\tau}^{T} \underline{F}_{C}^{(l+1 / 2)}-\underline{F}^{(l+1 / 2)} \tag{3.119}
\end{equation*}
$$

and enforce continuity of the 1st moment corrections:

$$
\begin{equation*}
\underline{\vec{G}}_{k+}^{(l+1 / 2)}=\underline{\vec{G}}^{(l+1 / 2)} . \tag{3.120}
\end{equation*}
$$

After we substitute these expressions, the interior boundaries terms for the 0th moment equation are:

$$
\begin{align*}
\int_{4 \pi} d \Omega & \sum_{k \in \text { Interior }} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega}) \\
& =\sum_{k \in \text { Interior }} \underline{A}_{\partial \tau_{k}}^{00}\left[\alpha_{i n c}^{F 0} \underline{F}_{k+}^{(l+1 / 2)}+\alpha_{o u t}^{F 0} \underline{F}^{(l+1 / 2)}+\vec{\alpha}_{\text {inc,k }}^{G 0} \cdot \underline{\vec{G}}_{k+}^{(l+1 / 2)}+\vec{\alpha}_{o u t, k}^{G 0} \cdot \underline{\vec{G}}^{(l+1 / 2)}\right], \\
& =\sum_{k \in \text { Interior }} \underline{A}_{\partial \tau_{k}}^{00}\left[\begin{array}{c}
\alpha_{i n c}^{F 0}\left(2 \underline{\underline{H}}_{\tau}^{T} \underline{F}_{C}^{(l+1 / 2)}-\underline{F}^{(l+1 / 2)}\right)+\alpha_{o u t}^{F 0} \underline{F}^{(l+1 / 2)} \\
+\vec{\alpha}_{\text {inc,k }}^{G 0} \cdot \underline{\vec{G}}^{(l+1 / 2)}+\vec{\alpha}_{o u t, k}^{G 0} \cdot \underline{\vec{G}}^{(l+1 / 2)}
\end{array}\right], \\
& =\sum_{k \in \text { Interior }} \underline{A}_{\partial \tau_{k}}^{00}\left[-2 \alpha_{o u t}^{F 0} \underline{\underline{H}}_{\tau}^{T} \underline{F}_{C}^{(l+1 / 2)}+2 \alpha_{o u t}^{F 0} \underline{F}^{(l+1 / 2)}+2 \vec{\alpha}_{o u t, k}^{G 0} \cdot \underline{G}^{(l+1 / 2)}\right] . \tag{3.121}
\end{align*}
$$

and the interior boundary terms for the 1 st moment equations are:

$$
\begin{align*}
\int_{4 \pi} d \Omega & \sum_{k \in \text { Interior }} \vec{\Omega} \vec{\Omega} \cdot \vec{n}_{k} \underline{\underline{A}}_{\partial \tau_{k}}^{00} \underline{f}_{k}^{(l+1 / 2)}(\vec{\Omega}) \\
& =\sum_{k \in \text { Interior }} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\vec{\alpha}_{\text {inc, }, k}^{F 1} \underline{F}_{k+}^{(l+1 / 2)}+\vec{\alpha}_{o u t, k}^{F 1} \underline{F}^{(l+1 / 2)}+\overrightarrow{\vec{\alpha}}_{\text {inc }}^{G 1} \cdot \overrightarrow{\underline{G}}_{k+}^{(l+1 / 2)}+\overrightarrow{\vec{\alpha}}_{o u t}^{G 1} \cdot \overrightarrow{\vec{G}}^{(l+1 / 2)}\right], \\
& =\sum_{k \in \text { Interior }} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[\begin{array}{l}
\left.\vec{\alpha}_{i n c, k}^{F 1}\left(2 \underline{\underline{H}}_{\tau}^{T} \underline{F}_{C}^{(l+1 / 2)}-\underline{F}^{(l+1 / 2)}\right)+\vec{\alpha}_{o u t, k}^{F 1} \underline{F}^{(l+1 / 2)}\right] \\
+\overrightarrow{\vec{\alpha}}_{\text {inc }}^{G 1} \cdot \underline{\vec{G}}^{(l+1 / 2)}+\overrightarrow{\vec{\alpha}}_{o u t}^{G 1} \cdot \underline{\vec{G}}^{(l+1 / 2)}
\end{array}\right], \\
& =\sum_{k \in \text { Interior }} \underline{\underline{A}}_{\partial \tau_{k}}^{00}\left[2 \vec{\alpha}_{o u t, k}^{F 1} \underline{\underline{H}}_{\tau}^{T} \underline{F}_{C}^{(l+1 / 2)}\right] . \tag{3.122}
\end{align*}
$$

This results in a locally invertible system of equations for each element.

### 3.3.3.1 Boundary Conditions: Alternate Interior Approximation

Though enforcing continuity of the correction on interior boundaries has shown to be effective, it is possible to approximate the 1 st moment corrections using the continuous correction. We may solve the first moment equations of the continuous operator for $\underline{\vec{G}}_{C}$ :

$$
\begin{equation*}
\overrightarrow{\underline{G}}_{C}=\underline{\underline{A}}_{G, C, 1}^{-1} \overrightarrow{\underline{A}}_{F, C, 1} \underline{\underline{F}}_{C}, \tag{3.123}
\end{equation*}
$$

where $\underline{\underline{A}}_{G, C, 1}$ is the combination of terms that multiply $\underline{\underline{G}}_{C}$ in the continuous 1 st moment equation, and $\underline{\underline{A}}_{F, C, 1}$ is the combination of terms that multiply $\underline{F}_{C}$ in the continuous 1 st moment equation.

We would then approximate the upstream discontinuous 1st moment corrections in a similar manner to the scalar correction:

$$
\begin{equation*}
\overrightarrow{\underline{G}}_{k+}=2 \underline{\underline{H}}_{\tau}^{T} \underline{\vec{G}}_{C}-\underline{\vec{G}} \tag{3.124}
\end{equation*}
$$

Because initial results did not show improvement of the semi-consistent CDFEM, this modification was not investigated further. However, we want to note that improving the approximation of the 1st moment correction is one of the ways to possibly prevent the degradation that has been shown for high-aspect ratio geometries. [19]

### 3.4 Summary

In this chapter we provided a detailed description of the discretization schemes we use for space, angle and energy. We also provided a description of source iteration, which is used by all methods that follow, and demonstrate the effectiveness of accelerating that iteration with a loworder operator. Finally, we showed the semi-consistent diffusion-like low-order operator. This method uses a combination of a continuous finite element method global solution and discontinuous finite element local solution. The global CFEM solution provides a reduced solution cost compared to fully-consistent diffusion, and the local DFEM solution has been shown to provide
enough consistency to effectively accelerate source iteration.
In the chapters that follow, we apply this semi-consistent diffusion-like low-order operator to thermal radiative transfer, $k$-eigenvalue, and thermal upscattering problems with the goal of using this method as the primary error reduction step per iteration by applying the low-order acceleration to the outermost iteration.

## 4. ADDITIVE SOURCE K-EIGENVALUE ITERATION FOR NEUTRON PROBLEMS

### 4.1 Method Motivation

In this chapter, we discuss solution methods for the multigroup discrete-ordinates $k$-eigenvalue neutron transport equation, which can be written as follows:

$$
\begin{gather*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) \Psi_{m}=\frac{1}{4 \pi} S_{m} \Phi+\frac{1}{4 \pi} \frac{1}{k} F \Phi_{0}, \quad m=1 \ldots M  \tag{4.1}\\
\Phi=W \Psi \tag{4.2}
\end{gather*}
$$

Here $\Psi$ is the vector of unknowns that represent the position-, direction-, and energy-dependent neutron angular flux, $M$ is the number of directions in the quadrature set (which can differ for different energy groups), $\Phi$ is the vector of angular moments needed to build the scattering source, $\Phi_{0}$ is the scalar flux ( $0^{t h}$ angular moment), $\vec{\Omega}_{m}$ is a unit vector in the $m^{t h}$ quadrature direction, $T$ is total collision operator, $S$ is the transfer operator (describing scattering, ( $\mathrm{n}, 2 \mathrm{n}$ ), and other non-fission neutron-emitting interactions), $F$ is the fission interaction operator, $W$ is the angularmoment operator, and $k$ is the eigenvalue to be determined.

A straightforward solution method for this problem is power iteration (PI):

$$
\begin{gather*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T-\frac{1}{4 \pi} W S_{m}\right) \Psi_{m}^{(t+1)}=\frac{1}{4 \pi} \frac{1}{k^{(t)}} F \Phi_{0}^{(t)}  \tag{4.3}\\
\Phi_{0}^{(t+1)}=W_{0} \Psi^{(t+1)}  \tag{4.4}\\
k^{(t+1)}=k^{(t)} \frac{\left\|F \Phi_{0}^{(t+1)}\right\|}{\left\|F \Phi_{0}^{(t)}\right\|} \tag{4.5}
\end{gather*}
$$

Upon convergence, $k$ is the largest of the $k$-eigenvalues and $\Psi$ is the associated eigenfunction. As written here, each power iteration requires solving for $\Psi^{(t+1)}$, which itself requires iteration. A
straightforward option for this "inner iteration" is source iteration (SI):

$$
\begin{equation*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) \Psi_{m}^{(i+1)}=\frac{1}{4 \pi} W S_{m} \Psi^{i}+\frac{1}{4 \pi} \frac{1}{k^{(t)}} F \Phi_{0}^{(t)}, \tag{4.6}
\end{equation*}
$$

with $\Psi_{m}^{(t+1)}$ set to $\Psi_{m}^{(i+1)}$ upon convergence.
The PI convergence rate depends on the eigenvalue dominance ratio, which can be arbitrarily close to one, in which case PI converges arbitrarily slowly. (See chapter VIII of [1].) The SI convergence rate depends on the scattering ratio (fraction of interactions that are scatters), which can also be close to one, in which case SI converges slowly. (See chapter II of [1].)

For many problems of practical interest, both the dominance ratio and scattering ratio are sufficiently close to one that it is beneficial to replace or modify both the outer and inner iteration methods to achieve faster convergence. $[25,39,40,29,30]$ In this chapter we consider methods that retain the basic outer / inner structure but employ "low-order" approximations of the transport operator to accelerate convergence. Our purpose is to help fill a gap in the theoretical foundation for a family of these methods that employ linear low-order operators.

Both linear and nonlinear low-order operators have been used effectively in $k$-eigenvalue problems. When nonlinear low-order operators are employed to accelerate convergence of outer iterations, the result is a series of low-order problems that are themselves $k$-eigenvalue problems, each with a unique largest eigenvalue and associated eigenfunction. This dominant \{eigenvalue, eigenfunction \} pair is the desired solution, and various techniques (including PI) can be employed to find this solution.[1, 25, 39, 40, 29, 30, 41, 27, 10, 9, 26]

In contrast, when linear low-order operators are employed to accelerate convergence of outer iterations, each resulting low-order problem is not itself an eigenvalue problem, for in addition to the fission term with its $1 / k$ multiplier there is also a fixed ("inhomogeneous") source term.[33, 42, $43,35,32$ ] For this problem there is not a unique largest $k$ for which the problem has a solution. In fact, the equation admits a solution for every value of $k$ greater than a certain well-defined value. In spite of this apparent theoretical issue, all applications of the linear methodology that we know of have been successful, with iterative performance comparable to that seen with nonlinear methods.

Each application that we know of has employed a power-like iteration scheme for the eigenvaluelike low-order problem, and this power-like iteration method apparently converges to a meaningful $k$ and associated function.

In this chapter we provide theoretical foundations for methods that employ linear operators to accelerate the convergence of outer iterations in $k$-eigenvalue problems. This includes analysis of the convergence of a power-like iteration scheme applied to the eigenvalue-like low-order problems as well as the convergence of the outer iteration (in which each iteration requires solution of a low-order eigenvalue-like problem) to the desired high-order eigenvalue and eigenfunction. Our approach is to perform convergence analyses of model problems for which we have devised analysis techniques. These problems are much simpler than real-world reactor problems, but they serve as a starting point for understanding the behavior of the iterative methods of interest here. The same kinds of simple model problems proved very helpful in the early days of understanding and developing rapidly convergent iterative methods for fixed-source problems.[1, 44, 37, 38, 34]

We remark that there are many approaches to solving $k$-eigenvalue problems that do not employ low-order operators in the way described above. These include subspace methods (Arnoldi iteration, Chebyshev iteration),[23, 24] casting the eigenvalue problem as a nonlinear PDE constraint problem and solving using a nonlinear solver such as a Newton-like method, and treating part of the fission source implicitly to reduce the dominance ratio (Weilandt shift). We do not address these methods here, but will mention that acceleration using low-order operators has been shown to improve these methods as well. [32, 28]

In the next section we describe the linear low-order methodology, including its developmental history as we understand it, and illustrate it using $P_{1}$ as the low-order approximation for transport. We compare and contrast this to the nonlinear low-order methodology, using QuasiDiffusion as the example. In Sec. 4.3 we present convergence analyses for two model problems. The first model problem employs transport and diffusion operators without spatial discretization and applies them to a one-energy-group problem in an infinite homogeneous medium. The second model problem employs spatial discretization for the transport and low-order operators and applies the method to
a single-cell problem with vacuum boundaries. We close the section with a discussion of spatialdiscretization considerations. In Sec. 4.4 we present numerical results from reactor test problems including those with strong heterogeneities, fine spatial features, large numbers of spatial cells, and large numbers of energy unknowns.

### 4.2 Linear Synthetic Acceleration for Eigenfunction Correction and Updated Eigenvalue

### 4.2.1 Description and History

In what follows we use equations without spatial discretization for illustration. The family of methods we study here employ nested iterations. If we let $(t)$ be the index of the outermost iteration and $(i)$ be the index of the scattering iteration, then the methods we consider have the following at the end of the transport portion of the $t$-th iteration:

$$
\begin{equation*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) \Psi_{m}^{(i+1)}=\frac{1}{4 \pi}\left(S_{m, c o n} \Phi^{(i+1)}+S_{m, r e c} \Phi^{(i+1 / 2)}+S_{m, l a g} \Phi^{(i)}+\frac{1}{k^{(t)}} F \Phi_{0}^{(t)}\right) \tag{4.7}
\end{equation*}
$$

Here $\Psi_{m}$ is a vector containing the angular flux for all energy groups for direction $m, \Phi$ is a vector containing all the angular moments needed to form the scattering source for all groups, $\Phi_{0}$ is a vector of scalar fluxes for all groups, $T$ contains the total cross section for each group, $\frac{1}{4 \pi} S_{m, c o n} \Phi^{(i+1)}$ is the scattering source rate density for direction $m$ that has been previously determined (e.g. downscattering from fast groups), $\frac{1}{4 \pi} S_{m, \text { rec }} \Phi^{(i+1 / 2)}$ is the scattering source rate density for direction $m$ that has been updated from the most recent transport step (iteration index $i+1 / 2$, e.g. within-group scattering), $\frac{1}{4 \pi} S_{m, l a g} \Phi^{(i)}$ is the scattering source rate density for direction $m$ that is evaluated at a previous iterate (e.g. upscattering), and $\frac{1}{4 \pi} \frac{1}{k^{(t)}} F \Phi_{0}^{(t)}$ is the fission source rate density.

As far as we know, the first derivation, implementation, and testing of a method in the family considered here appeared in a 1986 dissertation.[33] The author developed eigenproblem acceleration equations via a process that previous researchers had employed for scattering iterations: 1) define "converged" equations by setting all iteration indices to the same value; 2) subtract the equations satisfied by the latest solution, obtaining an exact equation for an additive correction;
3) replace the transport operator in this equation by a low-order operator. In the notation we have introduced, the first step produces:

$$
\begin{equation*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) \Psi_{m}^{(t+1)}=\frac{1}{4 \pi}\left(S_{m, c o n} \Phi^{(t+1)}+S_{m, r e c} \Phi^{(t+1)}+S_{m, l a g} \Phi^{(t+1)}+\frac{F \Phi_{0}^{(t+1)}}{k^{(t+1)}}\right) \tag{4.8}
\end{equation*}
$$

The second step subtracts Eq. (4.7) from this "converged" equation. We define the following corrections:

$$
\begin{align*}
& y^{(t+1)}=\Psi^{(t+1)}-\Psi^{(i+1)},  \tag{4.9}\\
& f^{(t+1)}=\Phi^{(t+1)}-\Phi^{(i+1)},  \tag{4.10}\\
& f_{0}^{(t+1)}=\Phi_{0}^{(t+1)}-\Phi_{0}^{(i+1)} . \tag{4.11}
\end{align*}
$$

Then we have an equation for a correction:

$$
\begin{equation*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) y_{m}^{(t+1)}=\frac{1}{4 \pi}\left(S_{m} f^{(t+1)}+\frac{F\left(f_{0}^{(t+1)}+\Phi_{0}^{(i+1)}\right)}{k^{(t+1)}}+R_{m}^{(i+1)}\right) \tag{4.12}
\end{equation*}
$$

where:

$$
\begin{equation*}
R_{m}^{(i+1)} \equiv S_{m, r e c}\left(\Phi^{(i+1)}-\Phi^{(i+1 / 2)}\right)+S_{m, l a g}\left(\Phi^{(i+1)}-\Phi^{(i)}\right)-\frac{1}{k^{(t)}} F \Phi_{0}^{(t)} \tag{4.13}
\end{equation*}
$$

The third step replaces the transport operator with a low-order operator, which for Adams was a diffusion operator.[33] We illustrate with a $P_{1}$ operator:

$$
\begin{equation*}
\vec{\nabla} \cdot \vec{g}^{(t+1)}+\left(T-S_{0}\right) f_{0}^{(t+1)}=\frac{1}{k^{(t+1)}} F\left(\Phi_{0}^{(i+1)}+f_{0}^{(t+1)}\right)+R_{0}^{(i+1)}, \tag{4.14}
\end{equation*}
$$

$$
\begin{equation*}
\frac{1}{3} \vec{\nabla} \cdot f_{0}^{(t+1)}+T \vec{g}^{(t+1)}=S_{1} \vec{g}^{(t+1)}+\vec{R}_{1}^{(i+1)} \tag{4.15}
\end{equation*}
$$

where $R_{0}$ and $\vec{R}_{1}$ are the $0^{t h}$ and $1^{s t}$ angular moments of $R_{m} / 4 \pi$.
Finally, an iterative method must be defined to solve for the new eigenvalue, $k^{(t+1)}$, and eigenfunction additive correction, $f_{0}^{(t+1)}$. An obvious choice, and the one made in Adams,[33] is a process that resembles power iteration, with starting guesses $f_{0}^{(0)}=0$ and $\left.k^{(n)}\right|_{n=0}=k^{(t)}$ :

$$
\begin{align*}
\vec{\nabla} \cdot \vec{g}^{(n+1)}+\left(T-S_{0}\right) f_{0}^{(n+1)} & =\frac{1}{k^{(n)}} F\left(\Phi_{0}^{(i+1)}+f_{0}^{(n)}\right)+R_{0}^{(i+1)}  \tag{4.16}\\
\frac{1}{3} \vec{\nabla} \cdot f_{0}^{(n+1)}+T \vec{g}^{(n+1)} & =S_{1} \vec{g}^{(n+1)}+\vec{R}_{1}^{(i+1)}  \tag{4.17}\\
k^{(n+1)} & =k^{(n)} \frac{\left\|F\left(f_{0}^{(n+1)}+\Phi_{0}^{(i+1)}\right)\right\|}{\left\|F\left(f_{0}^{(n)}+\Phi_{0}^{(i+1)}\right)\right\|} \tag{4.18}
\end{align*}
$$

Upon convergence, this low-order eigenvalue-like problem yields the next eigenvalue and eigenfunction iterates:

$$
\begin{equation*}
k^{(t+1)} \leftarrow k^{(n+1)} \quad \text { and } \quad \Phi_{0}^{(t+1)} \leftarrow \Phi_{0}^{(i+1)}+f_{0}^{(t+1)} \tag{4.19}
\end{equation*}
$$

We summarize the solution procedure in algorithm 1.
While the aforementioned 1986 dissertation reported excellent results, the method remained unpublicized because of theoretical concerns. Committee member E. W. Larsen observed that given the presence of a fixed source in Eq. (4.14) ( $R_{0}$ plus part of the fission source), the low-order problem is not an eigenvalue problem, and it appears to admit arbitrary solutions. For example, one could set $k^{(t+1)}$ to some arbitrary large value and solve the resulting fixed-source subcritical diffusion problem for the associated $f$. Setting a different value for $k^{(t+1)}$ would produce a different function for $f$. That is, infinitely many solutions ( $k$ and $f$ ) that are unrelated to the eigenproblem of interest are seen to satisfy Eqs. (4.14) and (4.15).

Numerical tests indicated that when the specific iteration process defined above was followed,

## Algorithm 1 Linear Acceleration of Power Iteration for $k$-Eigevalue Problems

$t \leftarrow 0$
Initialize $\phi^{(0)}, k^{(0)}$
repeat
Scattering Iteration for $\Phi^{(i+1)}: L_{m} \psi_{m}^{(i+1)}=\frac{S_{m}}{4 \pi} \Phi^{(i+1)}-R_{m}^{(i+1)}$
$n \leftarrow 0$
$\Phi^{(n)} \leftarrow \Phi^{(i+1)}$
$k^{(n)} \leftarrow k^{(t)}$
repeat
Solve low-order system of equations:
9:

10:
11: $\quad k^{(n+1)} \leftarrow k^{(n)} \frac{\left\|F \Phi^{(n+1)}\right\|}{\left\|F \Phi^{(n)}\right\|}$

$$
\left|1-\frac{k^{(n)}}{k^{(n+1)}}\right| \leq \epsilon_{k}\left(1-\frac{\left|k^{(n+1)}-k^{(n)}\right|}{\left|k^{(n)}-k^{(n-1)}\right|}\right)
$$

12:

$$
\text { until } \frac{\left\|\phi^{(n+1)}-\phi^{(n)}\right\|}{\left\|\phi^{(n+1)}\right\|}<\epsilon_{\phi}\left(1-\frac{\left\|\phi^{(n+1)}-\phi^{(n)}\right\|}{\left\|\phi^{(n)}-\phi^{(n-1)}\right\|}\right),
$$

else $n \leftarrow n+1$

$$
k^{(t+1)} \leftarrow k^{(n+1)}
$$

$$
\Phi^{(t+1)} \leftarrow \Phi^{(n+1)}
$$

$$
\left|1-\frac{k^{(t)}}{k^{(t+1)}}\right| \leq \epsilon_{k}\left(1-\frac{\left|k^{(t+1)}-k^{(t)}\right|}{\left|k^{(t)}-k^{(t-1)}\right|}\right)
$$

until $\frac{\left\|\phi^{(t+1)}-\phi^{(t)}\right\|}{\left\|\phi^{(t+1)}\right\|}<\epsilon_{\phi}\left(1-\frac{\left\|\phi^{(t+1)}-\phi^{(t)}\right\|}{\left\|\phi^{(t)}-\phi^{(t-1)}\right\|}\right)$,
else $t \leftarrow t+1$
the method worked quite well. Nevertheless, the absence of a theoretical understanding left a concern that the method might fail on some problems (for example, if the low-order power-like iteration failed to converge or converged to some additive correction that degraded instead of improved the latest transport solution). We remark that Adams and Larsen did publish a related linear method that was shown to converge rapidly, but it was defined only for the one-group case.[42]

Later, Suslov independently created the same basic method (with a different low-order operator) and provided an argument for why one would expect the low-order problem to converge to a useful solution.[43] We paraphrase Suslov's argument as follows: We cast Eqs. (4.7), (4.16), and (4.17) in operator notation, and for simplicity only include 0th moment scattering:

$$
\begin{gather*}
A \Phi_{0}^{(i+1)}=-R_{0}^{(i+1)}  \tag{4.20}\\
B f_{0}^{(n+1)}=\frac{1}{k^{(n)}} F\left(\Phi_{0}^{(i+1)}+f_{0}^{(n)}\right)+R_{0}^{(i+1)} \tag{4.21}
\end{gather*}
$$

Adding these two equations gives

$$
\begin{equation*}
A \Phi_{0}^{(i+1)}+B f_{0}^{(n+1)}=\frac{1}{k^{(n)}} F\left(\Phi_{0}^{(i+1)}+f_{0}^{(n)}\right) \tag{4.22}
\end{equation*}
$$

If we had $B=A$ (low-order $=$ high-order), then this method would be equivalent to solving a standard eigenvalue equation for the next eigenfunction iterate. That is, even though Eq. (4.21) does admit solutions that are not related to the eigenproblem, as Larsen had observed, solving it using a power-like iteration is algebraically equivalent to solving a problem-Eqs. (4.22) and (4.18) - that has no fixed source and is similar to (but if $B \neq A$ not quite that same as) a standard eigenvalue problem. Thus, Suslov justified using a low-order transport operator for $B$ and reported excellent results.[43]

Masiello and Rossi have also reported excellent results from the application of a method in the family of linear acceleration schemes that we study here for $k$-eigenvalue problems.[35] They applied the "Boundary-Projection Acceleration" (BPA) low-order operator to multigroup $k$ eigenvalue discrete-ordinates problems with anisotropic scattering.[34] They presented a Fourier
analysis of the iterative convergence rate of their BPA method for fixed-source problems, providing a sound theoretical basis for the application of BPA to such problems. They did not present theoretical analysis of convergence of the method for eigenvalue problems, but they provided results that demonstrated excellent performance.

### 4.2.2 Theoretical Questions

Theoretical questions remain if $B \neq A$. If an operator " $C$ " existed such that

$$
\begin{equation*}
A \Phi_{0}^{(i+1)}+B f_{0}^{(n+1)}=C\left(\Phi_{0}^{(i+1)}+f_{0}^{(n+1)}\right) \tag{4.23}
\end{equation*}
$$

for all possible $f_{0}^{(n+1)}$, then the given iteration method would be algebraically equivalent to power iteration on the operator $C^{-1} F$. This would find the largest eigenvalue and the associated eigenfunction, and the only theoretical question would be how rapidly this well-posed low-order problem would accelerate the overall iteration.

We now show that given the $A$ and $B$ operators studied here, there does exist an operator $C^{(n+1)}$ such that $A \Phi_{0}^{(i+1)}+B f_{0}^{(n+1)}=C^{(n+1)}\left(\Phi_{0}^{(i+1)}+f_{0}^{(n+1)}\right)$. However, this operator depends on $f_{0}^{(n+1)}$ and thus changes from iteration to iteration. If we take the $0^{t h}$ and $1^{\text {st }}$ angular moments of Eq. (4.7) we see that the following equations are satisfied at the end of the transport step:

$$
\begin{align*}
& \vec{\nabla} \cdot \vec{J}^{(i+1)}+T \Phi_{0}^{(i+1)}=S_{0} \Phi_{0}^{(i+1)}-R_{0}^{(i+1)},  \tag{4.24}\\
& \vec{\nabla} \cdot \overrightarrow{\vec{P}}^{(i+1)}+T \vec{J}^{(i+1)}=S_{1} \vec{J}^{(i+1)}-\vec{R}_{1}^{(i+1)} \tag{4.25}
\end{align*}
$$

where $\vec{J} \equiv \sum_{m} w_{m} \vec{\Omega}_{m} \Psi_{m} \quad$ and $\quad \overrightarrow{\vec{P}} \equiv \sum_{m} w_{m} \vec{\Omega}_{m} \vec{\Omega}_{m} \Psi_{m}$,
and subscripts 0 and 1 refer to $0^{t h}$ and $1^{\text {st }}$ angular moments. We define an Eddington tensor using the latest transport information: $\overrightarrow{\vec{E}}^{(i+1)} \equiv \overrightarrow{\vec{P}}^{(i+1)} / \Phi_{0}^{(i+1)}$, then add Eqs. (4.16) and (4.17) to

Eqs. (4.24) and (4.25) to obtain:

$$
\begin{align*}
\vec{\nabla} \cdot\left(\vec{J}^{(i+1)}+\vec{g}^{(n+1)}\right)+\left(T-S_{0}\right)\left(\Phi_{0}^{(i+1)}+f_{0}^{(n+1)}\right) & =\frac{1}{k^{(n)}} F\left(\Phi_{0}^{(i+1)}+f_{0}^{(n)}\right)  \tag{4.27}\\
\vec{\nabla} \cdot\left(\vec{E}^{(i+1)} \Phi_{0}^{(i+1)}+\frac{1}{3} \overrightarrow{\vec{I}} f_{0}^{(n+1)}\right)+\left(T-S_{1}\right)\left(\vec{J}^{(i+1)}+\vec{g}^{(n+1)}\right) & =0 \tag{4.28}
\end{align*}
$$

Here $\overrightarrow{\vec{I}}$ is the identity tensor. We define a new tensor, $\overrightarrow{\vec{M}}^{(n+1)}$, that is a weighted average of $\overrightarrow{\vec{I}} / 3$ and the Eddington tensor from the the latest transport step using the diffusion correction and transport scalar flux as weights:

$$
\begin{equation*}
\overrightarrow{\vec{M}}^{(n+1)} \equiv \frac{\left(\overrightarrow{\vec{E}}^{(i+1)} \Phi_{0}^{(i+1)}+\frac{1}{3} \overrightarrow{\vec{I}} f_{0}^{(n+1)}\right)}{\Phi_{0}^{(i+1)}+f_{0}^{(n+1)}} \tag{4.29}
\end{equation*}
$$

We also define the latest $\Phi_{0}$ and $\vec{J}$ quantities:

$$
\begin{equation*}
\Phi_{0}^{(n+1)} \equiv \Phi_{0}^{(i+1)}+f_{0}^{(n+1)} \quad \text { and } \quad \vec{J}^{(n+1)} \equiv \vec{J}^{(i+1)}+\vec{g}^{(n+1)} \tag{4.30}
\end{equation*}
$$

Then we see that our low-order $k$ iteration scheme satisfies the following equations:

$$
\begin{gather*}
\vec{\nabla} \cdot \vec{J}^{(n+1)}+\left(T-S_{0}\right) \Phi_{0}^{(n+1)}=\frac{1}{k^{(n)}} F \Phi_{0}^{(n)},  \tag{4.31}\\
\vec{\nabla} \cdot\left(\overrightarrow{\vec{M}}^{(n+1)} \Phi_{0}^{(n+1)}\right)+\left(T-S_{1}\right) \vec{J}^{(n+1)}=0,  \tag{4.32}\\
k^{(n+1)}=k^{(n)} \frac{\left\|F \Phi_{0}^{(n+1)}\right\|}{\left\|F \Phi_{0}^{(n)}\right\|} \tag{4.33}
\end{gather*}
$$

This method looks like power iteration, in particular the power iteration for the inner iteration of a Quasi-Diffusion method, except that the tensor $\vec{M}^{(n+1)}$ changes every iteration. A few remarks are in order.

1. While this is not a true eigenvalue problem, it is similar to problems and solution methods
that arise in multi-physics simulations, in which neutronics operators change as temperatures and densities change during the overall multi-physics iterative solution.
2. The change in $\overrightarrow{\vec{M}}$ from iteration to iteration is small when the correction, $f_{0}$, is small relative to the solution, $\Phi_{0}$, as is the case when the overall iteration is almost converged. In this limit the power-like iteration becomes algebraically equivalent to standard power iteration, which will converge.
3. The change in $\overrightarrow{\vec{M}}$ from iteration to iteration may not be small during the first overall iteration or two if the correction, $f_{0}$, is not small relative to $\Phi_{0}^{(i+1)}$. We do not know of a proof that the iteration given by Eqs. (4.31)-(4.33) will converge in such a case.
4. In the limit as $f_{0} \rightarrow 0, \overrightarrow{\vec{M}}^{(n+1)} \rightarrow \overrightarrow{\vec{E}}^{i+1}$. In this limit, this method produces precisely the QD method, which does not change as the $n$ iteration proceeds and has been shown to be rapidly convergent.
5. The arguments presented here depend on a power-like iteration method being used for the low-order problem. It is not clear that these arguments would apply if a different solution technique were used to solve Eqs. (4.14-4.15). Given our previous observation that infinitely many solutions exist to these equations, it seems all but certain that different iterative techniques would find different solutions.

In the next section we analyze the convergence behavior of the eigenvalues and eigenvectors of the two-step iteration process for simple model problems.

### 4.3 Convergence Analysis

### 4.3.1 Fourier Analysis of Infinite Homogeneous Model Problem

We analyze a particular setting of the linear low-order method where we perform one transport sweep per low-order diffusion problem solution. In the literature and our own experience, this "one-sweep" method has shown the most reduction to the total solution time. We apply this method to an infinite, homogeneous medium with isotropic scattering to determine the convergence rate
of both the diffusion eigenvalue and the transport eigenvalue problems. Because we only perform one-sweep per outer iteration, and because there is only within group scattering in the one-group problem, we write our transport iteration equation with only one iteration index. We denote the lack of group dependence with different symbols ( $\Psi_{m} \equiv \psi_{m}, \Phi_{m} \equiv \phi_{m}, T \equiv \sigma_{t}, S_{m} \equiv \sigma_{s}, F \equiv \nu \sigma_{f}$ ), and change of iteration index $((i+1) \equiv(i+1 / 2),(t) \equiv(i))$. The one-group, one-sweep transport equation is then given by the following:

$$
\begin{equation*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+\sigma_{t}\right) \psi_{m}^{(i+1 / 2)}=\frac{1}{4 \pi}\left(\sigma_{s}+\frac{\nu \sigma_{f}}{k^{(i)}}\right) \phi_{0}^{(i)} . \tag{4.34}
\end{equation*}
$$

We also derive the one-group diffusion problem that follows from Eq. (4.16-4.17), where we have solved the 1st moment equation analytically and substituted the resulting Ficks law equation into $\vec{g}^{(n+1)}$ :

$$
\begin{equation*}
\left(-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2}+\sigma_{a}\right) f_{0}^{(i+1 / 2, n+1)}=\frac{\nu \sigma_{f}}{k^{(i+1 / 2, n)}}\left(\tilde{\phi}_{0}^{(i+1 / 2, n)}\right)+R_{0}^{(i+1 / 2)}, \tag{4.35}
\end{equation*}
$$

where the low-order corrected unknown, $\tilde{\phi}_{0}^{(i+1 / 2, n)}$, is defined as:

$$
\begin{equation*}
\tilde{\phi}_{0}^{(i+1 / 2, n)}=\left(\phi_{0}^{(i+1 / 2)}+f_{0}^{(i+1 / 2, n)}\right) . \tag{4.36}
\end{equation*}
$$

and again, the residual source is:

$$
\begin{equation*}
R_{0}^{(i+1 / 2)}=-\frac{\nu \sigma_{f}}{k^{(i)}} \phi_{0}^{(i)}+\sigma_{s}\left(\phi_{0}^{(i+1 / 2)}-\phi_{0}^{(i)}\right) . \tag{4.37}
\end{equation*}
$$

Similar to Eq. (4.22), we add the 0th moment of the one group transport equation in Eq. (4.34):

$$
\begin{equation*}
\vec{\nabla} \cdot \vec{J}^{(i+1 / 2)}+\sigma_{a} \phi_{0}^{(i+1 / 2)}=-R_{0}^{(i+1 / 2)} . \tag{4.38}
\end{equation*}
$$

to the diffusion equation in Eq. (4.35):

$$
\begin{equation*}
\vec{\nabla} \cdot \vec{J}^{(i+1 / 2)}+\left(-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2}\right) f_{0}^{(i+1 / 2, n+1)}+\sigma_{a} \phi_{0}^{(i+1 / 2)}+\sigma_{a} f_{0}^{(i+1 / 2, n+1)}=\frac{\nu \sigma_{f}}{k^{(i+1 / 2, n)}} \tilde{\phi}_{0}^{(i+1 / 2, n)} \tag{4.39}
\end{equation*}
$$

We add $\left(-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2}\right) \phi_{0}^{(i+1 / 2)}$ to both sides and use the definition for $\tilde{\phi}^{i+1 / 2, n+1}$ to obtain an equivalent equation that is a power-like iteration for a diffusion operator:

$$
\begin{equation*}
\left(-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2}+\sigma_{a}\right) \tilde{\phi}_{0}^{(i+1 / 2, n+1)}=\frac{\nu \sigma_{f}}{k^{(i+1 / 2, n)}} \tilde{\phi}_{0}^{(i+1 / 2, n)}+Q_{L}^{(i+1 / 2)} \tag{4.40}
\end{equation*}
$$

where:

$$
\begin{equation*}
Q_{L}^{(i+1 / 2)}=\left(-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2} \phi_{0}^{(i+1 / 2)}-\vec{\nabla} \cdot \vec{J}^{(i+1 / 2)}\right) \tag{4.41}
\end{equation*}
$$

Now that we have obtained equations in a form that will be more easy to manipulate, we express the transport unknowns as integrals of infinite Fourier modes:

$$
\begin{align*}
\psi_{m}^{(i+1 / 2)} & =\iiint_{0}^{\infty} d^{3} \lambda \psi_{m, \dagger}(\vec{\lambda}) \omega_{H}^{i} e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}},  \tag{4.42}\\
\phi_{0}^{(i)} & =\iiint_{0}^{\infty} d^{3} \lambda \phi_{0, \dagger}(\vec{\lambda}) \omega_{H}^{i} e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}}, \tag{4.43}
\end{align*}
$$

and the low-order correction and corrected unknown as integrals of infinite Fourier modes:

$$
\begin{align*}
f^{(i+1 / 2, n)} & =\iiint_{0}^{\infty} d^{3} \lambda f_{\dagger}(\vec{\lambda}) \omega_{L}^{n} e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}}  \tag{4.44}\\
\tilde{\phi}_{0}^{(i+1 / 2, n)} & =\iiint_{0}^{\infty} d^{3} \lambda \tilde{\phi}_{0, \dagger}(\vec{\lambda}) \omega_{L}^{n} e^{\mathbf{i} \sigma_{t} \vec{\lambda} \cdot \vec{r}} \tag{4.45}
\end{align*}
$$

Here $\omega_{H}$ and $\omega_{L}$ are constants that describe the error reduction per iteration of the high-order system and low-order system respectively. The linear independence of each mode implies a separate equation for each $\vec{\lambda}$. That is, each mode evolves independently.

After substituting the Fourier integrals, the high-order equation implies:

$$
\begin{equation*}
\left(\mathbf{i} \vec{\Omega}_{m} \cdot \vec{\lambda}+1\right) \sigma_{t} \psi_{m, \dagger}^{(i+1 / 2)}(\vec{\lambda})=\frac{1}{4 \pi}\left(\sigma_{s}+\frac{\nu \sigma_{f}}{k^{(i)}}\right) \phi_{0, \dagger}^{(i)}(\vec{\lambda}) \tag{4.46}
\end{equation*}
$$

and the low-order equation implies:

$$
\begin{equation*}
\left(\frac{1}{3}|\vec{\lambda}|^{2} \sigma_{t}+\sigma_{a}\right) \tilde{\phi}_{\dagger, 0}^{(i+1 / 2, n+1)}(\vec{\lambda})=\frac{\nu \sigma_{f}}{k^{(i+1 / 2, n)}} \tilde{\phi}_{\dagger, 0}^{(i+1 / 2, n)}(\vec{\lambda})+Q_{L, \dagger}^{(i+1 / 2)}(\vec{\lambda}) \tag{4.47}
\end{equation*}
$$

We invert the high-order operator for each Fourier mode to determine $\psi_{m, \dagger}^{(i+1 / 2)}(\vec{\lambda})$ :

$$
\begin{align*}
\psi_{m, \dagger}^{(i+1 / 2)}(\vec{\lambda}) & =\frac{1}{4 \pi} \frac{1}{1+\mathbf{i} \vec{\Omega}_{m} \cdot \vec{\lambda}} \frac{1}{\sigma_{t}}\left(\sigma_{s}+\frac{\nu \sigma_{f}}{k^{(i)}}\right) \phi_{0, \dagger}^{(i)}(\vec{\lambda}), \\
& =\frac{1}{4 \pi} \frac{1-\mathbf{i} \vec{\Omega}_{m} \cdot \vec{\lambda}}{1+\left(\vec{\Omega}_{m} \cdot \vec{\lambda}\right)^{2}} \frac{1}{\sigma_{t}}\left(\sigma_{s}+\frac{\nu \sigma_{f}}{k^{(i)}}\right) \phi_{0, \dagger}^{(i)}(\vec{\lambda}), \tag{4.48}
\end{align*}
$$

and then determine modes of the next high-order iterate (assuming a symmetric quadrature set, which means the quadrature sum of the odd function in $\vec{\Omega}_{m}$ is zero):

$$
\begin{equation*}
\phi_{0, \dagger}^{(i+1 / 2)}(\vec{\lambda})=\frac{1}{4 \pi} \sum_{m} w_{m} \frac{1}{1+\left(\vec{\Omega}_{m} \cdot \vec{\lambda}\right)^{2}} \frac{1}{\sigma_{t}}\left(\sigma_{s}+\frac{\nu \sigma_{f}}{k^{(i)}}\right) \phi_{0, \uparrow}^{(i)}(\vec{\lambda}) \tag{4.49}
\end{equation*}
$$

Next we determine the source term for the power-like iteration that depends on the modes of $\phi_{0, \dagger}^{(i+1 / 2)}(\vec{\lambda})$ :

$$
\begin{equation*}
Q_{L, \dagger}^{(i+1 / 2)}(\vec{\lambda})=\frac{1}{3}|\vec{\lambda}|^{2} \sigma_{t}\left(1-3 \frac{\sum_{m} \frac{1}{4 \pi} w_{m} \frac{\left(\vec{\lambda} \cdot \vec{\Omega}_{m}\right)^{2}}{1+\left(\vec{\lambda} \cdot \vec{\Omega}_{m}\right)^{2}}}{\sum_{m} \frac{1}{4 \pi} w_{m} \frac{|\vec{\lambda}|^{2}}{1+\left(\vec{\lambda} \cdot \vec{\Omega}_{m}\right)^{2}}}\right) \phi_{0, \dagger}^{(i+1 / 2)}(\vec{\lambda}) \tag{4.50}
\end{equation*}
$$

or defining $\mu_{m}$ as the cosine between $\vec{\lambda}$ and $\vec{\Omega}_{m}$ :

$$
\begin{equation*}
Q_{L, \dagger}^{(i+1 / 2)}(\vec{\lambda})=\frac{1}{3}|\vec{\lambda}|^{2} \sigma_{t}\left(1-3 \frac{\sum_{m} \frac{1}{4 \pi} w_{m} \frac{|\vec{\lambda}|^{2} \mu_{m}^{2}}{1+|\vec{\lambda}|^{\prime} \mu_{m}^{2}}}{\sum_{m} \frac{1}{4 \pi} w_{m} \frac{|\vec{\lambda}|^{2}}{1+|\vec{\lambda}|^{2} \mu_{m}^{2}}}\right) \phi_{0, \dagger}^{(i+1 / 2)}(\vec{\lambda}) . \tag{4.51}
\end{equation*}
$$

Consider the first step of the power-like iteration for the flat mode, where all spatial gradients are 0 :

$$
\begin{equation*}
\tilde{\phi}_{0}^{(i+1 / 2,1)}=\frac{\nu \sigma_{f}}{\sigma_{a}} \frac{1}{k^{(i+1 / 2,0)}} \tilde{\phi}_{0}^{(i+1 / 2,0)} . \tag{4.52}
\end{equation*}
$$

The calculation of the next eigenvalue involves integrals that are non-zero only for the flat mode:

$$
\begin{equation*}
k^{(i+1 / 2,1)}=k^{(i+1 / 2,0)} \frac{\tilde{\phi}_{0}^{(i+1 / 2,1)}}{\tilde{\phi}_{0}^{(i+1 / 2,0)}} . \tag{4.53}
\end{equation*}
$$

On the next iteration, the diffusion equation produces:

$$
\begin{equation*}
\tilde{\phi}_{0}^{(i+1 / 2,2)}=\frac{\nu \sigma_{f}}{\sigma_{a}} \frac{1}{k^{(i+1 / 2,1)}}\left(\tilde{\phi}_{0}^{(i+1 / 2,1)}\right) . \tag{4.54}
\end{equation*}
$$

which is equal to $\tilde{\phi}_{0}^{(i+1 / 2,1)}$. Thus the power-like iteration must converge to the eigenvalue after one step, since $\tilde{\phi}_{0}^{(i+1 / 2,2)}=\tilde{\phi}_{0}^{(i+1 / 2,1)}$ and therefore $k^{(i+1 / 2,2)}=k^{(i+1 / 2,1)}$. We substitute initial conditions and $\tilde{\phi}_{0}^{(i+1 / 2,1)}$ into Eq. (4.53) to find the converged eigenvalue:

$$
\begin{align*}
k^{(i+1 / 2,1)} & =k^{(i+1 / 2,0)} \frac{\frac{\nu \sigma_{f}}{\sigma_{a}} \frac{1}{k^{(i+1 / 2,0)}} \tilde{\phi}_{0}^{(i+1 / 2,0)}}{\tilde{\phi}_{0}^{(i+1 / 2,0)}}  \tag{4.55}\\
& =\frac{\nu \sigma_{f}}{\sigma_{a}}
\end{align*}
$$

Thus the power-like iteration produces the correct infinite medium eigenvalue in one iteration. For this infinite homogeneous problem where there is no net leakage, Suslov's argument above shows that the power-like iteration is equivalent to power iteration and immediate convergence should be expected.

Next we consider non-flat modes for subsequent iterations, where the converged eigenvalue has
already been obtained. We define a converged diffusion equation:

$$
\begin{equation*}
\left(-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2}+\sigma_{a}\right) \tilde{\phi}_{0}^{(i+1 / 2, C)}=\frac{\nu \sigma_{f}}{k^{C}} \tilde{\phi}_{0}^{(i+1 / 2, C)}+Q_{L}^{(i+1 / 2)}, \tag{4.56}
\end{equation*}
$$

and an iteration error:

$$
\begin{equation*}
\tilde{\phi}_{\epsilon, 0}^{(i+1 / 2, n)}=\tilde{\phi}_{0}^{(i+1 / 2, C)}-\tilde{\phi}_{0}^{(i+1 / 2, n)}=f^{(i+1 / 2, C}-f^{(i+1 / 2, n)} . \tag{4.57}
\end{equation*}
$$

We subtract the diffusion iteration equation from the converged equation to obtain an equation for the error in the diffusion iteration, which for converged $k$ is equivalent to a diffusion equation for the correction in a purely scattering medium with scattering cross section $\sigma_{a}$ :

$$
\begin{equation*}
\left(-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2}+\sigma_{a}\right) f^{(i+1 / 2, n+1)}=\frac{\nu \sigma_{f}}{k^{C}} f^{(i+1 / 2, n)}=\sigma_{a} f^{(i+1 / 2, n)} . \tag{4.58}
\end{equation*}
$$

Using the Fourier integral representation for $f^{(i+1 / 2, n)}$ in Eq. (4.44), the equation above implies:

$$
\begin{equation*}
\left(\frac{1}{3} \frac{\sigma_{t}}{\sigma_{a}}|\vec{\lambda}|^{2}+1\right) \sigma_{a} \omega_{L}=\sigma_{a} \tag{4.59}
\end{equation*}
$$

which we solve for $\omega_{L}$ and obtain an expression that is less than one for all values of $\vec{\lambda}$ :

$$
\begin{equation*}
\omega_{L}=\frac{1}{\frac{1}{3} \frac{\sigma_{t}}{\sigma_{a}}|\vec{\lambda}|^{2}+1} . \tag{4.60}
\end{equation*}
$$

An error reduction per iteration less than one shows that all non-flat modes decrease in magnitude per iteration. Given the iteration converges, we now determine the coefficient of each eigenmode of the iteration.

From the the converged diffusion equation in Eq. (4.56):

$$
\begin{equation*}
\left(-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2}\right) \tilde{\phi}_{0}^{(i+1 / 2, C)}=Q_{L}^{(i+1 / 2)} \tag{4.61}
\end{equation*}
$$

we may solve for the Fourier coefficient for the low-order problem solution. From the eigenvector
update equation, and substituting expressions for $Q_{L, \dagger}^{(i+1 / 2)}(\vec{\lambda})$ and $\phi^{(i+1 / 2)}(\vec{\lambda})$ that we found above:

$$
\begin{align*}
\tilde{\phi}_{0, \dagger}^{(i+1)}(\vec{\lambda}) & =\left(1-3 \frac{\sum_{m} \frac{1}{4 \pi} w_{m} \frac{|\vec{\lambda}|^{2} \mu_{m}^{2}}{1+|\vec{\lambda}|^{2} \mu_{m}^{2}}}{\sum_{m} \frac{1}{4 \pi} w_{m} \frac{\mid \overrightarrow{\left.\right|^{2}}}{1+|\vec{\lambda}|^{2} \mu_{m}^{2}}}\right)  \tag{4.62}\\
& \times\left(\frac{1}{4 \pi} \sum_{m} w_{m} \frac{1}{1+|\vec{\lambda}|^{2} \mu_{m}^{2}}\right) \frac{1}{-\sigma_{t}}\left(\sigma_{s}+\frac{\nu \sigma_{f}}{k^{(i)}}\right)_{0, \dagger}^{(i)}(\vec{\lambda})
\end{align*} .
$$

The cross section terms cancel from the prior finding of a converged eigenvalue. The resulting equation gives the reduction per combined high- and low-operations for each non-zero mode of the eigenvector:

$$
\begin{equation*}
\tilde{\phi}_{0, \dagger}^{(i+1)}(\vec{\lambda})=\left(1-3 \frac{\sum_{m} \frac{1}{4 \pi} w_{m} \frac{|\vec{\lambda}|^{2} \mu_{m}^{2}}{1+|\vec{\lambda}|^{2} \mu_{m}^{2}}}{\sum_{m} \frac{1}{4 \pi} w_{m} \frac{|\vec{\lambda}|^{2}}{1+|\vec{\lambda}|^{2} \mu_{m}^{2}}}\right)\left(\frac{1}{4 \pi} \sum_{m} w_{m} \frac{1}{1+|\vec{\lambda}|^{2} \mu_{m}^{2}}\right) \phi_{0, \dagger}^{(i)}(\vec{\lambda}) . \tag{4.63}
\end{equation*}
$$

The maximum value of this expression is .2247 times a constant, which is the same value obtained from DSA for fixed-source problems.[1] Thus, the power-like iteration provides an error reduction similar to DSA for fixed-source problems per combined high- and low-operations. Another way to demonstrate the similarity to DSA for fixed-source problems is by substituting the converged eigenvalue $\nu \sigma_{f} / k^{(C)}=\sigma_{a}$ and the converged low-order equation:

$$
\begin{gather*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+\sigma_{t}\right) \psi_{m}^{(i+1 / 2)}=\frac{1}{4 \pi} \sigma_{t} \phi_{0}^{(i)}  \tag{4.64}\\
\left(-\frac{1}{3 \sigma_{t}} \vec{\nabla}^{2}\right) f_{0}^{(i+1 / 2, C)}=\sigma_{t}\left(\phi_{0}^{(i+1 / 2)}-\phi_{0}^{(i)}\right),  \tag{4.65}\\
\phi_{0}^{(i+1)}=\tilde{\phi}_{0}^{(i+1 / 2, n)}=\left(\phi_{0}^{(i+1 / 2)}+f_{0}^{(i+1 / 2, C)}\right) . \tag{4.66}
\end{gather*}
$$

This system of equations is equivalent to a DSA method for a purely scattering medium.
The preceding analysis for infinite homogeneous problems shows the power-like iteration algorithm produces the converged transport eigenvalue in one iteration, all modes are reduced similar to DSA for fixed-source problems, and the overall iteration becomes equivalent to DSA for fixedsource problems in a purely scattering medium once the eigenvalue is obtained.

### 4.3.2 Algebraic Analysis of One-Cell Problem

Consider a discretized one-cell homogeneous problem surrounded by vacuum, where we have a high-order operator accelerated with the power-like iteration by a low-order operator. We assume problem symmetry, a symmetric initial guess, and a spatial discretization such that a symmetric solution is characterized by a single scalar amplitude (for example, the scalar flux at each vertex). We can then write the net leakage rate as an escape cross section times a scalar-flux amplitude, denoted with $H$ for high-order and $L$ for low-order. The result from one high-order operation satisfies:

$$
\begin{equation*}
\left(\sigma_{e s c}^{H}+\sigma_{t}\right) \phi^{(i+1 / 2)}=\left(\sigma_{s}+\frac{\nu \sigma_{f}}{k^{(i)}}\right) \phi^{(i)} . \tag{4.67}
\end{equation*}
$$

The low-order problem that follows, following steps that led to Eq. (4.40):

$$
\begin{equation*}
\left(\sigma_{e s c}^{L}+\sigma_{a}\right) \tilde{\phi}^{(i+1 / 2, n+1)}=\frac{\nu \sigma_{f}}{k^{(i+1 / 2, n)}} \tilde{\phi}^{(i+1 / 2, n)}+\left(\sigma_{e s c}^{L}-\sigma_{e s c}^{H}\right) \phi^{(i+1 / 2)} \tag{4.68}
\end{equation*}
$$

with initial iterates:

$$
\begin{gather*}
\tilde{\phi}^{(i+1 / 2,1)}=\phi^{(i+1 / 2)},  \tag{4.69}\\
k^{(i+1 / 2, n)}=k^{(i)} . \tag{4.70}
\end{gather*}
$$

This simplified system allows us to solve for $\tilde{\phi}^{(i+1 / 2, n+1)}$ directly:

$$
\begin{equation*}
\tilde{\phi}^{(i+1 / 2, n+1)}=\frac{\frac{\nu \sigma_{f}}{k^{(i+1 / 2, n)}} \tilde{\phi}^{(i+1 / 2, n)}+\left(\sigma_{e s c}^{L}-\sigma_{e s c}^{H}\right) \phi^{(i+1 / 2)}}{\left(\sigma_{e s c}^{L}+\sigma_{a}\right)} . \tag{4.71}
\end{equation*}
$$

We show that the diffusion problem converges on the first diffusion power iteration. Using the initial conditions above, the diffusion eigenvector and eigenvalue after the first iteration:

$$
\begin{gather*}
\tilde{\phi}^{(i+1 / 2,1)}=\frac{\frac{\nu \sigma_{f}}{k^{(i)}}+\left(\sigma_{\text {esc }}^{L}-\sigma_{\text {esc }}^{H}\right)}{\left(\sigma_{\text {esc }}^{L}+\sigma_{a}\right)} \phi^{(i+1 / 2)},  \tag{4.72}\\
k^{(i+1 / 2,1)}=k^{(i)} \frac{\frac{\nu \sigma_{f}}{k^{(i)}}+\left(\sigma_{e s c}^{L}-\sigma_{e s c}^{H}\right)}{\left(\sigma_{e s c}^{L}+\sigma_{a}\right)} . \tag{4.73}
\end{gather*}
$$

On the second iteration we determine the diffusion eigenvector:

$$
\begin{equation*}
\tilde{\phi}^{(i+1 / 2,2)}=\frac{\frac{\nu \sigma_{f}}{k^{(i+1 / 2,1)}} \tilde{\phi}^{(i+1 / 2,1)}+\left(\sigma_{e s c}^{L}-\sigma_{e s c}^{H}\right) \phi^{(i+1 / 2)}}{\left(\sigma_{e s c}^{L}+\sigma_{a}\right)} \tag{4.74}
\end{equation*}
$$

From the update equation definition, $\frac{\tilde{\phi}^{(i+1 / 2,1)}}{k^{(i+1 / 2,1)}}=\frac{\phi^{(i+1 / 2)}}{k^{(i)}}$, and thus the second iteration eigenvector is the equal to the first:

$$
\begin{equation*}
\tilde{\phi}^{(i+1 / 2,2)}=\frac{\frac{\nu \sigma_{f}}{k^{(i)}} \phi^{(i+1 / 2)}+\left(\sigma_{\text {esc }}^{L}-\sigma_{e s c}^{H}\right) \phi^{(i+1 / 2)}}{\left(\sigma_{e s c}^{L}+\sigma_{a}\right)}=\tilde{\phi}^{(i+1 / 2,1)} . \tag{4.75}
\end{equation*}
$$

Because the eigenvector does not change, the second eigenvalue is also equal to the first, and that eigenvalue is the converged low-order eigenvalue:

$$
\begin{equation*}
k^{(i+1 / 2,2)}=k^{(i+1 / 2,1)} \frac{\tilde{\phi}^{(i+1 / 2,2)}}{\tilde{\phi}^{(i+1 / 2,1)}}=k^{(i+1 / 2,1)}=k^{(i+1 / 2, C)}=k^{(i)} \frac{\frac{\nu \sigma_{f}}{k^{(i)}}+\left(\sigma_{e s c}^{L}-\sigma_{\text {esc }}^{H}\right)}{\left(\sigma_{\text {esc }}^{L}+\sigma_{a}\right)} . \tag{4.76}
\end{equation*}
$$

We obtain the eigenvalue error reduction per combined high- and low-operations as follows. From the equation to update the high-order eigenvalue to the converged low-order eigenvalue:

$$
\begin{equation*}
k^{(i+1)}=k^{(i+1 / 2, C)} \tag{4.77}
\end{equation*}
$$

we subtract the converged transport eigenvalue, $k^{(C)}=\frac{\nu \sigma_{f}}{\sigma_{\text {esc }}^{H}+\sigma_{a}}$, from both sides:

$$
\begin{align*}
k^{(i+1)}-k^{(C)} & =k^{(i)} \frac{\nu \frac{\nu \sigma_{f}}{k^{(i)}}+\left(\sigma_{\text {esc }}^{L}-\sigma_{\text {esc }}^{H}\right)}{\left(\sigma_{\text {esc }}^{L}+\sigma_{a}\right)}-\frac{\nu \sigma_{f}}{\sigma_{\text {esc }}^{H}+\sigma_{a}},  \tag{4.78}\\
& =\frac{\nu \sigma_{f}+k^{(i)}\left(\sigma_{\text {esc }}^{L}-\sigma_{\text {esc }}^{H}\right)-\frac{\nu \sigma_{f}}{\sigma_{\text {esc }}^{H}+\sigma_{a}}\left(\sigma_{\text {esc }}^{L}+\sigma_{a}\right)}{\left(\sigma_{\text {esc }}^{L}+\sigma_{a}\right)} .
\end{align*}
$$

We add and subtract $\sigma_{\text {esc }}^{H}$ and regroup terms:

$$
\begin{align*}
k^{(i+1)}-k^{(C)} & =\frac{\nu \sigma_{f}+k^{(i)}\left(\sigma_{\text {esc }}^{L}-\sigma_{\text {esc }}^{H}\right)-\frac{\nu \sigma_{f}}{\sigma_{\text {esc }}^{H}+\sigma_{a}}\left(\sigma_{\text {esc }}^{L}+\sigma_{a}+\sigma_{\text {esc }}^{H}-\sigma_{\text {esc }}^{H}\right)}{\left(\sigma_{\text {esc }}^{L}+\sigma_{a}\right)}, \\
& =\frac{\nu \sigma_{f}+k^{(i)}\left(\sigma_{\text {esc }}^{L}-\sigma_{\text {esc }}^{H}\right)-\frac{\nu \sigma_{f}}{\sigma_{\text {esc }}^{H}+\sigma_{a}}\left(\sigma_{\text {esc }}^{L}-\sigma_{\text {esc }}^{H}\right)-\frac{\nu \sigma_{f}}{\sigma_{\text {esc }}^{H}+\sigma_{a}}\left(\sigma_{\text {esc }}^{H}+\sigma_{a}\right)}{\left(\sigma_{\text {esc }}^{L}+\sigma_{a}\right)},  \tag{4.79}\\
& =\frac{\sigma_{\text {esc }}^{L}-\sigma_{\text {esc }}^{H}}{\sigma_{\text {esc }}^{L}+\sigma_{a}}\left(k^{(i)}-k^{(C)}\right) .
\end{align*}
$$

Thus the eigenvalue iteration converges if the following term is less than one in magnitude:

$$
\begin{equation*}
\left|\frac{\sigma_{e s c}^{L}-\sigma_{e s c}^{H}}{\sigma_{e s c}^{L}+\sigma_{a}}\right|<1 \tag{4.80}
\end{equation*}
$$

Since $\sigma_{\text {esc }}^{L}+\sigma_{a}$ is strictly positive, the convergence condition can be written as:

$$
\begin{equation*}
\left|\sigma_{e s c}^{L}-\sigma_{e s c}^{H}\right|<\sigma_{e s c}^{L}+\sigma_{a} . \tag{4.81}
\end{equation*}
$$

This analysis shows that for this simplified problem the iteration will diverge if the high-order leakage and low-order leakage disagree to a large degree-more specifically, the requirement for convergence is that the two leakage probabilities must differ by less than the sum of the low-order absorption and leakage probabilities. (Simple algebra shows that this is equivalent to the low- and high-order $k$ eigenvalues differing by less than a factor of two.) It is not surprising that convergence requires the low-order operator to be sufficiently "consistent" with the high-order operator. This kind of "consistency" requirement also exists for fixed-source problems.[1] In the next section we compare the consistency requirement derived here to the requirement for a similar fixed-source
problem.

### 4.3.3 Algebraic Analysis of One-Cell Fixed-Source Problem

An interesting question is how the consistency requirements compare for fixed-source and $k$-eigenvalue versions of the one-cell problem studied in the previous section. We demonstrate a derivation of the consistency requirement from a one-cell fixed-source problem with a DSA scheme.

The converged fixed-source problem satisfies the following equation:

$$
\begin{equation*}
\left(\sigma_{e s c}^{H}+\sigma_{t}\right) \phi^{(C)}=\sigma_{s} \phi^{(C)}+Q_{H} \tag{4.82}
\end{equation*}
$$

and the DSA iteration scheme is given by the following equations:

$$
\begin{gather*}
\left(\sigma_{\text {esc }}^{H}+\sigma_{t}\right) \phi^{(i+1 / 2)}=\sigma_{s} \phi^{(i)}+Q_{H},  \tag{4.83}\\
\left(\sigma_{e s c}^{L}+\sigma_{a}\right) f^{(i+1 / 2)}=\sigma_{s}\left(\phi^{(i+1 / 2)}-\phi^{(i)}\right),  \tag{4.84}\\
\phi^{(i+1)}=\phi^{(i+1 / 2)}+f^{(i+1 / 2)} . \tag{4.85}
\end{gather*}
$$

We obtain an expression for the high-order error- $\left(\phi^{(C)}-\phi^{(i+1 / 2)}\right)$ —by subtracting the highorder equation in Eq. (4.83) from the converged equation in Eq. (4.82):

$$
\begin{equation*}
\left(\sigma_{e s c}^{H}+\sigma_{t}\right)\left(\phi^{(C)}-\phi^{(i+1 / 2)}\right)=\sigma_{s}\left(\phi^{(C)}-\phi^{(i)}\right) \tag{4.86}
\end{equation*}
$$

Next we obtain an equation for the error after the low-order operation and subsequent update. From the high-order equation in Eq. (4.83), we perform algebra to obtain the following form:

$$
\begin{equation*}
\left(\sigma_{e s c}^{L}+\sigma_{a}\right) \phi^{(i+1 / 2)}=\left(\sigma_{e s c}^{L}-\sigma_{e s c}^{H}\right) \phi^{(i+1 / 2)}+\sigma_{s}\left(\phi^{(i)}-\phi^{(i+1 / 2)}\right)+Q_{H}, \tag{4.87}
\end{equation*}
$$

and we add this to the low-order equation in Eq. (4.84):

$$
\begin{equation*}
\left(\sigma_{e s c}^{L}+\sigma_{a}\right) \phi^{(i+1)}=\left(\sigma_{e s c}^{L}-\sigma_{e s c}^{H}\right) \phi^{(i+1 / 2)}+Q_{H} . \tag{4.88}
\end{equation*}
$$

Similarly, from the converged equation in Eq. (4.82) we obtain:

$$
\begin{equation*}
\left(\sigma_{e s c}^{L}+\sigma_{a}\right) \phi^{(C)}=\left(\sigma_{e s c}^{L}-\sigma_{e s c}^{H}\right) \phi^{(C)}+Q_{H} . \tag{4.89}
\end{equation*}
$$

We subtract the previous two equations-Eq. (4.88) and (4.89)-to obtain an equation for the iteration error of the next high-order iterate:

$$
\begin{equation*}
\left(\sigma_{\text {esc }}^{L}+\sigma_{a}\right)\left(\phi^{(C)}-\phi^{(i+1)}\right)=\left(\sigma_{\text {esc }}^{L}-\sigma_{\text {esc }}^{H}\right)\left(\phi^{(C)}-\phi^{(i+1 / 2)}\right) . \tag{4.90}
\end{equation*}
$$

We combine Eq. (4.90) and (4.86) and obtain an equation for the error after the combined highand low-operations:

$$
\begin{equation*}
\left(\phi^{(C)}-\phi^{(i+1)}\right)=\frac{\sigma_{s}}{\left(\sigma_{e s c}^{H}+\sigma_{t}\right)} \frac{\left(\sigma_{\text {esc }}^{L}-\sigma_{\text {esc }}^{H}\right)}{\left(\sigma_{\text {esc }}^{L}+\sigma_{a}\right)}\left(\phi^{(C)}-\phi^{(i)}\right) . \tag{4.91}
\end{equation*}
$$

The previous equation implies the iteration converges if:

$$
\begin{equation*}
\left|\frac{\sigma_{s}}{\left(\sigma_{e s c}^{H}+\sigma_{t}\right)} \frac{\left(\sigma_{e s c}^{L}-\sigma_{e s c}^{H}\right)}{\left(\sigma_{e s c}^{L}+\sigma_{a}\right)}\right|<1, \tag{4.92}
\end{equation*}
$$

and after multiplying by terms that are strictly positive, we obtain a convergence criteria similar to that of the $k$-eigenvalue criteria in the previous section:

$$
\begin{equation*}
\left|\sigma_{e s c}^{L}-\sigma_{e s c}^{H}\right|<\frac{1}{\sigma_{s}}\left(\sigma_{e s c}^{L}+\sigma_{a}\right)\left(\sigma_{e s c}^{H}+\sigma_{t}\right) . \tag{4.93}
\end{equation*}
$$

Previously we found that the one-cell $k$ problem converges if the magnitude of the difference in high- and low-order escape cross sections is less than the sum of the absorption and low-order escape cross sections. Here we find a less stringent requirement for convergence of the one-cell
fixed-source problem, because the magnitude of the difference in escape cross sections is permitted to be larger by a factor of $\left(\sigma_{e s c}^{H}+\sigma_{t}\right) / \sigma_{s}$, which is greater than 1 . We remark that in the problems that are most difficult to converge, $\sigma_{t} \approx \sigma_{s} \gg \sigma_{e s c}^{H}$, so this factor approaches unity and the "consistency" conditions for convergence of the fixed-source and $k$ problems become approximately the same.

### 4.4 Results

In the numerical results that follow, we employ the PieceWise Linear Discontinuous (PWLD) finite element method for our transport spatial discretization.[45, 46, 47] We use the Semi-Consistent "CDFEM" diffusion operator that we previously developed, which solves a continuous finite element (CFEM) discretization of the diffusion equation and then employs a cell-by-cell calculation to create a discontinuous (DFEM) additive correction.[19] The use of a CFEM greatly reduces the number of degrees of freedom of the global diffusion matrix, and ensures this matrix is symmetric positive definite, unlike the matrix resulting from fully consistent DSA for DFEMs.

The first test problem is the well-known 2D C5G7 reactor benchmark problem.[48] We model one quarter of the lattice, with reflecting boundary conditions on left and bottom sides, and vacuum boundary conditions on right and top sides. We use a mesh refinement that was shown to produce very small spatial discretization error, shown in Fig. (4.1).[49] Multi-group cross sections are defined in the problem specification. We use discrete ordinates with a Gauss-Legendre-Chebyshev product quadrature, with 8 polar and 16 azimuthal directions per quadrant, which has been shown to be sufficient to resolve the angular discretization error to within a few pcm.[49] These problems were run on the Quartz supercomputer at LLNL (Lawrence Livermore National Lab), on 6 nodes and 196 concurrent processes. The problem was split by into 14 processes in x by 14 processes in y. We note that this is not the optimal layout for parallelism of transport sweeps, but is a better distribution for parallelism of the diffusion solution.

Table 4.1 presents results for four different iterative strategies-two strategies for scattering iterations within the transport steps, with and without the use a diffusion problem for acceleration. One scattering strategy is to fully converge the scattering source during each transport step


Figure 4.1: Mesh and materials for one quarter geometry of the C5G7 reactor benchmark (left) and mesh detail for a single pin cell (right).
(labeled Converged and meaning $S_{c o n}=S$ and $S_{\text {rec }}=S_{\text {lag }}=0$ in Eq. (4.7)); the other is to perform a single transport sweep independently across all groups (labeled 1-Sweep and meaning $S_{\text {lag }}=S$ and $S_{\text {con }}=S_{\text {rec }}=0$ in Eq. (4.7)). (There are possible levels of scattering convergence between these two limits. We have not explored these in detail.) Problems that use the diffusion eigenvalue-like acceleration are labeled k -Accel. We compare the effect of performing the cell-by-cell DFEM update step at various points in the iteration: end of iteration (labeled End); after every diffusion operation (labeled CDFEM, since this is the original CDFEM method); and performing no consistency step (labeled CFEM, as this is the same as using a CFEM basis for the diffusion problem). For this problem, we used Richardson iteration when we fully converged the within-group scattering transport problems.

As expected, we have found that the optimal method is to perform only one transport sweep per power iteration. The number of transport sweeps required to converge the eigenvalue to $1.0 E-7$ and the eigenvector to $1.0 E-5$ without acceleration is around 2000 . For this problem, a CFEM
diffusion additive correction is remarkably effective, reducing the overall iteration count to 17 even when only one transport sweep is executed per iteration. Employing the one-cell discontinuouscorrection updates, either after every CFEM diffusion solution or only after convergence of the CFEM diffusion power iterations, does improve the correction, reducing the iteration count even further, to 15 . We note that discontinuous update step is an inexpensive operation, requiring only the independent solutions of single-cell linear systems, with number of unknowns equaling the number of vertices in each cell.

Table 4.1: Results from 2D C5G7 problem

| Transport Scattering | Converged | Converged | 1-Sweep | 1-Sweep | 1-Sweep | 1-Sweep |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Accel. Method | N/A | k-Accel. | N/A | k-Accel. | k-Accel. | k-Accel. |
| Disc. Update | N/A | End | N/A | End | CDFEM | CFEM |
| Transport Steps | 49 | 6 | 2038 | 15 | 15 | 17 |
| Sweep Time [s] | 8515 | 1187 | 2677 | 41.7 | 41.3 | 47.2 |
| Diffusion Time [s] | N/A | 90.7 | N/A | 15.2 | 15.1 | 15.8 |

Next we study a problem that is a modification of the C5G7 design. In this problem the spatial mesh resolves fuel, gap, guide tubes, instrumentation tubes, and cladding. We employ the Finite-Element-with-Discontiguous-Support (FEDS) energy discretization with 191 energy unknowns (including 59 in the resolved-resonance range).[50] We used only $\mathrm{UO}_{2}$ assemblies to simplify cross-section generation. The mesh is illustrated in Fig. 4.2. The FEDS energy discretization provides increased accuracy over standard multigroup, but adds upscattering in the resolved-resonance range even when scattering is physically only downscattering. This problem is meant to test the applicability of the linear DSA for eigenvalues with a more complicated scattering operator, and also to test the ability of the CDFEM DSA to handle small transparent regions such as the gap between fuel and cladding.

We set the eigenvalue residual tolerance to $1.0 E-5$ and the eigenvector residual tolerance of the $L_{2}$ norm to $1.0 E-5$. We use adaptive error estimates to guard against false convergence, which


Figure 4.2: Mesh and materials for one quarter geometry of the C5G191 reactor (left) and mesh detail for a single pin cell (right).
requires smaller relative difference between successive iterates if the observed error-reduction factor is close to one.[1]

The previous problem made it clear that a single transport sweep per overall iteration is the most efficient strategy, so here we test that strategy with and without DSA. Results are summarized in Table 4.2. We observe that the within group scattering problem is computationally expensive to converge. Iterating on only the scattering operator does not efficiently reduce the eigenvalue residual.

Without acceleration, the 1-Sweep method has an error-reduction factor near unity. This is remedied by using the diffusion eigenvalue-like problem to accelerate the solution, not only speeding convergence but removing the issue of false convergence.

Table 4.2: Results from 2D C5G191 problem

| Transport Scattering | 1-Sweep | 1-Sweep |
| :---: | :---: | :---: |
| Accel. Method | N/A | k-Accel. |
| Error-Reduction Factor | 0.991 | 0.743 |
| Transport Steps | 852 | 23 |
| Total Time [hours] | 12.2 | 1.14 |

The final problem we test is a C5G7 problem in three dimensions, which we include to demonstrate that the linear DSA methodology with our chosen CDFEM low-order operator also works well in 3D. This is the C5G7 problem with the same mesh in the $x y$ plane, extruded in the third dimension according to the benchmark designation with axial meshing sufficient to accurately resolve the solution. As before, we set the eigenvalue residual tolerance to $1.0 E-5$ and the eigenvector residual tolerance of the $L_{2}$ norm to $1.0 E-5$. Results are shown in Table 4.3. The performance of the iterative method is similar to that in 2 D , reducing the required number of transport sweeps for $1.0 E-5$ convergence to only 14 . The unaccelerated method was converging so slowly that we terminated the run to avoid wasting compute cycles.

Table 4.3: Results from 3D C5G7 problem

| Transport Scattering | 1-Sweep | 1-Sweep |
| :---: | :---: | :---: |
| Accel. Method | N/A | k-Accel. |
| Error-Reduction Factor | 0.980 | 0.633 |
| Transport Steps | $128^{*}$ | 14 |
| Total Time [hours] | $24^{*}$ | 2.35 |

* Terminated without converging after 24 hours of run time


### 4.5 Summary

In this chapter we have studied the use of diffusion operators to accelerate the convergence of eigenvalue iterations. Here we have explored a family of methods, developed by Adams in 1986 and independently by Suslov in 2003, that employs a low-order eigenvalue-like problem
with a fixed source to obtain an updated eigenvalue estimate and an additive correction to the eigenfunction. We have shown that the low-order linear diffusion problem becomes algebraically equivalent to the QuasiDiffusion low-order problem as the solution approaches the converged solution. Through a Fourier analysis in an infinite homogeneous medium, we have shown the iteration rapidly converges to the correct eigenvalue and eigenvector and not an arbitrary solution. We have shown that for one-cell homogeneous problems the iteration procedure is convergent and converges to the correct eigenvalue if the high-order and low-order operators satisfy a mild consistency requirement, namely, that they produce eigenvalues that are within a factor of two of each other.

We have also shown the effectiveness of our Continuous / Discontinuous finite-element diffusion operator for reactor problems. We have demonstrated that the method provides convergence of $k$ problems to $1 E-5$ with only $\approx 15$ transport sweeps for the well-known C5G7 benchmarks in 2D and 3D, and also for a similar problem with more spatial detail and with 191 energy unknowns. We emphasize that if a transport code already uses a diffusion preconditioner to accelerate convergence of scattering iterations, then using the low-order eigenvalue-like problem it is easy to apply the same diffusion operator to eigenvalue acceleration using the equations described herein, without the need to develop nonlinear functionals or discretize operators more complicated than diffusion.

## 5. LINEAR ACCELERATION OF THERMAL RADIATIVE TRANSFER ITERATION

### 5.1 Method Motivation

In this chapter, we discuss solution methods for time dependent thermal radiative transfer. For photon frequencies at which photon absorption dominates photon scattering, and motion of the material is ignored, the thermal radiation follows a Boltzmann transport equation:

$$
\begin{align*}
& \frac{1}{c} \frac{\partial}{\partial t} \psi(\vec{r}, \vec{\Omega}, E, t)+\vec{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, \vec{\Omega}, E, t)+\sigma(\vec{r}, E, t, T(\vec{r}, t)) \psi(\vec{r}, \vec{\Omega}, E, t)  \tag{5.1}\\
&=\frac{1}{4 \pi} \sigma(\vec{r}, E, t, T(\vec{r}, t)) B(T(\vec{r}, t), E)+q(\vec{r}, \vec{\Omega}, E, t)
\end{align*}
$$

and an equation that describes the change in material energy, ignoring thermal conduction:

$$
\begin{equation*}
C_{v}(\vec{r}, t) \frac{\partial}{\partial t} T(\vec{r}, t)=\rho(\vec{r}, t)-\int_{0}^{\infty} d E \sigma(\vec{r}, E, t, T(\vec{r}, t)) B(T(\vec{r}, t), E)+Q_{e x t}(\vec{r}, t) . \tag{5.2}
\end{equation*}
$$

The independent variables in these equations are the spatial position, $\vec{r}$, direction of particle motion, $\vec{\Omega}$, photon energy, $E$, and time, $t$. These equations couple the unknown quantities of radiation intensity, $\psi(\vec{r}, \vec{\Omega}, E, t)$, and material temperature, $T(\vec{r}, t)$. The macroscopic material opacity $\sigma(\vec{r}, E, t, T(\vec{r}, t))$ is calculated from the space- and time-dependent material density, $\rho_{M}(\vec{r}, t)$, and the microscopic opacity of the material, $\kappa(\vec{r}, E, T(\vec{r}, t))$ at position $\vec{r}$ and time $t$ for photons of energy $E$ given a material temperature of $T(\vec{r}, t)$ :

$$
\begin{equation*}
\sigma(\vec{r}, E, t, T(\vec{r}, t))=\rho_{M}(\vec{r}, t) \kappa(\vec{r}, E, T(\vec{r}, t)) \tag{5.3}
\end{equation*}
$$

The Planckian emission spectrum, $B(T(\vec{r}, t), E)$, is a known function:

$$
\begin{equation*}
B(T(\vec{r}, t), E) \approx \frac{2 E^{3}}{h^{3} c^{2}}\left(e^{E /(k T(\vec{r}, t))}-1\right)^{-1} \tag{5.4}
\end{equation*}
$$

In the material energy equation, $C_{v}(\vec{r}, t)$ is the material specific heat at constant volume, and
$\rho(\vec{r}, t)$ is the absorption rate density (ARD) of thermal radiation in the material, which is the integral quantity of the radiation intensity that couples angular and energy dependence:

$$
\begin{equation*}
\rho(\vec{r}, t)=\int_{0}^{\infty} d E \sigma(\vec{r}, E, t, T(\vec{r}, t)) \int_{4 \pi} d \Omega \psi(\vec{r}, \vec{\Omega}, E, t), \tag{5.5}
\end{equation*}
$$

For completeness we have included a fixed radiation source, $q(\vec{r}, \vec{\Omega}, E, t)$, and an external source of material heating, $Q_{\text {ext }}(\vec{r}, t)$, but omit these interior sources from equations henceforward as they do not introduce significant difficulty in the solution procedure.

We solve this system with Newton's Method, resulting in a transport equation that contains absorption/re-emission terms that are a pseudo-scattering problem for the ARD (details of the pseudo-scattering problem are found in subsection 5.2.3). The pseudo-scattering problem is then solved with an iterative method, which is itself sometimes called lambda iteration, at each step of the Newton iteration.

Linear acceleration methods have been devised to effectively accelerate the convergence of the iterative method used to solve the pseudo-scattering problem, such as Grey Transport Acceleration (GTA),[17] and Linear Multifrequency-Grey Acceleration (LMFGA).[18] These methods are devised to exactly capture the dominant energy spectrum of an infinite homogeneous medium problem while using only one energy group. However, these methods accelerate the pseudo-scattering iteration and thus have no effect on the Newton iteration itself.

Gol'din devised a scheme that uses Newton's Method again in an inner iteration with a loworder Quasi-Diffusion (QD) operator to approximate the transport operator.[51, 52] The low-order solution is then used to update the high-order using a nonlinear closure, and the outer Newton iteration is resumed. While effective, these methods introduce an additional nonlinearity to the low-order operator that is poorly behaved when the solution is near zero.

Paul Nowak has devised a linear modification to the Newton iteration that also introduces an inner Newton iteration, but uses a local (infinite medium) low-order operator for each degree of freedom. Brunner et al. have described this method as a local inversion of the material energy
operator.[21] They also state that the local solve is sufficient in the thick limit, where the material energy coupling (high absorption/re-emission fraction) dominates the equations.

The method we propose is an amalgamation of these methods. We make a linear modification to the outer Newton iteration and introduce an inner Newton-like iteration with a global low-order operator, which is a grey low-order operator similar to GTA and LMFGA. In future sections we show the similarity of this method to the QD method described above, where our method obtains a different Eddington tensor that changes at each iteration.

In the coming sections we discuss discretizations that are unique to this chapter's derivation. Then we discuss the application of Newton's Method to this nonlinear system and how it is equivalent to a Taylor series linearization of the Planckian emission term. We then derive a grey low-order operator from a $P 1$ approximation to the GTA equations. Finally, we discuss the method we have devised that uses an inner Newton iteration with a low-order operator to obtain a linear correction to the high-order solution, and compare this method to QD for thermal radiative transfer. In our results, we demonstrate an analytic Fourier analysis and numerical results of Marshak wave and crooked pipe (tophat) problems.

### 5.2 Thermal Radiative Transfer Discretizations and Nonlinear Iteration Scheme

### 5.2.1 Multigroup Discretization of Thermal Radiative Transfer Equations

The spatial discretization is covered in Chapter chapter 3, but will not be expressed here as this chapter focuses on the iterative method used to solve the nonlinear coupled system. However, we do include the angle and energy discretizations, as these discretizations influence and simplify the upcoming iterative method derivation.

Several terms arise in these equations that are different enough from previous discretizations to warrant a detailed description. The multigroup Planckian emission term can be evaluated as a direct integral:

$$
\begin{equation*}
\int_{E_{g}}^{E_{g-1}} d E \sigma(\vec{r}, E, t, T(\vec{r}, t)) B(T(\vec{r}, t), E)=[\sigma B]_{g}(\vec{r}, t, T(\vec{r}, t)) . \tag{5.6}
\end{equation*}
$$

However, we define an opacity that is a weighted integral of $B(T(\vec{r}, t), E)$, which also allows us to separate the opacity and Planckian emission spectrum into separate group integrated quantities:

$$
\begin{gather*}
\sigma_{g}(\vec{r}, t, T(\vec{r}, t))=\frac{\int_{E_{g}}^{E_{g-1}} d E \sigma(\vec{r}, E, t, T(\vec{r}, t)) B(T(\vec{r}, t), E)}{\int_{E_{g}}^{E_{g-1}} d E B(T(\vec{r}, t), E)},  \tag{5.7}\\
B_{g}(T(\vec{r}, t))=\int_{E_{g}}^{E_{g-1}} d E B(T(\vec{r}, t), E) . \tag{5.8}
\end{gather*}
$$

The multigroup Planckian emission term is then expressed as:

$$
\begin{equation*}
\int_{E_{g}}^{E_{g-1}} d E \sigma(\vec{r}, E, t, T(\vec{r}, t)) B(T(\vec{r}, t), E)=\sigma_{g}(\vec{r}, t, T(\vec{r}, t)) B_{g}(\vec{r}, T(\vec{r}, t)) . \tag{5.9}
\end{equation*}
$$

It is a common practice to weight the opacity multiplying the radiation intensity with a Planckian spectrum as well, since the true radiation intensity spectrum is unknown. Thus, we make the approximation that the radiation intensity spectrum opacitiy is equal to the Planckian spectrum opacity:

$$
\begin{equation*}
\sigma_{\psi, g}(\vec{r}, t, T(\vec{r}, t))=\frac{\int_{E_{g}}^{E_{g-1}} d E \sigma(\vec{r}, E, t, T(\vec{r}, t)) \psi(\vec{r}, \vec{\Omega}, E, t)}{\int_{E_{g}}^{E_{g-1}} d E \psi(\vec{r}, \vec{\Omega}, E, t)} \approx \sigma_{g}(\vec{r}, t, T(\vec{r}, t)) \tag{5.10}
\end{equation*}
$$

Using these definitions, the multigroup discrete ordinates equations for radiation intensity and material energy are:

$$
\begin{align*}
\frac{1}{c} \frac{\partial}{\partial t} \psi_{m, g}(\vec{r}, t) & +\vec{\Omega} \cdot \vec{\nabla} \psi_{m, g}(\vec{r}, t)+\sigma_{g}(\vec{r}, t, T(\vec{r}, t)) \psi_{m, g}(\vec{r}, t)  \tag{5.11}\\
& =\frac{1}{4 \pi} \sigma_{g}(\vec{r}, t, T(\vec{r}, t)) B_{g}(\vec{r}, T(\vec{r}, t)),
\end{align*}
$$

$$
\begin{gather*}
C_{v}(\vec{r}, t) \frac{\partial}{\partial t} T(\vec{r}, t)=\rho(\vec{r}, t)-\sum_{g=1}^{G} \sigma_{g}(\vec{r}, t, T(\vec{r}, t)) B_{g}(\vec{r}, T(\vec{r}, t)),  \tag{5.12}\\
\rho(\vec{r}, t)=\sum_{g=1}^{G} \sigma_{g}(\vec{r}, t, T(\vec{r}, t)) \sum_{m=1}^{M} w_{m} \psi_{m, g}(\vec{r}, t) . \tag{5.13}
\end{gather*}
$$

### 5.2.2 Time Discretization of Thermal Radiative Transfer Equations

We now introduce a discretization in the time domain by evaluating the time-average of the equations over a discrete time-step. We denote quantities at the time-step boundaries with half integer indices, and time-averaged quantities at integer indices. In general the size of each timestep can change, and we define the time-step size for each discrete interval:

$$
\begin{equation*}
\Delta t^{(n)}=t^{(n+1 / 2)}-t^{(n-1 / 2)} . \tag{5.14}
\end{equation*}
$$

The time-averaged integrals that appear in the transport equation are:

$$
\begin{gather*}
\frac{1}{\Delta t^{(n)}} \int_{t^{(n-1 / 2)}}^{t^{(n+1 / 2)}} d t \frac{\partial}{\partial t} \psi_{m, g}(\vec{r}, t)=\frac{1}{\Delta t^{(n)}} \psi_{m, g}^{n+1 / 2}(\vec{r})-\frac{1}{\Delta t^{(n)}} \psi_{m, g}^{n-1 / 2}(\vec{r}),  \tag{5.15}\\
\psi_{m, g}^{(n)}(\vec{r}) \equiv \frac{1}{\Delta t^{(n)}} \int_{t^{(n-1 / 2)}}^{t^{(n+1 / 2)}} d t \psi_{m, g}(\vec{r}, t) \tag{5.16}
\end{gather*}
$$

Because the time distribution of $\psi_{m, g}(\vec{r}, t)$ and $T(\vec{r}, t)$ are not known, in practice $\sigma_{g}^{n}(\vec{r}, T(\vec{r}))$ is approximated by evaluating the opacity at the time-averaged temperature for that step.

$$
\begin{equation*}
\sigma_{g}^{(n)}(\vec{r}) \equiv \frac{\frac{1}{\Delta t^{(n)}} \int_{t^{(n-1 / 2)}}^{t^{(n+1 / 2)}} d t \sigma_{g}(\vec{r}, t, T(\vec{r}, t)) \psi_{m, g}(\vec{r}, t)}{\frac{1}{\Delta t^{(n)}} \int_{t^{(n-1 / 2)}}^{t^{(n+1 / 2)}} d t \psi_{m, g}(\vec{r}, t)} \approx \sigma_{g}\left(\vec{r}, T^{(n)}(\vec{r})\right) \tag{5.17}
\end{equation*}
$$

Similarly, the time-averaged Planckian emission spectrum is approximated at the time-averaged temperature:

$$
\begin{equation*}
B_{g}^{(n)}(\vec{r}) \approx B_{g}\left(\vec{r}, T^{(n)}(\vec{r})\right), \tag{5.18}
\end{equation*}
$$

$$
\begin{equation*}
\left[\sigma_{g} B_{g}\right]^{(n)}(\vec{r}, T(\vec{r})) \equiv \frac{1}{\Delta t^{(n)}} \int_{t^{(n-1 / 2)}}^{t^{(n+1 / 2)}} d t \sigma_{g}(\vec{r}, t, T(\vec{r}, t)) B_{g}(\vec{r}, T(\vec{r}, t)) \approx \sigma_{g}^{(n)}(\vec{r}) B_{g}^{(n)}(\vec{r}) . \tag{5.19}
\end{equation*}
$$

The time-averaged integrals in the material energy equation that have not already been defined are:

$$
\begin{align*}
\frac{1}{\Delta t^{(n)}} \int_{t^{(n-1 / 2)}}^{t^{(n+1 / 2)}} d t \frac{\partial}{\partial t} T(\vec{r}, t) & =\frac{1}{\Delta t^{(n)}} T^{(n+1 / 2)}(\vec{r})-\frac{1}{\Delta t^{(n)}} T^{(n-1 / 2)}(\vec{r})  \tag{5.20}\\
\rho^{(n)}(\vec{r}) & \equiv \frac{1}{\Delta t^{(n)}} \int_{t^{(n-1 / 2)}}^{t^{(n+1 / 2)}} d t \rho(\vec{r}, t) \tag{5.21}
\end{align*}
$$

We choose weighted diamond differencing to close the equations between the time average and time boundary terms. The weighted diamond closure defines time averaged terms as a weighted average of the terms at the time-step boundaries, e.g. for a generic time averaged term, $x^{(n)}$, the weighted average with weight $\theta$ is:

$$
\begin{equation*}
x^{(n)}=\theta x^{(n+1 / 2)}+(1-\theta) x^{(n-1 / 2)} . \tag{5.22}
\end{equation*}
$$

We use this closure to solve for the next time-step, and substitute the next time-step values where applicable:

$$
\begin{equation*}
x^{(n+1 / 2)}=\frac{1}{\theta} x^{(n)}-\frac{1}{\theta} x^{(n-1 / 2)}+x^{(n-1 / 2)} . \tag{5.23}
\end{equation*}
$$

By varying the weight value, we implement different time discretizations using the same equation. Some notable time integration methods are Backward Euler when $\theta$ is 1, and Crank-Nicholson
when $\theta$ is $1 / 2$. Other higher order time integration methods can be made from combinations of choices of $\theta$ and additional subdivisions of the time-step. We define a term, $\tau^{(n)}$, that frequently appears in the TRT equations:

$$
\begin{equation*}
\tau^{(n)}=\frac{1}{c \Delta t^{(n)} \theta} \tag{5.24}
\end{equation*}
$$

Using these definitions, the discrete time-integrated, multigroup, discrete ordinates equations for radiation intensity and material energy are:

$$
\begin{gather*}
\tau^{(n)}\left(\psi_{m, g}^{(n)}(\vec{r})-\psi_{m, g}^{(n-1 / 2)}(\vec{r})\right) \\
+\vec{\Omega} \cdot \vec{\nabla} \psi_{m, g}^{(n)}(\vec{r})+\sigma_{g}^{(n)}(\vec{r}) \psi_{m, g}^{(n)}(\vec{r})  \tag{5.25}\\
=\frac{1}{4 \pi} \sigma_{g}^{(n)}(\vec{r}) B_{g}^{(n)}(\vec{r}), \\
\rho^{(n)}(\vec{r})=\sum_{g=1}^{G} \sigma_{g}^{(n)}(\vec{r}) \sum_{m=1}^{M} w_{m} \psi_{m, g}^{(n)}(\vec{r}),  \tag{5.26}\\
\frac{C_{v}^{(n)}}{\Delta t^{(n)} \theta}\left(T^{(n)}(\vec{r})-T^{(n-1 / 2)}(\vec{r})\right)=\rho^{(n)}(\vec{r})-\sum_{g=1}^{G} \sigma_{g}^{(n)}(\vec{r}) B_{g}^{(n)}(\vec{r}) . \tag{5.27}
\end{gather*}
$$

### 5.2.3 Linearized Planckian Iteration Equations

In the system of equations above, all unknowns are at the time averaged index, $n$. However, it is not feasible to solve the nonlinear system directly when the Planckian is evaluated implicitly. Similarly, evaluating the Planckian explicitly results in an iterative method where the stability condition is dominated by the speed of radiation, and is prohibitively expensive to take such small time-steps. Thus we introduce an iteration with index $p$ to resolve the nonlinearities of the coupled radiation intensity and material energy.

For simplicity, we ignore the nonlinearity introduced by the temperature dependence of $\sigma_{g}^{n}(\vec{r}, T(\vec{r}))$. Though it is possible to devise methods that include this nonlinear dependence, in practice the opacities are evaluated at index $p$ and if desired they are updated when a new
temperature is obtained. In the equations that follow, we no longer explicitly state the spatial dependence of terms and define an operator for the radiation intensity transfer equation to lower the length of the equations:

$$
\begin{equation*}
L_{m, g}^{(n)}=\vec{\Omega}_{m} \cdot \vec{\nabla}+\sigma_{g}^{(p)}+\tau^{(n)} . \tag{5.28}
\end{equation*}
$$

The coupled system of nonlinear equations for an iterative method at index $p+1$ are:

$$
\begin{gather*}
L_{m, g}^{(n)} \psi_{m, g}^{(p+1)}=\frac{1}{4 \pi} \sigma_{g}^{(p)} B_{g}^{(p+1)}+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)},  \tag{5.29}\\
\rho^{(p+1)}=\sum_{g=1}^{G} \sigma_{g}^{(p)} \sum_{m=1}^{M} w_{m} \psi_{m, g}^{(p+1)},  \tag{5.30}\\
\frac{C_{v}}{\Delta t^{(n)} \theta}\left(T^{(p+1)}-T^{(n-1 / 2)}\right)=\rho^{(p+1)}-\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(p+1)} . \tag{5.31}
\end{gather*}
$$

We make a linear semi-implicit (this is semi-implicit because we have ignored some temperature dependence) approximation by using the linear terms of a Taylor series expansion of the Planckian about an intermediate temperature, $T^{(p)}$ :

$$
\begin{equation*}
B_{g}^{(p+1)} \approx B_{g}\left(T^{(p)}\right)+\frac{d B_{g}}{d t}\left(T^{(p)}\right)\left(T^{(p+1)}-T^{(p)}\right)={B_{g}^{(p)}}_{+{\frac{d B_{g}}{}{ }^{(p)}}_{d t}\left(T^{(p+1)}-T^{(p)}\right) . . . . . .} \tag{5.32}
\end{equation*}
$$

We substitute the linearized Planckian into the radiation intensity and material energy equations:

$$
\begin{equation*}
L_{m, g}^{(n)} \psi_{m, g}^{(p+1)}=\frac{1}{4 \pi} \sigma_{g}^{(p)}\left(B_{g}^{(p)}+\frac{d B_{g}{ }^{(p)}}{d t}\left(T^{(p+1)}-T^{(p)}\right)\right)+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)}, \tag{5.33}
\end{equation*}
$$

$$
\begin{equation*}
\frac{C_{v}}{\Delta t^{(n)} \theta}\left(T^{(p+1)}-T^{(n-1 / 2)}\right)=\rho^{(p+1)}-\sum_{g=1}^{G} \sigma_{g}^{(p)}\left({\left.B_{g}^{(p)}+{\frac{d B_{g}}{d t}}^{(p)}\left(T^{(p+1)}-T^{(p)}\right)\right) . . ~ . ~}_{d}\right. \tag{5.34}
\end{equation*}
$$

We add and subtract $\frac{C_{v}}{\Delta t^{(n) \theta}} T^{(p)}$ on the left hand side of the material energy equation and solve for $\left(T^{(p+1)}-T^{(p)}\right)$ so that we may eliminate this term from the radiation intensity equation:

$$
\begin{equation*}
\left(T^{(p+1)}-T^{(p)}\right)=\frac{\rho^{(p+1)}-\frac{C_{v}}{\Delta t^{(n)} \theta}\left(T^{(p)}-T^{(n-1 / 2)}\right)-\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(p)}}{\left(\frac{C_{v}}{\Delta t^{(n)} \theta}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(p)}{d t}\right)} \tag{5.35}
\end{equation*}
$$

Next we substitute the expression for $T^{(p+1)}-T^{(p)}$ into the equation for radiation intensity:

$$
\begin{align*}
& L_{m, g}^{(n)} \psi_{m, g}^{(p+1)} \\
& =\frac{1}{4 \pi} \sigma_{g}^{(p)}\left(B_{g}^{(p)}+\frac{d B_{g}}{d t}{ }^{(p)}\left(\frac{\rho^{(p+1)}-\frac{C_{v}}{\Delta t^{(n)} \theta}\left(T^{(p)}-T^{(n-1 / 2)}\right)-\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(p)}}{\left(\frac{C_{v}}{\Delta t^{(n)}}+\sum_{g=1}^{G} \sigma_{g}^{(p) \frac{d B_{g}}{d t}}{ }^{(p)}\right)}\right)\right)  \tag{5.36}\\
& +\tau^{(n)} \psi_{m, g}^{(n-1 / 2)} .
\end{align*}
$$

We define several quantities, $\eta^{(p)}, \iota^{(p)}$, and $\chi^{(p)}$, to simplify the radiation intensity equation:

$$
\begin{gather*}
\eta^{(p)}=\frac{\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(p)}{d t}}{\frac{C_{v}}{\Delta t^{(n)} \theta}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(p)}{d t}},  \tag{5.37}\\
\iota^{(p)}=\frac{\frac{C_{v}}{\Delta t^{(n)} \theta}}{\frac{C_{v}}{\Delta t^{(n)} \theta}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(p)}{d t}}=1-\eta^{(p)}, \tag{5.38}
\end{gather*}
$$

$$
\begin{gather*}
\chi_{g}^{(p)}=\frac{\sigma_{g}^{(p)} \frac{d B_{g}(p)}{d t}}{\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(p)}{d t}},  \tag{5.39}\\
Q_{r a d, g}^{(p)}=\sigma_{g}^{(p)}\left(B_{g}^{(p)}+{\frac{d B_{g}}{d t}}^{(p)}\left(-\iota^{(p)}\left(T^{(p)}-T^{(n-1 / 2)}\right)-\frac{\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(p)}}{\left(\frac{C_{v}}{\Delta t^{(n)}}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}{ }^{(p)}}{d t}\right)}\right)\right) \tag{5.40}
\end{gather*}
$$

This results in the following iterative system of equations:

$$
\begin{gather*}
L_{m, g}^{(n)} \psi_{m, g}^{(p+1)}=\frac{1}{4 \pi} \eta^{(p)} \chi_{g}^{(p)} \rho^{(p+1)}+\frac{1}{4 \pi} Q_{r a d, g}^{(p)}+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)},  \tag{5.41}\\
\frac{C_{v}}{\Delta t^{(n)} \theta}\left(T^{(p+1)}-T^{(n-1 / 2)}\right)=\rho^{(p+1)}-\sum_{g=1}^{G} \sigma_{g}^{(p)}\left(B_{g}^{(p)}+{\frac{d B_{g}}{d t}}^{(p)}\left(T^{(p+1)}-T^{(p)}\right)\right) \tag{5.42}
\end{gather*}
$$

We introduce an iteration at index $k$ that is sometimes called a pseudo-scattering iteration or lambda iteration, where the effective total cross section is $\sigma_{g}^{(p)}+\tau^{(n)}$, and the effective $g^{\prime}$ - to $g$-scattering cross section is $\eta^{(p)} \chi_{g}^{(p)} \sigma_{g^{\prime}}^{(p)}$. The pseudo-scattering iteration determines the ARD at $k+1$ from the previous ARD at $k$ :

$$
\begin{gather*}
L_{m, g}^{(n)} \psi_{m, g}^{(k+1)}=\frac{1}{4 \pi} \eta^{(p)} \chi_{g}^{(p)} \rho^{(k)}+\frac{1}{4 \pi} Q_{r a d, g}^{(p)}+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)}  \tag{5.43}\\
\rho^{(k+1)}=\sum_{g=1}^{G} \sigma_{g}^{(p)} \sum_{m=1}^{M} w_{m} \psi_{m, g}^{(k+1)} \tag{5.44}
\end{gather*}
$$

Upon convergence of the pseudo-scattering iteration, the ARD at iteration $p+1$ is set:

$$
\begin{equation*}
\left|\rho^{(k+1)}-\rho^{(k)}\right| \leq \epsilon \Rightarrow \rho^{(p+1)}=\rho^{(k+1)} \tag{5.45}
\end{equation*}
$$

We now show that this system is equivalent to Newton's method for temperature if we also ignore any temperature dependence of $C_{v}$ and $\sigma^{(n)}$. We apply Newton's Method to the original system of equations. Using the previously defined transport operator, the ARD is determined as follows:

$$
\begin{equation*}
\rho^{(p)}=\sum_{m=1}^{M} w_{m} \sum_{g=1}^{G}\left[L_{m, g}^{(n)}\right]^{-1}\left[\sigma_{g}^{(p)} B_{g}^{(p)}+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)}\right] \tag{5.46}
\end{equation*}
$$

We may then write the system of equations as:

$$
\begin{equation*}
F\left(x^{(p)}\right)=0, \tag{5.47}
\end{equation*}
$$

where we define a vector of the unknown variables:

$$
x^{(p)}=\left[\begin{array}{c}
\rho^{(p)}  \tag{5.48}\\
T^{(p)}
\end{array}\right],
$$

and we define a function, $F$, that the thermal radiative transfer equations satisfy:

$$
F\left(x^{(p)}\right)=\left[\begin{array}{c}
\rho^{(p)}-\sum_{m=1}^{M} w_{m} \sum_{g=1}^{G}\left[L_{m, g}^{(n)}\right]^{-1}\left[\sigma_{g}^{(p)} B_{g}^{(p)}+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)}\right]  \tag{5.49}\\
\frac{C_{v}}{\Delta t^{(n) \theta}}\left(T^{(p)}-T^{(n-1 / 2)}\right)-\rho^{(p)}+\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(p)}
\end{array}\right] .
$$

The Jacobian of $F$, if we ignore temperature dependence of $C_{v}$ and $\sigma_{g}^{(p)}$, is:

$$
J_{F}\left(x^{(p)}\right)=\left[\begin{array}{cc}
\frac{d F_{1}}{d \rho^{(p)}} & \frac{d F_{1}}{d T^{(p)}}  \tag{5.50}\\
\frac{d F_{2}}{d \rho^{(p)}} & \frac{d F_{2}}{d T^{(p)}}
\end{array}\right]=\left[\begin{array}{cc}
1 & -\sum_{m=1}^{M} w_{m} \sum_{g=1}^{G}\left[L_{m, g}^{(n)}\right]^{-1}\left[\sigma_{g}^{(p)} \frac{d B_{g}}{d T}{ }^{(p)}\right] \\
-1 & \frac{C_{v}}{\Delta t^{(n) \theta}}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(p)}{d T}
\end{array}\right] .
$$

Then we determine Newton's Method on this system:

$$
\begin{equation*}
J_{F}\left(x^{(p)}\right)\left[x^{(p+1)}-x^{(p)}\right]=-F\left(x^{(p)}\right) . \tag{5.51}
\end{equation*}
$$

After we substitute the expressions for $J_{F}\left(x^{(p)}\right), x^{(p)}$, and $F\left(x^{(p)}\right)$ :

$$
\begin{align*}
& {\left[\begin{array}{cc}
1 & -\sum_{m=1}^{M} w_{m} \sum_{g=1}^{G}\left[L_{m, g}^{(n)}\right]^{-1}\left[\sigma_{g}^{(p)} \frac{d B_{g}(p)}{d T}\right] \\
-1 & \frac{C_{v}}{\Delta t^{(n) \theta}}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(p)}{d T}
\end{array}\right]\left[\begin{array}{l}
\rho^{(p+1)}-\rho^{(p)} \\
T^{(p+1)}-T^{(p)}
\end{array}\right]}  \tag{5.52}\\
& =-\left[\begin{array}{c}
\rho^{(p)}-\sum_{m=1}^{M} w_{m} \sum_{g=1}^{G}\left[L_{m, g}^{(n)}\right]^{-1}\left[\sigma_{g}^{(p)} B_{g}^{(p)}+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)}\right] \\
\frac{C_{v}}{\Delta t^{(n)} \theta}\left(T^{(p)}-T^{(n-1 / 2)}\right)-\rho^{(p)}+\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(p)}
\end{array}\right],
\end{align*}
$$

we expand the left hand side:

$$
\begin{align*}
& {\left[\begin{array}{c}
\rho^{(p+1)}-\rho^{(p)}-\sum_{m=1}^{M} w_{m} \sum_{g=1}^{G}\left[L_{m, g}^{(n)}\right]^{-1}\left[\sigma_{g}^{(p)} \frac{d B_{g}(p)}{d T}\left(T^{(p+1)}-T^{(p)}\right)\right] \\
-\left(\rho^{(p+1)}-\rho^{(p)}\right)+\left(\frac{C_{v}}{\Delta t^{(n)}}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(p)}{d T}\right)\left(T^{(p+1)}-T^{(p)}\right)
\end{array}\right]} \\
& =-\left[\begin{array}{c}
\rho^{(p)}-\sum_{m=1}^{M} w_{m} \sum_{g=1}^{G}\left[L_{m, g}^{(n)}\right]^{-1}\left[\sigma_{g}^{(p)} B_{g}^{(p)}+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)}\right] \\
\frac{C_{v}}{\Delta t^{(n)} \theta}\left(T^{(p)}-T^{(n-1 / 2)}\right)-\rho^{(p)}+\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(p)}
\end{array}\right],
\end{align*}
$$

and we simplify the equations:

$$
\begin{gather*}
\rho^{(p+1)}=\sum_{m=1}^{M} w_{m} \sum_{g=1}^{G}\left[L_{m, g}^{(n)}\right]^{-1}\left[\sigma_{g}^{(p)}\left(B_{g}^{(p)}+\frac{d B_{g}^{(p)}}{d T}\left(T^{(p+1)}-T^{(p)}\right)\right)+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)}\right],  \tag{5.54}\\
\frac{C_{v}}{\Delta t^{(n)} \theta}\left(T^{(p+1)}-T^{(n-1 / 2)}\right)=\rho^{(p+1)}-\sum_{g=1}^{G} \sigma_{g}^{(p)}\left(B_{g}^{(p)}+{\frac{d B_{g}}{d T}}^{(p)}\left(T^{(p+1)}-T^{(p)}\right)\right) . \tag{5.55}
\end{gather*}
$$

From here it is apparent that these are the same equations in Eqs. (5.33) and (5.34) that were obtained by approximating the Planckian emission spectrum as a linear Taylor series.

We summarize the iterative method to determine the unknown variables at the end of the current time-step, $(n+1 / 2)$, which is a pseudo-scattering iteration to determine ARD, and a Newton-like
iteration to couple ARD and temperature in algorithm 2:

```
Algorithm 2 Newton's Method for Thermal Radiative Transfer
    \(p \leftarrow 0\)
    \(T^{(p)} \leftarrow T^{(n-1 / 2)}, \rho^{(p)} \leftarrow \rho^{(n-1 / 2)}\)
    repeat
        Compute \(B_{g}^{(p)}, \frac{d B_{g}{ }^{(p)}}{d T}, \eta^{(p)}, \chi_{g}^{(p)}, Q_{g, \text { rad }}^{(p)}\)
        \(k \leftarrow 0\)
        \(\rho^{(k)} \leftarrow \rho^{(p)}\)
        repeat
            Sweep \(L_{m, g}^{(n)} \psi_{m, g}^{(k+1)}=\frac{\eta^{(p)} \chi_{g}^{(p)} \rho^{(k)}+Q_{g, r a d}^{(p)}}{4 \pi}+q_{m, g}+\tau \psi_{m, g}^{n-1 / 2}\)
            \(\rho^{(k+1)} \leftarrow \sum_{g=1}^{G} \sigma_{g}^{(p)} \sum_{m=1}^{M} w_{m} \psi_{m, g}^{(k+1)}\)
            until \(\left|\rho^{(k+1)}-\rho^{(k)}\right| \leq \epsilon_{\rho}\), else \(k \leftarrow k+1\)
            \(\rho^{(p+1)} \leftarrow \rho^{(k+1)}\)
            \(T^{(p+1)} \leftarrow T^{(p)}+\frac{-\frac{C_{v}}{\Delta t^{(n)}}\left(T^{(p)}-T^{(n-1 / 2)}\right)+\rho^{(p+1)}-\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(p)}+Q_{e x t}}{\frac{C_{v}}{\Delta t^{(n)}}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(p)}{d T}}\)
    until \(\left|T^{(p+1)}-T^{(p)}\right| \leq \epsilon_{T},\left|\rho^{(p+1)}-\rho^{(p)}\right| \leq \epsilon_{\rho}\), else \(p \leftarrow p+1\)
    \(T^{(n)} \leftarrow T^{(p+1)} \Rightarrow T^{(n+1 / 2)} \leftarrow \frac{1}{\theta} T^{(n)}-\left(\frac{1}{\theta}-1\right) T^{(n-1 / 2)}\)
    \(\rho^{(n)} \leftarrow \rho^{(p+1)} \Rightarrow \rho^{(n+1 / 2)} \leftarrow \frac{1}{\theta} \rho^{(n)}-\left(\frac{1}{\theta}-1\right) \rho^{(n-1 / 2)}\)
```


### 5.3 Gray Diffusion Synthetic Acceleration

We apply techniques to devise a DSA scheme for the pseudo-scattering iteration. Larsen[17] and Morel[18] each identified the slowest converging modes of the high-order system and developed energy collapse scheme to exactly eliminate these modes with a low-order additive correction. We follow the logic of Larsen and determine an equation for the transport error.

The converged pseudo-scattering iteration obtains radiation intensity and ARD that satisfy the following transport equation:

$$
\begin{equation*}
L_{m, g}^{(n)} \psi_{m, g}=\frac{1}{4 \pi}\left[\chi_{g}^{(p)} \eta^{(p)} \rho+Q_{g, r a d}^{(p)}\right]+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)} . \tag{5.56}
\end{equation*}
$$

We introduce an equation for a half-step radiation intensity:

$$
\begin{equation*}
L_{m, g}^{(n)} \psi_{m, g}^{(k+1 / 2)}=\frac{1}{4 \pi}\left[\chi_{g}^{(p)} \eta^{(p)} \rho^{(k)}+Q_{g, r a d}^{(p)}\right]+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)}, \tag{5.57}
\end{equation*}
$$

and define errors for angular radiation intensity and ARD, and the Fourier decomposition of these terms:

$$
\begin{gather*}
\delta \rho^{(k)}=\rho-\rho^{(k)}=\iiint_{0}^{\infty} d^{3} \lambda \omega^{k} e^{\mathbf{i} \vec{\lambda} \cdot \vec{r}},  \tag{5.58}\\
\delta \psi_{m, g}^{(k+1 / 2)}=\psi_{m, g}-\psi_{m, g}^{(k+1 / 2)}=\iiint_{0}^{\infty} d^{3} \lambda \delta \psi_{m, g, \dagger}(\vec{\lambda}) \omega^{k} e^{\mathbf{i} \vec{\lambda} \cdot \vec{r}} . \tag{5.59}
\end{gather*}
$$

After we subtract the half-step radiation intensity equation from the converged radiation intensity equation we obtain an equation for the error:

$$
\begin{equation*}
L_{m, g}^{(n)} \delta \psi_{m, g}^{(k+1 / 2)}=\frac{1}{4 \pi} \chi_{g}^{(p)} \eta^{(p)} \delta \rho^{(k)} . \tag{5.60}
\end{equation*}
$$

The linear independence of each mode of the Fourier expanded error implies a separate equation for each $\vec{\lambda}$. That is, each mode evolves independently. After substituting the Fourier integrals, the high-order equation implies:

$$
\begin{equation*}
\delta \psi_{m, g, \dagger}(\vec{\lambda})=\frac{1}{4 \pi} \frac{\chi_{g}^{(p)} \eta^{(p)}}{\mathbf{i} \vec{\lambda} \cdot \vec{\Omega}+\sigma_{g}^{(p)}+\tau^{(n)}} \delta \rho^{(k)} . \tag{5.61}
\end{equation*}
$$

Larsen recognized the slowest converging modes were for $|\vec{\lambda}|=0$. He found shape function of the two largest leading order terms of this expression by expanding this function as a Taylor series about $|\vec{\lambda}| \approx 0$ :

$$
\begin{equation*}
\delta \psi_{m, g, \dagger}(|\vec{\lambda}| \approx 0)=\frac{1}{4 \pi} \eta^{(p)} \frac{\chi_{g}^{(p)}}{\sigma_{g}^{(p)}+\tau^{(n)}}-\frac{1}{4 \pi} \eta^{(p)} \mathbf{i} \vec{\lambda} \cdot \vec{\Omega}_{m} \frac{\chi_{g}^{(p)}}{\left(\sigma_{g}^{(p)}+\tau^{(n)}\right)^{2}}+\mathcal{O}\left(|\vec{\lambda}|^{2}\right) . \tag{5.62}
\end{equation*}
$$

The shape function of the two most slowly converging Fourier modes are, as determined by Larsen:

$$
\begin{gather*}
y_{g, 0}^{(p)}=\frac{\chi_{g}^{(p)}}{\sigma_{g}^{(p)}+\tau^{(n)}},  \tag{5.63}\\
y_{g, 1}^{(p)}=\frac{\chi_{g}^{(p)}}{\left(\sigma_{g}^{(p)}+\tau^{(n)}\right)^{2}} . \tag{5.64}
\end{gather*}
$$

Larsen then defines a gray equation by integrating the half-step radiation intensity iteration equation over energy, expressed here as a summation over energy groups:

$$
\begin{equation*}
\sum_{g=1}^{G}\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+\sigma_{g}^{(p)}+\tau^{(n)}\right) \psi_{m, g}^{(k+1 / 2)}=\sum_{g=1}^{G} \frac{1}{4 \pi}\left[\chi_{g}^{(p)} \eta^{(p)} \rho^{(k)}+Q_{g, r a d}^{(p)}\right]+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)}, \tag{5.65}
\end{equation*}
$$

and defines group integrated quantities:

$$
\begin{gather*}
\langle\psi\rangle_{m}^{(k+1 / 2)}=\sum_{g=1}^{G} \psi_{m, g}^{(k+1 / 2)},  \tag{5.66}\\
\langle Q\rangle_{m}^{(p)}=\sum_{g=1}^{G}\left[\frac{1}{4 \pi} Q_{g, r a d}^{(p)}+\tau^{(n)} \psi_{m, g}^{(n-1 / 2)}\right] . \tag{5.67}
\end{gather*}
$$

Larsen then rearranges the equation and adds terms to both sides containing gray opacities that will soon be determined:

$$
\begin{align*}
\vec{\Omega}_{m} \cdot \vec{\nabla}\langle\psi\rangle_{m}^{(k+1 / 2)} & +\langle\sigma\rangle_{T}^{(p)}\langle\psi\rangle_{m}^{(k+1 / 2)}-\frac{1}{4 \pi}\langle\sigma\rangle_{S}^{(p)} \sum_{m} w_{m}\langle\psi\rangle_{m}^{(k+1 / 2)} \\
& =\frac{1}{4 \pi} \sum_{g=1}^{G}\left[\langle\sigma\rangle_{T}^{(p)}-\sigma_{g}^{(n)}-\tau^{(n)}\right] \psi_{m, g}^{(k)}  \tag{5.68}\\
& +\frac{1}{4 \pi} \sum_{g=1}^{G} \sum_{m} w_{m}\left[\eta^{(p)} \sigma_{g}^{(n)}-\langle\sigma\rangle_{S}^{(p)}\right] \psi_{m, g}^{(k)} \\
& +\langle Q\rangle_{m}^{(p)}
\end{align*}
$$

Similarly, he adds and subtracts a term in the ARD update equation:

$$
\begin{equation*}
\rho^{(k+1 / 2)}=\frac{1}{4 \pi}\langle\sigma\rangle^{(p)} \sum_{m} w_{m}\langle\psi\rangle_{m}^{(k+1 / 2)}+\frac{1}{4 \pi} \sum_{g=1}^{G} \sum_{m} w_{m}\left[\sigma_{g}^{(n)}-\langle\sigma\rangle^{(p)}\right] \psi_{m, g}^{(k+1 / 2)} . \tag{5.69}
\end{equation*}
$$

The gray opacities are defined such that the terms in brackets in the previous two equations are exactly zero for the two slowest converging modes determined above. This results in the following system of equations:

$$
\begin{gather*}
0=\sum_{g=1}^{G}\left(\left[\langle\sigma\rangle_{T}^{(p)}-\sigma_{g}^{(n)}-\tau^{(n)}\right]+\left[\eta^{(p)} \sigma_{g}^{(n)}-\langle\sigma\rangle_{S}^{(p)}\right]\right) y_{g, 0}^{(p)}  \tag{5.70}\\
0=\sum_{g=1}^{G}\left(\left[\langle\sigma\rangle_{T}^{(p)}-\sigma_{g}^{(n)}-\tau^{(n)}\right]\right) \vec{y}_{g, 1}^{(p)}  \tag{5.71}\\
0=\sum_{g=1}^{G}\left(\left[\sigma_{g}^{(n)}-\langle\sigma\rangle^{(p)}\right]\right) \vec{y}_{g, 0}^{(p)} \tag{5.72}
\end{gather*}
$$

that have the following solutions:

$$
\begin{equation*}
\langle\sigma\rangle^{(p)}=\frac{\sum_{g=1}^{G} \frac{\sigma_{g}^{(n)} \chi_{g}^{(p)}}{\sigma_{g}^{(n)}+\tau^{(n)}}}{\sum_{g=1}^{G} \frac{\chi_{g}^{(p)}}{\sigma_{g}^{(n)}+\tau^{(n)}}} \tag{5.73}
\end{equation*}
$$

$$
\begin{gather*}
\langle\sigma\rangle_{T}^{(p)}=\frac{\sum_{g=1}^{G} \frac{\chi_{g}^{(p)}}{\sigma_{g}^{(n)}+\tau^{(n)}}}{\sum_{g=1}^{G} \frac{\chi_{g}^{(p)}}{\left(\sigma_{g}^{(n)}+\tau^{(n)}\right)^{2}}}  \tag{5.74}\\
\langle\sigma\rangle_{S}^{(p)}=\langle\sigma\rangle_{T}^{(p)}-\iota^{(p)}\langle\sigma\rangle^{(p)}-\tau \tag{5.75}
\end{gather*}
$$

The final step Larsen takes is to define an equation for a gray additive correction:

$$
\begin{equation*}
\vec{\Omega}_{m} \cdot \vec{\nabla} \delta\langle\psi\rangle_{m}^{(k+1)}+\langle\sigma\rangle_{T}^{(p)} \delta\langle\psi\rangle_{m}^{(k+1)}-\frac{1}{4 \pi}\langle\sigma\rangle_{S}^{(p)} \sum_{m} w_{m} \delta\langle\psi\rangle_{m}^{(k+1)}=\frac{1}{4 \pi} \eta^{(p)}\left(\rho^{(k+1 / 2)}-\rho^{(k)}\right), \tag{5.76}
\end{equation*}
$$

where,

$$
\begin{equation*}
\delta\langle\psi\rangle_{m}^{(k+1)}=\langle\psi\rangle_{m}^{(k+1)}-\langle\psi\rangle_{m}^{(k+1 / 2)} . \tag{5.77}
\end{equation*}
$$

We make the additional step of replacing the high-order angle operator by making a $P_{1}$ approximation to the correction:

$$
\begin{equation*}
\delta\langle\psi\rangle_{m}^{(k+1)}=\frac{1}{4 \pi}\left(\delta\langle\phi\rangle^{(k+1)}+3 \vec{\Omega} \cdot \delta\langle\vec{J}\rangle^{(k+1)}\right) \tag{5.78}
\end{equation*}
$$

The resulting system of equations, after evaluating the $0^{t h}$ and $1^{\text {st }}$ angular moments of the correction equation:

$$
\begin{align*}
\vec{\nabla} \cdot \delta\langle\vec{J}\rangle^{(k+1)}+ & \left(\langle\sigma\rangle_{T}^{(p)}-\langle\sigma\rangle_{S}^{(p)}\right) \delta\langle\phi\rangle^{(k+1)}=\eta^{(p)}\left(\rho^{(k+1 / 2)}-\rho^{(k)}\right),  \tag{5.79}\\
& \vec{\nabla} \delta\langle\phi\rangle^{(k+1)}+\langle\sigma\rangle_{T}^{(p)} \delta\langle\vec{J}\rangle_{m}^{(k+1)}=0, \tag{5.80}
\end{align*}
$$

with update equation:

$$
\begin{equation*}
\rho^{(k+1)}=\rho^{(k+1 / 2)}+\langle\sigma\rangle^{(p)} \tag{5.81}
\end{equation*}
$$

We summarize the Newton's method iteration scheme that includes gray DSA (GDSA) in algorithm 3.

```
Algorithm 3 Newton's Method with Gray DSA for Thermal Radiative Transfer
    \(p \leftarrow 0\)
    \(T^{(p)} \leftarrow T^{(n-1 / 2)}, \rho^{(p)} \leftarrow \rho^{(n-1 / 2)}\)
    repeat
        Compute \(B_{g}^{(p)}, \frac{d B_{g}{ }^{(p)}}{d T}, \eta^{(p)}, \chi_{g}^{(p)}, Q_{g, \text { rad }}^{(p)}\)
        Compute \(\langle\sigma\rangle_{T}^{(p)},\langle\sigma\rangle_{S}^{(p)},\langle\sigma\rangle^{(p)}\)
        \(k \leftarrow 0\)
        \(\rho^{(k)} \leftarrow \rho^{(p)}\)
        repeat
            Sweep \(L_{m, g}^{(n)} \psi_{m, g}^{(k+1)}=\frac{\eta^{(p)} \chi_{g}^{(p)} \rho^{(k)}+Q_{g, r a d}^{(p)}}{4 \pi}+q_{m, g}+\tau \psi_{m, g}^{n-1 / 2}\)
            \(\rho^{(k+1 / 2)} \leftarrow \sum_{g=1}^{G} \sigma_{g}^{(p)} \sum_{m=1}^{M} w_{m} \psi_{m, g}^{(k+1 / 2)}\)
```

            Solve Gray LO System:
    11:

$$
\begin{gathered}
\vec{\nabla} \cdot \delta\langle\vec{J}\rangle^{(k+1)}+\left(\langle\sigma\rangle_{T}^{(p)}-\langle\sigma\rangle_{S}^{(p)}\right) \delta\langle\phi\rangle^{(k+1)}=\eta^{(p)}\left(\rho^{(k+1 / 2)}-\rho^{(k)}\right) \\
\vec{\nabla} \delta\langle\phi\rangle^{(k+1)}+\langle\sigma\rangle_{T}^{(p)} \delta\langle\vec{J}\rangle_{m}^{(k+1)}=0 \\
\begin{array}{c}
\rho^{(k+1)} \leftarrow \rho^{(k+1 / 2)}+\langle\sigma\rangle \delta\langle\phi\rangle^{(k+1)} \\
\text { until }\left|\rho^{(k+1)}-\rho^{(k)}\right| \leq \epsilon_{\rho}, \text { else } k \leftarrow k+1 \\
\rho^{(p+1)} \leftarrow \rho^{(k+1)}
\end{array} \\
T^{(p+1)} \leftarrow T^{(p)}+\frac{-\frac{C_{v}}{\Delta t^{(n)}}\left(T^{(p)}-T^{(n-1 / 2)}\right)+\rho^{(p+1)}-\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(p)}+Q_{e x t}}{\frac{C_{v}}{\Delta t^{(n)}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(p)}{d T}}} \\
\text { until }\left|T^{(p+1)}-T^{(p)}\right| \leq \epsilon_{T},\left|\rho^{(p+1)}-\rho^{(p)}\right| \leq \epsilon_{\rho}, \mathbf{e l s e} p \leftarrow p+1 \\
T^{(n)} \leftarrow T^{(p+1)} \Rightarrow T^{(n+1 / 2)} \leftarrow \frac{1}{\theta} T^{(n)}-\left(\frac{1}{\theta}-1\right) T^{(n-1 / 2)} \\
\rho^{(n)} \leftarrow \rho^{(p+1)} \Rightarrow \rho^{(n+1 / 2)} \leftarrow \frac{1}{\theta} \rho^{(n)}-\left(\frac{1}{\theta}-1\right) \rho^{(n-1 / 2)}
\end{gathered}
$$

Accelerating the pseudo-scattering iteration can greatly reduce the number of transport sweeps. However, if the pseudo-scattering iteration is converged at each step, the next temperature iterate is
the same whether the iteration was accelerated or not. Thus, this form of acceleration has no affect on how many temperature iterations are necessary to converge the Newton iteration, and future pseudo-scattering iterations may be just as difficult to solve once the temperature is updated and new properties and sources are calculated.

In the next section we devise a Linear HOLO method that instead solves a low-order problem for a new ARD and temperature, similar to nonlinear HOLO methods.

### 5.4 Linear HOLO Derivation

We follow a process that many researchers have employed for scattering iterations: 1) define "converged" equations; 2) subtract the equations satisfied by the latest solution, obtaining an exact equation for an additive correction; 3) replace the transport operator in this equation by a low-order operator.

We begin with equations for radiation intensity and material energy that satisfy the converged Newton iteration:

$$
\begin{gather*}
\vec{\Omega}_{m} \cdot \vec{\nabla} \psi_{m, g}^{(n)}+\left(\sigma_{g}^{(p)}+\tau^{(n)}\right) \psi_{m, g}^{(n)}=\frac{1}{4 \pi}\left[\chi_{g}^{(n)} \eta^{(n)} \rho^{(n)}+Q_{g, r a d}^{(n)}\right]+Q_{m, g}^{(n-1 / 2)}  \tag{5.82}\\
\frac{C_{v}}{\Delta t^{(n)} \theta}\left(T^{(n)}-T^{(n-1 / 2)}\right)=\rho^{(n)}-\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(n)}+Q_{e x t} \tag{5.83}
\end{gather*}
$$

where we recall:

$$
\begin{align*}
& \rho^{(n)}=\sum_{g=1}^{G} \sigma_{g}^{(p)} \sum_{m} w_{m} \psi_{m, g}^{(n)}  \tag{5.84}\\
& Q_{m, g}^{(n-1 / 2)}=\tau \psi_{m, g}^{(n-1 / 2)}+q_{m, g} \tag{5.85}
\end{align*}
$$

$$
\begin{equation*}
\left.Q_{r a d, g}^{(n)}=\sigma_{g}^{(p)}\left(B_{g}^{(n)}+{\frac{d B_{g}}{d t}}^{(n)}\left(-\iota^{(n)}\left(T^{(n)}-T^{(n-1 / 2)}\right)-\frac{\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(n)}}{\left(\frac{C_{v}}{\Delta t^{(n)}}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}}{d t}\right.}\right)\right)\right) \tag{5.86}
\end{equation*}
$$

We reiterate the iteration transport equation for the latest pseudo-scattering iteration at index $k+1 / 2$; we note that if the pseudo-scattering iteration is converged, then quantities at $(p+1 / 2)$, $(k+1 / 2)$, and $(k)$ are equivalent:

$$
\begin{equation*}
\vec{\Omega}_{m} \cdot \vec{\nabla} \psi_{m, g}^{(k+1 / 2)}+\left(\sigma_{g}^{(p)}+\tau^{(n)}\right) \psi_{m, g}^{(k+1 / 2)}=\frac{1}{4 \pi}\left[\chi_{g}^{(p)} \eta^{(p)} \rho^{(k)}+Q_{g, r a d}^{(p)}\right]+Q_{m, g}^{(n-1 / 2)} \tag{5.87}
\end{equation*}
$$

In the second step, we subtract the iteration transport equation from the converged Newton iteration equation:

$$
\begin{align*}
& \vec{\Omega}_{m} \cdot \vec{\nabla}\left(\psi_{m, g}^{(n)}-\psi_{m, g}^{(k+1 / 2)}\right)+\left(\sigma_{g}^{(p)}+\tau^{(n)}\right)\left(\psi_{m, g}^{(n)}-\psi_{m, g}^{(k+1 / 2)}\right) \\
& =\frac{1}{4 \pi}\left[\chi_{g}^{(n)} \eta^{(n)} \rho^{(n)}-\chi_{g}^{(n)} \eta^{(n)} \rho^{(k+1 / 2)}\right]  \tag{5.88}\\
& +\frac{1}{4 \pi}\left[\chi_{g}^{(n)} \eta^{(n)} \rho^{(k+1 / 2)}-\chi_{g}^{(p)} \eta^{(p)} \rho^{(k)}+Q_{g, r a d}^{(n)}-Q_{g, r a d}^{(p)}\right]
\end{align*}
$$

define additive corrections:

$$
\begin{gather*}
\delta \psi_{m, g}^{(n)}=\psi_{m, g}^{(n)}-\psi_{m, g}^{(k+1 / 2)}  \tag{5.89}\\
\delta \rho^{(n)}=\rho^{(n)}-\rho^{(k+1 / 2)} \tag{5.90}
\end{gather*}
$$

and obtain an equation for an additive correction:

$$
\begin{align*}
& \vec{\Omega}_{m} \cdot \vec{\nabla} \delta \psi_{m, g}^{(n)}+\left(\sigma_{g}^{(p)}+\tau^{(n)}\right) \delta \psi_{m, g}^{(n)}-\frac{1}{4 \pi} \chi_{g}^{(n)} \eta^{(n)} \delta \rho^{(n)} \\
& =\frac{1}{4 \pi}\left[\chi_{g}^{(n)} \eta^{(n)} \rho^{(k+1 / 2)}-\chi_{g}^{(p)} \eta^{(p)} \rho^{(k)}+Q_{g, \text { rad }}^{(n)}-Q_{g, \text { rad }}^{(p)}\right] . \tag{5.91}
\end{align*}
$$

The previous equation suggests another iterative process, denoted by index $s$ :

$$
\begin{align*}
& \vec{\Omega}_{m} \cdot \vec{\nabla} \delta \psi_{m, g}^{(s+1 / 2)}+\left(\sigma_{g}^{(p)}+\tau^{(n)}\right) \delta \psi_{m, g}^{(s+1 / 2)}-\frac{1}{4 \pi} \chi_{g}^{(s)} \eta^{(s)} \delta \rho^{(s+1 / 2)}  \tag{5.92}\\
& =\frac{1}{4 \pi}\left[\chi_{g}^{(s)} \eta^{(s)} \rho^{(k+1 / 2)}-\chi_{g}^{(p)} \eta^{(p)} \rho^{(k)}+Q_{g, \text { rad }}^{(s)}-Q_{g, r a d}^{(p)}\right]
\end{align*}
$$

with update equations:

$$
\begin{gather*}
\delta \rho^{(s+1 / 2)}=\sum_{g=1}^{G} \sigma_{g}^{(p)} \sum_{m=1}^{M} w_{m} \delta \psi_{m, g}^{(s+1 / 2)},  \tag{5.93}\\
\rho^{(s+1)}=\rho^{(k+1 / 2)}+\delta \rho^{(s+1 / 2)}, \tag{5.94}
\end{gather*}
$$

and material energy equation:

$$
\begin{equation*}
T^{(s+1)}=T^{(s)}-\iota^{(s)}\left(T^{(s)}-T^{(n-1 / 2)}\right)+\frac{\rho^{(s+1)}-\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(s)}+Q_{e x t}}{\frac{C_{v}}{\Delta t \theta}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(s)}{d T}} \tag{5.95}
\end{equation*}
$$

This system of equations is as difficult to solve as the original system; thus we make a $P_{1}$ approximation to the angular dependence of the correction:

$$
\begin{equation*}
\delta \psi_{m, g}^{(s+1 / 2)} \approx \frac{1}{4 \pi}\left(\delta \phi_{g}^{(s+1 / 2)}+3 \vec{\Omega}_{m} \cdot \delta \vec{J}_{g}^{(s+1 / 2)}\right) \tag{5.96}
\end{equation*}
$$

Then the $0^{\text {th }}$ and $1^{\text {st }}$ angular moments of the low-order iteration equation are given by:

$$
\begin{align*}
& \vec{\nabla} \cdot \delta \vec{J}_{g}^{(s+1 / 2)}+\left(\sigma_{g}^{(p)}+\tau^{(n)}\right) \delta \phi_{g}^{(s+1 / 2)}-\chi_{g}^{(s)} \eta^{(s)} \sum_{g=1}^{G} \sigma_{g}^{(p)} \delta \phi_{g}^{(s+1 / 2)}  \tag{5.97}\\
& =\left[\chi_{g}^{s} \eta^{(s)} \rho^{(k+1 / 2)}-\chi_{g}^{(p)} \eta^{(p)} \rho^{(k)}+Q_{g, r a d}^{(s)}-Q_{g, r a d}^{(p)}\right] \\
& \vec{\nabla} \frac{1}{3} \delta \phi_{g}^{(s+1 / 2)}+\left(\sigma_{g}^{(p)}+\tau^{(n)}\right) \delta \vec{J}_{g}^{(s+1 / 2)}=0 \tag{5.98}
\end{align*}
$$

The preceding system is very costly to solve, requiring a diffusion solution for each group,
and solving a scattering problem through the absorption/re-emission phenomenon. Following the steps of Larsen for Grey Transport Acceleration [17], we can obtain a gray diffusion equation, with opacities determined in the same manner. The resulting spectrum is different from that determined by Larsen, as the spectrum is dependent on the right hand side of the equation. In practice, we have found the spectrum determined by Larsen to be sufficient, as it obtains the same opacities upon convergence, and the increased complexity only provides minor corrections to the Larsen spectrum. We derive the gray opacities using the energy error spectrum of these equations in the next section, but in general this gray system can be written as:

$$
\begin{equation*}
\vec{\nabla} \cdot \delta\langle\vec{J}\rangle^{(s+1 / 2)}+\left(\langle\sigma\rangle_{T}^{(s)}-\langle\sigma\rangle_{S}^{(s)}\right) \delta\langle\phi\rangle^{(s+1 / 2)}=\eta^{(s)} \rho^{(k+1 / 2)}-\eta^{(p)} \rho^{(k)}+\langle Q\rangle_{r a d}^{(s)}-\langle Q\rangle_{r a d}^{(p)} \tag{5.99}
\end{equation*}
$$

$$
\begin{equation*}
\vec{\nabla} \frac{1}{3} \delta\langle\phi\rangle^{(s+1 / 2)}+\langle\sigma\rangle_{T}^{(s)} \delta\langle\vec{J}\rangle^{(s+1 / 2)}=0 \tag{5.100}
\end{equation*}
$$

$$
\begin{equation*}
\rho^{s+1}=\rho^{k+1 / 2}+\langle\operatorname{sigma}\rangle \delta\langle\phi\rangle^{(s+1 / 2)} \tag{5.101}
\end{equation*}
$$

$$
\begin{equation*}
T^{(s+1)}=T^{(s)}-\iota^{(s)}\left(T^{(s)}-T^{(n-1 / 2)}\right)+\frac{\rho^{(s+1)}-\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(s)}+Q_{e x t}}{\frac{C_{v}}{\Delta t \theta}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}(s)}{d T}} \tag{5.102}
\end{equation*}
$$

We propose the iteration given by algorithm 4 .
This algorithm uses a low-order (gray $P_{1}$ diffusion) operator to iterate on the material temperature in an inner Newton-like iteration, which reduces the number of Newton iterations that uses a high-order operator. We have included the steps to fully converge the pseudo-scattering iteration in this algorithm, but our numerical results show that performing only one sweep per outer iteration to be the fastest iterative method.

If we insert the converged iteration solution, $\rho^{(n+1 / 2)}$ and $T^{(n+1 / 2)}$, as the solution we obtain a

```
Algorithm 4 Linear Acceleration of Newton's Method for Thermal Radiative Transfer
    \(p \leftarrow 0\)
    \(T^{(p)} \leftarrow T^{(n-1 / 2)}, \rho^{(p)} \leftarrow \rho^{(n-1 / 2)}\)
    repeat
        Compute \(B_{g}^{(p)}, \frac{d B_{g}(p)}{d T}, \eta^{(p)}, \chi_{g}^{(p)}, Q_{g, \text { rad }}^{(p)}\)
        \(k \leftarrow 0\)
        \(\rho^{(k)} \leftarrow \rho^{(p)}\)
        repeat
            Sweep \(L_{m, g}^{(n)} \psi_{m, g}^{(k+1)}=\frac{\eta^{(p)} \chi_{g}^{(p)} \rho^{(k)}+Q_{g, r a d}^{(p)}}{4 \pi}+q_{m, g}+\tau \psi_{m, g}^{n-1 / 2}\)
            \(\rho^{(k+1)} \leftarrow \sum_{g=1}^{G} \sigma_{g}^{(p)} \sum_{m=1}^{M} w_{m} \psi_{m, g}^{(k+1)}\)
        until \(\left|\rho^{(k+1)}-\rho^{(k)}\right| \leq \epsilon_{\rho}, k \geq k_{m} a x\), else \(k \leftarrow k+1\)
        \(\rho^{(p+1 / 2)} \leftarrow \rho^{(k+1)}\)
        \(T^{(p+1 / 2)} \leftarrow T^{(p)}+\frac{-\frac{C_{v}}{\Delta t^{(n)}}\left(T^{(p)}-T^{(n-1 / 2)}\right)+\rho^{(p+1 / 2)}-\sum_{g=1}^{G} \sigma_{g}^{(p)} B_{g}^{(p)}+Q_{e x t}}{\frac{C_{v}}{\Delta t^{(n)}}+\sum_{g=1}^{G} \sigma_{g}^{(p)} \frac{d B_{g}}{d T}{ }^{(p)}}\)
        \(s \leftarrow 0\)
        \(T^{(s)} \leftarrow T^{(p+1 / 2)}\)
        repeat
            Compute \(\eta^{(s)}, Q_{\text {rad }}^{(s)}\)
            Solve \(-\vec{\nabla} \cdot\langle D\rangle \vec{\nabla} F^{(s+1)}+\langle\sigma\rangle_{a} F^{(s+1)}=\eta^{(s)} \rho^{(p+1 / 2)}-\eta^{(p)} \rho^{(p)}+Q_{r a d}^{(s)}-Q_{r a d}^{(p)}\)
            \(\rho^{(s+1)} \leftarrow \rho^{(p+1 / 2)}+\langle\sigma\rangle F^{(s+1)}\)
            \(T^{(s+1)} \leftarrow T^{(s)}+\frac{-\frac{C_{v}}{\Delta t}\left(T^{(s)}-T^{(n-1 / 2)}\right)+\rho^{(s+1)}-\langle\sigma\rangle_{B} B^{(s)}+Q_{e x t}}{\frac{C_{v}}{\Delta t}+\langle\sigma\rangle_{B} \frac{d B}{d T}(s)}\)
            until \(\left|T^{(s+1)}-T^{(s)}\right| \leq \epsilon_{T},\left|\rho^{(s+1)^{\Delta t}}-\rho^{(s)}\right| \stackrel{\epsilon_{\rho}}{ }\) else \(s \leftarrow s+1\)
            \(T^{(p+1)} \leftarrow T^{(s+1)}\)
            \(\rho^{(p+1)} \leftarrow \rho^{(s+1)}\)
    until \(\left|T^{(p+1)}-T^{(p)}\right| \leq \epsilon_{T},\left|\rho^{(p+1)}-\rho^{(p)}\right| \leq \epsilon_{\rho}\), else \(p \leftarrow p+1\)
    \(T^{(n)} \leftarrow T^{(p+1)} \Rightarrow T^{(n+1 / 2)} \leftarrow \frac{1}{\theta} T^{(n)}-\left(\frac{1}{\theta}-1\right) T^{(n-1 / 2)}\)
    \(\rho^{(n)} \leftarrow \rho^{(p+1)} \Rightarrow \rho^{(n+1 / 2)} \leftarrow \frac{1}{\theta} \rho^{(n)}-\left(\frac{1}{\theta}-1\right) \rho^{(n-1 / 2)}\)
```

zero correction because the right hand side is zero.

### 5.4.1 Linear HOLO Energy Error Spectrum and Gray Opacities

We now seek an energy collapse scheme that will eliminate the slowest converging error modes of the following transport equation for a correction:

$$
\begin{align*}
& \vec{\Omega}_{m} \cdot \vec{\nabla} \delta \psi_{m, g}^{(s+1 / 2)}+\left(\sigma_{g}^{(p)}+\tau^{(n)}\right) \delta \psi_{m, g}^{(s+1 / 2)}-\frac{1}{4 \pi} \chi_{g}^{(s)} \eta^{(s)} \delta \rho^{(s+1 / 2)}  \tag{5.103}\\
& =\frac{1}{4 \pi}\left[\chi_{g}^{(s)} \eta^{(s)} \rho^{(k+1 / 2)}-\chi_{g}^{(p)} \eta^{(p)} \rho^{(k)}+Q_{g, r a d}^{(s)}-Q_{g, r a d}^{(p)}\right]
\end{align*}
$$

One choice of solving this system is a pseudo-scattering iteration, that we denote with index $l+1 / 2$ :

$$
\begin{align*}
& \vec{\Omega}_{m} \cdot \vec{\nabla} \delta \psi_{m, g}^{(l+1 / 2)}+\left(\sigma_{g}^{(p)}+\tau^{(n)}\right) \delta \psi_{m, g}^{(l+1 / 2)}-\frac{1}{4 \pi} \chi_{g}^{(s)} \eta^{(s)} \delta \rho^{(l)}  \tag{5.104}\\
& =\frac{1}{4 \pi}\left[\chi_{g}^{(s)} \eta^{(s)} \rho^{(k+1 / 2)}-\chi_{g}^{(p)} \eta^{(p)} \rho^{(k)}+Q_{g, r a d}^{(s)}-Q_{g, r a d}^{(p)}\right] .
\end{align*}
$$

The although there are many more terms on the right hand side of the equation than the equation in Larsen's paper, the resulting system has the same form for the pseudo-scattering iteration as Larsen's equations. Thus, we obtain the same energy collapsed cross sections as Larsen, which we have detailed above, except quantities are evaluated at index $s$.

### 5.5 Analysis of Gray Diffusion Synthetic Acceleration

We are interested in the convergence properties of the gray-diffusion linear preconditioning method for multi-group energy discretization. The success of the linear HOLO iterative method is predicated on the ability of the linear preconditioning method to approximate the slowest converging error mode in space, angle, and energy. We analyze an infinite homogeneous system to determine the effects of energy discretization on the gray preconditioner.

We postulate a Fourier ansatz for the errors of the pseudo-scattering iteration at $k$ from the converged pseudo-scattering solution at iteration $p+1 / 2$ :

$$
\begin{equation*}
\delta \rho^{(k)}=\rho^{(p+1 / 2)}-\rho^{(k)}=\iiint_{0}^{\infty} d^{3} \lambda \omega^{k} e^{\mathbf{i} \vec{\lambda} \cdot \vec{r}} \tag{5.105}
\end{equation*}
$$

$$
\begin{align*}
\delta \psi_{m, g}^{(k+1 / 2)} & =\psi_{m, g}^{(p+1 / 2)}-\psi_{m, g}^{(k+1 / 2)}=\iiint_{0}^{\infty} d^{3} \lambda \omega^{k} \delta \psi_{m, g, \dagger}(\vec{\lambda}) e^{\mathrm{i} \lambda \cdot \vec{r}},  \tag{5.106}\\
\delta \phi^{(k+1)} & =\phi^{(p+1 / 2)}-\phi^{k+1 / 2}=\iiint_{0}^{\infty} d^{3} \lambda \delta \phi_{\dagger}(\vec{\lambda}) \omega^{k+1} e^{\overrightarrow{\mathrm{\lambda}} \cdot \vec{r}} . \tag{5.107}
\end{align*}
$$

We substitute the Fourier ansatz into the transport error equation:

$$
\begin{equation*}
\left(\mathbf{i} \vec{\Omega}_{m} \cdot \vec{\lambda}+\sigma_{g}^{(p)}+\tau\right) \delta \psi_{m, g, \dagger}(\vec{\lambda})=\frac{1}{4 \pi} \eta^{(p)} \chi_{g}^{(p)}, \tag{5.108}
\end{equation*}
$$

and solve for $\delta \psi_{m, g, \dagger}(\vec{\lambda})$ :

$$
\begin{equation*}
\delta \psi_{m, g, \dagger}(\vec{\lambda})=\frac{1}{4 \pi} \frac{\chi_{g}^{p} \eta^{p}}{\mathbf{i} \vec{\Omega}_{m} \cdot \vec{\lambda}+\sigma_{g}^{(p)}+\tau} \tag{5.109}
\end{equation*}
$$

We use the definition of $\delta \rho^{(k+1 / 2)}$ :

$$
\begin{equation*}
\delta \rho^{(k+1 / 2)}(\vec{\lambda})=\sum_{g} \sum_{m} \sigma_{g}^{(p)} \delta \psi_{m, g, \dagger}(\vec{\lambda}) . \tag{5.110}
\end{equation*}
$$

and solve the $P_{1}$ diffusion equations for $\delta \phi^{\dagger}$ :

$$
\begin{equation*}
\delta \phi_{\dagger}(\vec{\lambda})=\frac{\eta^{p}}{\left(\frac{|\vec{\lambda}|^{2}}{3\langle\sigma\rangle_{T}}+\langle\sigma\rangle_{T}-\langle\sigma\rangle_{S}\right)}\left(\delta \rho^{(k+1 / 2)}(\vec{\lambda})-1\right) \tag{5.111}
\end{equation*}
$$

Finally, we substitute into the update equation for $\rho^{(k+1)}$ :

$$
\begin{equation*}
\omega=\delta \rho^{(k+1 / 2)}(\vec{\lambda})+\langle\sigma\rangle \delta \phi_{\dagger}(\vec{\lambda}) . \tag{5.112}
\end{equation*}
$$

We analyze a Fourier problem that has two energy groups. The problem's two opacities are chosen such that $\langle\sigma\rangle=1000\left[\mathrm{~cm}^{2} / \mathrm{g}\right]$, and $\sigma_{2}=\sigma_{1} * M_{\sigma}$, where $M_{\sigma}$ is a multiplier that ranges from $1 e-6$ to $1 e 6 . \frac{C_{v}}{\Delta t}$ was chosen to be $10, \Delta t$ was chosen to be $1 / c$ such that $\tau=1 / c \Delta t=1$, and $\eta$ was chosen to be .9. To satisfy these constraints, we assumed a group structure such that $d B / d T$

Figure 5.1: Spectral radius from Fourier analysis of a 2 energy group problem.

is the same for each energy group, and we solve the quadratic equation that arises from solving the averaged opacity for $\sigma_{1}$ :

$$
\begin{gather*}
\frac{d B}{d T}=[1,1] \frac{d B_{1}}{d T}  \tag{5.113}\\
\sigma=\left[1, M_{\sigma}\right] \sigma_{1},  \tag{5.114}\\
\chi=\left[\frac{1}{1+M_{\sigma}}, \frac{M_{\sigma}}{1+M_{\sigma}}\right],  \tag{5.115}\\
\langle\sigma\rangle=\frac{\sigma_{1} \frac{1}{1+M_{\sigma}} \frac{1}{\sigma_{1}+\tau}+M_{\sigma} \sigma_{1} \frac{M_{\sigma}}{1+M_{\sigma}} \frac{1}{\sigma_{1} M_{\sigma}+\tau}}{1+M_{\sigma}} \frac{1}{\sigma_{1}+\tau}+\frac{M_{\sigma}}{1+M_{\sigma}} \frac{1}{\sigma_{1} M_{\sigma}+\tau} \tag{5.116}
\end{gather*} 1000 .
$$

Figure 5.1 shows the spectral radii of the GDSA scheme as a function of the opacity ratio $M_{\sigma}=\sigma_{2} / \sigma_{1}$. We demonstrate that even with no discretization error, as the difference in opacities between groups increases the spectral radius of the GDSA scheme degrades to approximately the energy averaged "scattering ratio" $\left(\frac{\langle\sigma\rangle_{S}}{\langle\sigma\rangle_{T}}\right)$, but is always less than one in magnitude.

Next, we compare behavior of the linear preconditioning method between a 2D Fourier analysis and a 2D infinite homogeneous problem run with PDT, a massively parallel transport code developed at Texas A\&M University [53] using the STAPL parallel library [54, 55, 56]. We use 50 group multi-group plastic opacities at $5[\mathrm{eV}]$ generated during the CRASH project led by the University of Michigan. We have found it necessary to set a maximum opacity value of the cross section set, which we choose to be $1 \times 10^{6}\left[\mathrm{~cm}^{2} / \mathrm{g}\right]$. For the test problems, we choose problem dimensions such that cells have an optical thickness of 10 mean free paths in each dimension, and we choose 30 by 30 cells. In Table 5.1, column $S(A)$ is the spectral radius of the transport operator, and column $S(P A)$ is the spectral radius of the GDSA scheme.

This set of test problems shows that the gray diffusion preconditioner's effectiveness does not degrade as the number of energy groups is increased. These results are similar to previous results

Table 5.1: Plastic Spectral Radius Comparison

|  | $S(A)$ |  | $S(P A)$ |  |
| :---: | :---: | :---: | :---: | :---: |
| groups | Fourier | Model | Fourier | Model |
| 2 | .5107 | .5107 | .1772 | .1147 |
| 10 | .9999 | .9999 | .4120 | .4241 |
| 50 | .9999 | .9999 | .4112 | .4152 |
| 99 | .9999 | .9999 | .4112 | .4150 |

for Linear Multifrequency Gray (LMFG) [18] and Gray Transport Acceleration (GTA) [17].

### 5.6 Results

We have tested our two methods for a variety of difficult radiative transfer problems, and we present results from the following: a Marshak wave in plastic using realistic opacities, a tophat problem using a one-group analytic function for opacity, and a tophat problem using multi-group plastic opacities. We investigate the behavior of the unpreconditioned GMRES iteration with no restarts $(A)$, linear-preconditioned GMRES iteration with no restarts $(P A)$, and the proposed linear HOLO acceleration iteration ( $N L A$ ). All problems were run with Backward Euler time differencing, with opacities evaluated at beginning-of-step temperatures.

Convergence is determined by three conditions. The inner iteration for ARD is tested with the $L_{2}$ norm of the ARD residual relative to the ARD associated with the uncollided intensity given the effective fixed source at iteration $p$ :

$$
\begin{equation*}
\frac{\left\|\rho^{s+1}-\rho^{s}\right\|_{2}}{\left\|b^{p}\right\|_{2}} \leq \epsilon_{\rho, 2} \tag{5.117}
\end{equation*}
$$

the $L_{\infty}$ norm of the relative ARD residual:

$$
\begin{equation*}
\left\|\frac{\rho^{s+1}-\rho^{s}}{\rho^{s+1}}\right\|_{\infty} \leq \epsilon_{\rho, \infty} \tag{5.118}
\end{equation*}
$$

The outer Newton iteration is tested with the $L_{\infty}$ norm of the relative difference in temperature iterates:

$$
\begin{equation*}
\left\|\frac{T^{p+1}-T^{p}}{T^{p+1}}\right\|_{\infty} \leq \epsilon_{T, \infty} \tag{5.119}
\end{equation*}
$$

The tolerances used are specified in each problem description.
Unaccelerated problems were solved with GMRES, as Richardson iteration is prohibitively expensive for problems with spectral radii near unity. Problems solved with linear-preconditioning used a preconditioned GMRES iteration. From our observations, the convergence is often limited by the $L_{\infty}$ norm of the relative ARD residual. Preconditioned GMRES iteration may re-excite error modes of the $L_{\infty}$ norm even when the $L_{2}$ norm is satisfied. Preconditioned Richardson iteration monotonically decreases the iteration residual of the $L_{\infty}$ and $L_{2}$ norms. Once the $L_{2}$ norm is satisfied, the iteration to converge the $L_{\infty}$ norm becomes a preconditioned Richardson iteration. We note that the linear HOLO reduces to a preconditioned Richardson iteration for ARD when the temperature is converged.

In all problems, the low-order one-group diffusion system is solved with preconditioned Conjugate Gradient (PCG) using algebraic-multigrid (AMG) as the preconditioner. We link to the implementation of PCG and AMG in HYPRE. A $L_{2}$ norm tolerance of $1 \times 10^{-15}$ is chosen for all diffusion solutions. This tight tolerance was chosen to eliminate the possibility of confusion from poorly converged diffusion. We are exploring how much we can relax this to improve run time without degrading performance.

In the iteration statistics for each problem, we list the number of sweeps (Sweeps), temperature iterations (Te It.), diffusion solutions (Diffusion), total solution time in seconds (Time), sweep reduction factor (Swp. RF), and time reduction factor (Time RF). Reduction factors are calculated as ratio of unpreconditioned iteration value to preconditioned iteration value.

### 5.6.1 Marshak wave in plastic

The Marshak wave problem is a plastic square $.0012[\mathrm{~cm}]$ by $.0012[\mathrm{~cm}]$, discretized into 20 by 20 cells, an $S 8$ quadrature and one energy group. The plastic is initially at $1[\mathrm{eV}]$ with an incoming blackbody intensity of $100[\mathrm{eV}]$ at the left boundary. We solve the system to $3 \times 10^{-9}[\mathrm{~s}]$ using fixed

Table 5.2: Marshak Wave Plastic Iteration Statistics

|  | $A$ | $P A$ | $N L A$ |
| :---: | :---: | :---: | :---: |
| Sweeps | 1864 | 926 | 87 |
| Te It. | 93 | 92 | 87 |
| Diffusion | - | 926 | 158 |
| Time[s] | 36 | 56 | 11 |
| Swp. RF | - | 2.0130 | 21.4253 |
| Time RF | - | 0.6429 | 3.2727 |

timesteps of $1 \times 10^{-10}[s]$. We choose convergence tolerances of $\epsilon_{\rho, 2}=1 \times 10^{-10}, \epsilon_{\rho, \infty}=1 \times 10^{-2}$, and $\epsilon_{T, \infty}=1 \times 10^{-2}$.

Table 5.2 shows the number of sweeps, temperature iterations, diffusion solutions, and total time to completion to solve the problem described above. The linear-preconditioning method shows a significant reduction in the number of transport sweeps (a factor of 2). However, the computational effort expended in reducing the error of ARD at each Newton iteration for temperature is wasted to some extent if later temperature updates produce a significantly different temperature field. Because the solution of the diffusion operator is relatively expensive compared to a one group transport sweep, the linear-preconditioning method was not effective at reducing total solution time for this problem.

Iterative convergence in this particular test problem is dominated by error reduction of the temperature field. The linear HOLO acceleration method reduced the temperature error using a diffusion operator before resolving the ARD error, and thus avoided over converging ARD. Because the problem is highly diffusive, the temperature field and diffusion error is effectively approximated by the linear HOLO acceleration method. The linear HOLO acceleration method resulted in a factor of three reduction in solution time compared to unpreconditioned iteration, and a factor of 20 fewer transport sweeps. The time reduction is much greater in multi-frequency problems, because transport sweeps are relatively more expensive in such problems.

Figure 5.2: Tophat Geometry and Meshing


### 5.6.2 Tophat with Model Opacity

The tophat model-opacity problem embodies many of the challenges that arise from spatial dependence in realistic thermal radiation transport problems, but treats the opacity as a simple analytic function. The optically thick region introduces boundary layers and makes the ARD iteration difficult to converge. The optically thin region allows streaming, which is challenging for angular and temporal discretizations. Transient effects of radiation propagation must be resolved with sufficiently small time-steps to obtain an accurate solution.

We begin with a tophat-geometry problem that has one-group opacities that are independent of temperature. The tophat model-opacity problem is a cylinder $7[\mathrm{~cm}]$ long with $4[\mathrm{~cm}]$ radius, which we approximate with cartesian geometry in 2D with $50 \times 35$ cells and an $S_{8}$ discrete ordinates quadrature. We solve the system to $1 \times 10^{-8}[s]$ using adaptive timesteps with an initial time of $1 \times 10^{-12}[s]$, a maximum increase in timestep of 1.25 , and a maximum relative difference in temperature and ARD of 0.125 per timestep. The remaining problem definition is listed in Table 5.3, and the geometry is shown in Fig. (5.2). We choose convergence tolerances of $\epsilon_{\rho, 2}=1 \times 10^{-5}$, $\epsilon_{\rho, \infty}=1 \times 10^{-3}$, and $\epsilon_{T, \infty}=1 \times 10^{-3}$.

Table 5.3: Tophat Model Problem Description

| Property | Thin | Thick | Units |
| :---: | :---: | :---: | :---: |
| Density | .01 | 10 | $[\mathrm{~g} / \mathrm{cc}]$ |
| Opacity | 20 | 20 | $\left[\mathrm{~cm}^{2} / \mathrm{g}\right]$ |
| $T_{0}$ | .05 | .05 | $[\mathrm{keV}]$ |
| $C_{v}$ | .05 | .05 | $1 \mathrm{e} 16[\mathrm{ergs} / \mathrm{g}-\mathrm{keV}]$ |
| $\psi(x=0)^{0}$ | .3 | .3 | $[\mathrm{keV}]$ |

Table 5.4: Tophat Model Opacity Iteration Statistics

|  | $A$ | $P A$ | $N L A$ |
| :---: | :---: | :---: | :---: |
| Sweeps | 2125 | 971 | 415 |
| Te It. | 254 | 254 | 415 |
| Diffusion | - | 971 | 572 |
| Time[s] | 494 | 400 | 362 |
| Swp. RF | - | 2.1885 | 5.1205 |
| Time RF | - | 1.2350 | 1.3646 |

The spectral radius of the unpreconditioned operator was close to one in magnitude. The GDSA scheme did not degrade from spatial discretization due to high-aspect ratio mesh or from energy discretization because the problem only had one group. However, the GDSA scheme still requires converging the high-order scattering problem sufficiently at each temperature iteration. The linear HOLO acceleration method was effective at reducing the number of transport sweeps, cutting them by approximately a factor of two compared to the linear-preconditioning method because only one sweep was performed per temperature iteration, and the primary solution was performed during the low-order Newton iteration.

### 5.6.3 Tophat with Plastic Opacities

We show the iterative method behavior for a 50 -group multi-group plastic opacity. Except for the opacities and energy group structure, this problem definition (cells, angles, time-step control) is identical to the tophat model-opacity problem in Table 5.3. We choose convergence tolerances of $\epsilon_{\rho, 2}=1 \times 10^{-5}, \epsilon_{\rho, \infty}=1 \times 10^{-4}$, and $\epsilon_{T, \infty}=1 \times 10^{-3}$.

Table 5.5: Tophat Plastic Opacity Iteration Statistics

|  | $A$ | $P A$ | $N L A$ |
| :---: | :---: | :---: | :---: |
| Sweeps | 3194 | 2112 | 1334 |
| Te It. | 302 | 292 | 1334 |
| Diffusion | - | 2112 | 1680 |
| Time[s] | 8929 | 4491 | 3209 |
| Swp. RF | - | 1.5052 | 2.3943 |
| Time RF | - | 1.9882 | 2.7825 |

We noticed the opacity values in the this data set were non-physical, with low energy opacities reaching $1 \times 10^{22}\left[\mathrm{~cm}^{2} / \mathrm{g}\right]$. We set a maximum opacity of $1 \times 10^{6} \mathrm{~cm}^{2} / \mathrm{g}$ to limit the otherwise extreme ill-conditioning of the problem. Table 5.5 shows the number of sweeps, temperature iterations, diffusion precoditioner solutions, and total solution time. The sweep operation for this problem is considerably more expensive than the one-group model problem, and the sweep operation occupies essentially all of the solution time. Thus, a reduction in the number of sweeps had more effect on reducing the solution time.

This problem shows the importance of reducing the error of the temperature field not only the ARD. The linear HOLO method reduced the number of transport sweeps taken at the significantly lower cost of added temperature iterations, source calculations, and diffusion solutions. We note that the transport problem that was solved had relatively low number of energy groups and angles in the quadrature. As the fidelity of angle and energy treatment increases the sweep time will dominate the problem, and thus time reduction factor will limit to the same value as the sweep reduction factor.

### 5.7 Summary

Previous work has shown that accelerating the pseudo-scattering iteration with a gray loworder operator can effectively reduce the number of sweeps during that iteration. However, HOLO methods that use nonlinear functionals in a low-order Newton iteration can perform significantly fewer transport sweeps. We devise a linear HOLO method that only uses linear functionals of the transport solution to determine the ARD and material temperature in an Newton iteration on a
low-order operator.
The linear HOLO method is effective when the problem is highly diffusive, and when iteration error is dominated by error in the temperature field. For problems that are limited by error in the ARD, the linear HOLO method quickly resolves the temperature field, and effectively becomes a DSA scheme for a preconditioned Richardson iterative method. The linear HOLO method is an improvement to the linear preconditioned method for all problems studied, because it avoids excessive iteration on the pseudo-scattering problems when the problem is dominated by the error in the temperature field.

## 6. ONE-GROUP DIFFUSION ACCELERATION OF JACOBI ITERATION FOR THERMAL NEUTRON UPSCATTERING ITERATION

### 6.1 Method Motivation

We are interested in methods that solve thermal neutron upscattering iterations efficiently on state of the art computer architectures. As processes increase, we seek higher fidelity of our physical models. Thus we seek to refine space, angle, and energy resolution. As the number of energy groups increases, it is necessary to use methods that have good weak scaling efficiency with increasing energy groups. It is well known that a Gauss-Seidel operator splitting with a DSA preconditioner produces an efficient solution method, but has poor weak scaling efficiency because the method requires sequential operations. Although there are paths to extend the scaling of GaussSeidel methods (prefix sums [57], FEDS [50, 58]), at some point poor scaling efficiency dominates. Alternatively, Jacobi operator splitting (block and non-block) produce methods with poor solution efficiency (operator spectral radii near unity) even when preconditioned with DSA, and excellent weak scaling efficiency.

Hanuš and Ragusa have devised a method that combines within-group DSA and a one-group DSA to accelerate thermal neutron upscattering.[59] In their paper, they perform thorough analysis of Gauss-Seidel and Jacobi methods, combinations of within-group and two-grid (TG) DSA, and study the effects of converging or partially converging the within-group scattering iteration. They present numerical results using the Modified Interior Penalty (MIP) Diffusion operator, which is a low-order operator that has spatial degrees of freedom equal to the DFEM discretization. Their results show that the optimal procedure for a Jacobi iteration is to perform one DSA iteration independently across all energies ( $\mathrm{J} 1+\mathrm{wgDSA}$ ), and accelerate the upscattering iteration using onegroup (also known as Two-Grid, or TG) DSA. This combination, labeled as " $\mathrm{J} 1+\mathrm{wgDSA}+\mathrm{TG}$ " in their paper, is shown to recover the iterative performance of fully converging the within-group scattering iteration while requiring far fewer transport sweeps.

In this work, we analyze linearly anisotropic scattering for Gauss-Seidel and Jacobi splitting using the Two-Grid energy collapsed low-order scheme, to determine if accelerating only the scalar moment is sufficient. We also perform numerical tests of the optimal Jacobi method devised by Hanuš and Ragusa, J1+wgDSA+TG, using the CDFEM Diffusion operator in chapter 3, which has fewer spatial degrees of freedom than the MIP discretization.

### 6.2 Thermal Neutron Upscattering Iteration

From the transport equation in Eq. (3.24), neutrons in steady state with upscattering satisfy the following equation:

$$
\begin{equation*}
(\vec{\Omega} \cdot \vec{\nabla}+T) \Psi_{m}=S_{m} \Phi+Q_{m}^{f i x e d} \tag{6.1}
\end{equation*}
$$

where,

$$
\begin{equation*}
S_{m} \Phi \equiv \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right) \Phi_{l, n} \tag{6.2}
\end{equation*}
$$

This system is solved iteratively by lagging some part of the scattering source, resulting two nested iterations at index $k$ and $i$. The way the scattering operator is split has a large effect on the performance of the method, but in general the operator is split into three parts: a "recent" part that represents the current iterate from a "within-group" iteration denoted here by index $k$, which are on the diagonal; a "lagged" part that represents terms that are calculated using the previous iterate (i), which are typically terms below the diagonal of the scattering matrix; and a "converged" part that represents terms that are at the next iterate (i+1), which are typically terms below the diagonal. In operator notation, the within-group iteration at index $k$ is determined as follows:

$$
\begin{equation*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) \Psi_{m}^{(k+1)}=S_{m, r e c} \Phi^{(k)}+S_{m, c o n} \Phi^{(i+1)}+S_{m, l a g} \Phi^{(i)}+\frac{1}{4 \pi} Q_{m}^{f i x e d} \tag{6.3}
\end{equation*}
$$

This iteration may be slow to converge, dependent on the ratio of the within-group scattering cross section to the group total cross section. As previously discussed, acceleration of the
within-group scattering using a diffusion operator has been called Diffusion Synthetic Acceleration (DSA). Instead, methods have been devised to accelerate the outer (upscattering) iteration. One such method, is the Two-Grid (TG) method devised by B.T. Adams and J.E. Morel, which we discuss in the next section.[36]

### 6.3 Two-Grid Acceleration

Although the two-grid method has previously been devised, we find it instructional to derive this method again using the steps from the previous chapters. Step (1): We write the "converged" equation:

$$
\begin{equation*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) \Psi_{m}^{(i+1)}=S_{m} \Phi^{(i+1)}+\frac{1}{4 \pi} Q_{m, e x t} \tag{6.4}
\end{equation*}
$$

and a half-step equation at the end of the within-group iteration:

$$
\begin{equation*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) \Psi_{m}^{(i+1 / 2)}=S_{m, r e c} \Phi^{(k)}+S_{m, c o n} \Phi^{(i+1 / 2)}+S_{m, l a g} \Phi^{(i)}+\frac{1}{4 \pi} Q_{m}^{f i x e d} \tag{6.5}
\end{equation*}
$$

We note that if the within-group scattering iteration is converged, then $\Phi^{(k)}=\Phi^{(i+1 / 2)}$, and if only one sweep is performed per outer iteration then $\Phi^{(k)}=\Phi^{(i)}$.

Step (2): We subtract the equation satisfied by the latest solution from the converged equation to obtaining an exact equation for an additive correction:

$$
\begin{align*}
& \left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) \delta \Psi_{m}^{(i+1)} \\
& =S_{m, \text { rec }}\left(\Phi^{(i+1)}-\Phi^{(i+1 / 2)}+\Phi^{(i+1 / 2)}-\Phi^{(k)}\right) \\
& +S_{m, \text { con }}\left(\Phi^{(i+1)}-\Phi^{(i+1 / 2)}\right)  \tag{6.6}\\
& +S_{m, \text { lag }}\left(\Phi^{(i+1)}-\Phi^{(i+1 / 2)}+\Phi^{(i+1 / 2)}-\Phi^{(i)}\right) \\
& +\frac{1}{4 \pi} Q_{m}^{f i x e d}
\end{align*}
$$

where:

$$
\begin{gather*}
\delta \Psi_{m}^{(i+1)}=\Psi_{m}^{(i+1)}-\Psi_{m}^{(i+1 / 2)},  \tag{6.7}\\
\delta \Phi^{(i+1)}=\Phi^{(i+1)}-\Phi^{(i+1 / 2)} . \tag{6.8}
\end{gather*}
$$

After we simplify the equation and define a residual source, the equation for the exact correction is:

$$
\begin{equation*}
\left(\vec{\Omega}_{m} \cdot \vec{\nabla}+T\right) \delta \Psi_{m}^{(i+1)}=S_{m} \delta \Phi^{(i+1)}+R_{m}^{(i+1 / 2)} \tag{6.9}
\end{equation*}
$$

where the residual source is defined as:

$$
\begin{equation*}
R_{m}^{(i+1 / 2)} \equiv=S_{m, \text { rec }}\left(\Phi^{(i+1 / 2)}-\Phi^{(k)}\right)+S_{m, l a g}\left(\Phi^{(i+1 / 2)}-\Phi^{(i)}\right) . \tag{6.10}
\end{equation*}
$$

3) replace the transport operator in this equation by a low-order operator. Here we have employed a $P_{1}$ diffusion equation by finding the $W_{0}$ and $\vec{W}_{1}$ moments of the transport equation:

$$
\begin{align*}
& \vec{\nabla} \cdot \delta \vec{J}^{(i+1)}+T \delta \Phi^{(i+1)}=S_{0} \delta \Phi_{0}^{(i+1)}+R_{0}^{(i+1 / 2)}  \tag{6.11}\\
& \frac{1}{3} \vec{\nabla} \delta \Phi^{(i+1)}+T \delta \vec{J}^{(i+1)}=S_{1} \delta \vec{J}^{(i+1)}+\vec{R}_{1}^{(i+1 / 2)}, \tag{6.12}
\end{align*}
$$

with update equation:

$$
\begin{equation*}
\Phi_{0}^{i+1}=\Phi_{0}^{(i+1 / 2)}+\delta \Phi_{0}^{(i+1)}, \tag{6.13}
\end{equation*}
$$

and moments of the residual source are given by:

$$
\begin{align*}
R_{0}^{(i+1 / 2)} \equiv & W_{0} \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l, \text { rec }} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right)\left(\Phi_{l, n}^{(i+1 / 2)}-\Phi_{l, n}^{(k)}\right) \\
& +W_{0} \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l, l a g} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right)\left(\Phi_{l, n}^{(i+1 / 2)}-\Phi_{l, n}^{(i)}\right)  \tag{6.14}\\
& =S_{0, \text { rec }}\left(\Phi_{0}^{(i+1 / 2)}-\Phi_{0}^{(k)}\right)+S_{0, \text { lag }}\left(\Phi_{0}^{(i+1 / 2)}-\Phi_{0}^{(i)}\right), \\
\vec{R}_{1}^{(i+1 / 2)} \equiv & \vec{W}_{1} \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l, \text { rec }} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right)\left(\Phi_{l, n}^{(i+1 / 2)}-\Phi_{l, n}^{(k)}\right) \\
& +\vec{W}_{1} \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} S_{l, l a g} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right)\left(\Phi_{l, n}^{(i+1 / 2)}-\Phi_{l, n}^{(i)}\right)  \tag{6.15}\\
= & S_{1, \text { rec }}\left(\vec{J}^{(i+1 / 2)}-\vec{J}^{(k)}\right)+S_{1, l a g}\left(\vec{J}^{(i+1 / 2)}-\vec{J}^{(i)}\right),
\end{align*}
$$

This low-order system still requires costly iteration to resolve upscattering. We note that this low-order system has a choice of how to split the scattering operator, but we are unaware of any low-order methods that do not employ the same operator splitting as the high-order operator.

Instead of solving the upscattering problem, Adams and Morel[36] recognized that the slowest converging error mode could be eliminated by solving a one-group problem with cross sections collapsed with an energy spectrum, $\xi$, equal to the energy eigenvector of the slowest converging mode, which they approximate with the slowest converging mode of an infinite homogeneous problem. In practice, $\xi$ must be determined for each unique material within the problem, each requiring an eigenvalue solution to determine the largest eigenvalue and its eigenvector. Using the two-grid energy collapse scheme we obtain a one-group system of $P_{1}$ diffusion equations:

$$
\begin{gather*}
\vec{\nabla} \cdot \delta\langle\vec{J}\rangle^{(i+1)}+\langle T\rangle \delta\langle\Phi\rangle_{0}^{(i+1)}=\langle S\rangle_{0} \delta\langle\Phi\rangle_{0}^{(i+1)}+\langle R\rangle_{0}^{(i+1 / 2)},  \tag{6.16}\\
\frac{1}{3} \vec{\nabla} \delta\langle\Phi\rangle_{0}^{(i+1)}+\langle T\rangle \delta\langle\vec{J}\rangle^{(i+1)}=\langle S\rangle_{1} \delta\langle\vec{J}\rangle^{(i+1)}+\langle\vec{R}\rangle_{1}^{(i+1 / 2)}, \tag{6.17}
\end{gather*}
$$

For completeness we have included $\langle\vec{R}\rangle_{1}^{(i+1 / 2)}$ in the $1^{\text {st }}$ moment equation, but the original TG derivation ignores this term; in future equations we also choose to ignore this term. The next
iterate is calculated with update equation given by:

$$
\begin{equation*}
\Phi_{0}^{(i+1)}=\Phi_{0}^{(i+1 / 2)}+\xi \delta\langle\Phi\rangle_{0}^{(i+1)} . \tag{6.18}
\end{equation*}
$$

The group collapsed cross sections are defined as follows, also given in block matrix form using a vector of ones, $P$ :

$$
\begin{equation*}
\langle T\rangle=\sum_{g=1}^{N} \xi_{g} \sigma_{t, g}=P^{T} T \xi \tag{6.19}
\end{equation*}
$$

$$
\begin{equation*}
\langle S\rangle_{0} \delta\langle\Phi\rangle_{0}^{(i+1)}=W_{0} \sum_{g=1}^{N} \sum_{g^{\prime}=1}^{N} \xi_{g}^{\prime} \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} \sigma_{s, g^{\prime} \rightarrow g, l} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right) \delta \phi_{g^{\prime}, l, n}^{(i+1)}=P^{T} S_{0} \xi^{T} \delta \Phi_{0}^{(i+1)} \tag{6.20}
\end{equation*}
$$

$$
\begin{equation*}
\langle S\rangle_{1} \delta\langle\vec{J}\rangle_{0}^{(i+1)}=\vec{W}_{1} \sum_{g=1}^{N} \sum_{g^{\prime}=1}^{N} \xi_{g}^{\prime} \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} \sigma_{s, g^{\prime} \rightarrow g, l} \sum_{n=-l}^{l} Y_{l}^{n}\left(\vec{\Omega}_{m}\right) \delta \phi_{g^{\prime}, l, n}^{(i+1)}=P^{T} S_{1} \xi^{T} \delta \vec{J}^{(i+1)}, \tag{6.21}
\end{equation*}
$$

$$
\langle D\rangle=\frac{1}{3\left(\langle T\rangle-\langle S\rangle_{1}\right)},
$$

$$
\langle A\rangle=\langle T\rangle-\langle S\rangle_{0}
$$

$$
\langle R\rangle_{0}^{(i+1 / 2)}=P R_{0}^{(i+1 / 2)}
$$

$$
\begin{equation*}
\langle\vec{R}\rangle_{1}^{(i+1 / 2)}=P \vec{R}_{1}^{(i+1 / 2)} \tag{6.25}
\end{equation*}
$$

This system of equations defines the two-grid DSA method, and includes linearly anisotropic scattering sources, but only accelerates the $0^{\text {th }}$ moment of $\Phi$.

### 6.4 Analysis

### 6.4.1 Block Matrix Form of the Iteration Operator

We define our system of equations in block matrix form. For simplicity, we treat the withingroup scattering as either fully converged so that $S_{l, \text { rec }}$ is included in $S_{l, \text { con }}$, or only one transport step and $S_{l, \text { rec }}$ is included in $S_{l, l a g}$. We also limit this analysis to $P_{1}$ scattering, and do not discretize the angle dependence. We find the angular intensity after a within-group solve for $P_{1}$ scattering:

$$
\begin{align*}
\Psi^{(i+1 / 2)}(\vec{\Omega}) & =L^{-1} \frac{1}{4 \pi}\left[S_{0, c o n} \Phi_{0}^{(i+1 / 2)}+S_{1, \text { con }} 3 \vec{\Omega} \cdot \vec{J}^{(i+1 / 2)}\right] \\
& +L^{-1} \frac{1}{4 \pi}\left[S_{0, \text { lag }} \Phi_{0}^{(i)}+S_{1, \text { lag }} 3 \vec{\Omega} \cdot \vec{J}^{(i)}\right]  \tag{6.26}\\
& +\frac{1}{4 \pi} L^{-1} Q^{\text {fixed }}(\vec{\Omega}) .
\end{align*}
$$

We find the $0^{t h}$ and $1^{\text {st }}$ moments of the previous equation:

$$
\begin{align*}
\Phi_{0}^{(i+1 / 2)} & =W_{0} L^{-1}\left[S_{0, \text { con }} \Phi_{0}^{(i+1 / 2)}+S_{1, \text { con }} 3 \vec{\Omega} \cdot \vec{J}^{(i+1 / 2)}\right] \\
& +W_{0} L^{-1}\left[S_{0, \text { lag }} \Phi_{0}^{(i)}+S_{1, \text { lag }} 3 \vec{\Omega} \cdot \vec{J}^{(i)}\right]  \tag{6.27}\\
& +W_{0} L^{-1}(\vec{\Omega}) Q^{\text {fixed }}(\vec{\Omega}) \\
\vec{J}^{(i+1 / 2)} & =\vec{W}_{1} L^{-1}\left[S_{0, \text { con }} \Phi_{0}^{(i+1 / 2)}+S_{1, \text { con }} 3 \vec{\Omega} \cdot \vec{J}^{(i+1 / 2)}\right] \\
& +\vec{W}_{1} L^{-1}\left[S_{0, \text { lag }} \Phi_{0}^{(i)}+S_{1, l a g} 3 \vec{\Omega} \cdot \vec{J}^{(i)}\right]  \tag{6.28}\\
& +\vec{W}_{1} L^{-1} Q^{\text {fixed }}(\vec{\Omega}) .
\end{align*}
$$

In in block matrix form, these equations are:

$$
\begin{equation*}
\left[\mathcal{I}-\mathcal{A}_{\text {con }}\right] \Phi^{(i+1 / 2)}=\mathcal{A}_{\text {lag }} \Phi^{(i)}+\mathcal{Q}, \tag{6.29}
\end{equation*}
$$

where:

$$
\mathcal{I}=\left[\begin{array}{cc}
I & 0  \tag{6.30}\\
0 & \overrightarrow{\vec{I}}
\end{array}\right]
$$

$$
\begin{align*}
& \mathcal{F}=\left[\begin{array}{ll}
W_{0} L^{-1} & W_{0} L^{-1} \vec{\Omega} \\
\vec{W}_{1} L^{-1} & \vec{W}_{1} L^{-1} \vec{\Omega}
\end{array}\right],  \tag{6.31}\\
& \mathcal{S}_{0, \text { con } / \text { lag }}=\left[\begin{array}{ccc}
S_{0, \text { con } / l a g} & 0 \\
0 & 3 S_{1, \text { con } / \text { lag }} \vec{I}
\end{array}\right]  \tag{6.32}\\
& \mathcal{A}_{\text {con }}=\left[\begin{array}{ll}
W_{0} L^{-1} S_{0, c o n} & W_{0} L^{-1} S_{1, c o n} 3 \vec{\Omega} \\
\vec{W}_{1} L^{-1} S_{0, c o n} & \vec{W}_{1} L^{-1} S_{1, c o n} 3 \vec{\Omega}
\end{array}\right]=\left[\begin{array}{ll}
W_{0} L^{-1} & W_{0} L^{-1} \vec{\Omega} \\
\vec{W}_{1} L^{-1} & \vec{W}_{1} L^{-1} \vec{\Omega}
\end{array}\right]\left[\begin{array}{cc}
S_{0, c o n} & 0 \\
0 & 3 S_{1, c o n} \vec{I}
\end{array}\right]  \tag{6.33}\\
& =\mathcal{F} \mathcal{S}_{\text {con }}, \\
& \mathcal{A}_{\text {lag }}=\left[\begin{array}{ll}
W_{0} L^{-1} S_{0, l a g} & W_{0} L^{-1} S_{1, l a g} 3 \vec{\Omega} \\
\vec{W}_{1} L^{-1} S_{0, l a g} & \vec{W}_{1} L^{-1} S_{1, l a g} 3 \vec{\Omega}
\end{array}\right]=\mathcal{F} \mathcal{S}_{\text {lag }},  \tag{6.34}\\
& \mathcal{Q}=\left[\begin{array}{l}
W_{0} L^{-1} Q^{\text {fixed }}(\vec{\Omega}) \\
\vec{W}_{1} L^{-1} Q^{\text {fixed }}(\vec{\Omega})
\end{array}\right], \tag{6.35}
\end{align*}
$$

Next we solve for $\Phi^{(i+1 / 2)}$ :

$$
\begin{equation*}
\Phi^{(i+1 / 2)}=\left[\mathcal{I}-\mathcal{A}_{\text {con }}\right]^{-1}\left[\mathcal{A}_{\text {lag }} \Phi^{(i)}+\mathcal{Q}\right], \tag{6.36}
\end{equation*}
$$

We show a two-grid step with no spatial discretization and $P_{1}$ scattering:

$$
\begin{equation*}
\delta\langle\Phi\rangle_{0}^{(i+1)}=\left[\vec{\nabla} \cdot \frac{1}{3}\left(\langle T\rangle-\langle S\rangle_{1}\right)^{-1} \vec{\nabla}+\left(\langle T\rangle-\langle S\rangle_{0}\right)\right]^{-1} P S_{0, l a g}\left(\Phi_{0}^{(i+1 / 2)}-\Phi_{0}^{(i)}\right), \tag{6.37}
\end{equation*}
$$

and define a two-grid operator $\hat{A}_{T G}$ :

$$
\begin{equation*}
\hat{A}_{T G}=\xi\left[\vec{\nabla} \cdot \frac{1}{3}\left(\langle T\rangle-\langle S\rangle_{1}\right)^{-1} \vec{\nabla}+\left(\langle T\rangle-\langle S\rangle_{0}\right)\right]^{-1} P S_{0, l a g} \tag{6.38}
\end{equation*}
$$

that is a component of a block matrix operator:

$$
\mathcal{A}_{T G}=\left[\begin{array}{cc}
\hat{A}_{T G} & 0  \tag{6.39}\\
0 & 0
\end{array}\right]
$$

Then the update equations for the next scattering moments are:

$$
\begin{gather*}
\Phi_{0}^{(i+1)}=\Phi_{0}^{(i+1 / 2)}+\hat{A}_{T G}\left(\Phi_{0}^{(i+1 / 2)}-\Phi_{0}^{(i)}\right),  \tag{6.40}\\
\vec{J}^{(i+1)}=\vec{J}^{(i+1 / 2)}, \tag{6.41}
\end{gather*}
$$

We write this system in block matrix form:

$$
\begin{align*}
\Phi^{(i+1)} & =\left[\left[\mathcal{I}-\mathcal{A}_{c o n}\right]^{-1} \mathcal{A}_{\text {lag }}+\mathcal{A}_{T G}\left[\left[\mathcal{I}-\mathcal{A}_{c o n}\right]^{-1}\left[\mathcal{A}_{l a g}\right]-\mathcal{I}\right]\right] \Phi^{(i)}  \tag{6.42}\\
& +\left[\mathcal{I}+\mathcal{A}_{T G}\right]\left[I-\mathcal{A}_{c o n}\right]^{-1} \mathcal{Q}
\end{align*}
$$

This class of iteration schemes is equivalent to a Richardson iteration for an operator $\mathcal{A}_{\text {all }}$ such that:

$$
\begin{equation*}
\Phi^{(i+1)}=\left(\mathcal{I}-\mathcal{A}_{\text {all }}\right) \Phi^{(i)}+\tilde{\mathcal{Q}}, \tag{6.43}
\end{equation*}
$$

where:

$$
\begin{gather*}
\mathcal{A}_{\text {all }}=\mathcal{I}-\left[\left[\mathcal{I}-\mathcal{A}_{\text {con }}\right]^{-1} \mathcal{A}_{\text {lag }}+\mathcal{A}_{T G}\left[\left[I-\mathcal{A}_{\text {con }}\right]^{-1} \mathcal{A}_{\text {lag }}-\mathcal{I}\right]\right]  \tag{6.44}\\
\tilde{\mathcal{Q}}=\left[\mathcal{I}+\mathcal{A}_{T G}\right]\left[\mathcal{I}-\mathcal{A}_{c o n}\right]^{-1} \mathcal{Q} \tag{6.45}
\end{gather*}
$$

and eigenvalues of $\mathcal{I}-\mathcal{A}_{\text {all }}$ determine how quickly the Richardson iteration will converge.

### 6.4.2 Fourier Decomposition of Modes

To evaluate the spatial operators of the infinite system, we expand the solution error using the Fourier ansatz:

$$
\begin{equation*}
\delta\langle\Phi\rangle(\vec{r})^{(i)}=\iiint_{0}^{\infty} d^{3} \lambda \delta \Phi_{+} e^{2 \vec{\lambda} \cdot \vec{r}} . \tag{6.46}
\end{equation*}
$$

We use the linear independence of modes to define equations for one mode, and we can analytically determine the spatial dependence from that equation as a function of the error mode. We substitute this ansatz into the expression for $\mathcal{F}$ to determine inverse of the transport operator for a mode $\vec{\lambda}$ :

$$
\mathcal{F}=\left[\begin{array}{cc}
W_{0} L^{-1} & W_{0} L^{-1} \vec{\Omega}  \tag{6.47}\\
\vec{W}_{1} L^{-1} & \vec{W}_{1} L^{-1} \vec{\Omega}
\end{array}\right]=\frac{1}{4 \pi} \int_{4 \pi} d \Omega(\imath \vec{\lambda} \cdot \vec{\Omega}+T)^{-1}\left[\begin{array}{cccc}
1 & \Omega_{x} & \Omega_{y} & \Omega_{z} \\
\Omega_{x} & \Omega_{x} \Omega_{x} & \Omega_{x} \Omega_{y} & \Omega_{x} \Omega_{z} \\
\Omega_{y} & \Omega_{y} \Omega_{x} & \Omega_{y} \Omega_{y} & \Omega_{y} \Omega_{z} \\
\Omega_{z} & \Omega_{z} \Omega_{x} & \Omega_{z} \Omega_{y} & \Omega_{z} \Omega_{z}
\end{array}\right]
$$

Because this expression is rotationally symmetric, we choose to orient our $\vec{e}_{z}$ axis to coincide with the $\vec{\lambda}$ mode, and define a cosine in the direction of $\vec{\lambda}$ :

$$
\begin{equation*}
\Omega \cdot \vec{\lambda}=|\vec{\lambda}| \mu \tag{6.48}
\end{equation*}
$$

Then we may write the direction $\Omega$ as a function of $\mu$ and $\gamma$, the azimuthal angle about the $\vec{e}_{z}$ axis from the $\vec{e}_{x}$ axis:

$$
\begin{equation*}
\vec{\Omega}=\left[\left(1-\mu^{2}\right)^{1 / 2} \cos (\gamma) \vec{e}_{x}+\left(1-\mu^{2}\right)^{1 / 2} \sin (\gamma) \vec{e}_{y}+\mu \vec{e}_{z}\right] . \tag{6.49}
\end{equation*}
$$

We manipulate the inverse of the operator in $\mathcal{F}$ :

$$
\begin{equation*}
(\imath \vec{\lambda} \cdot \vec{\Omega}+T)^{-1} \equiv(\imath \vec{\lambda} \cdot \vec{\Omega}+T)^{-1}(-\imath \vec{\lambda} \cdot \vec{\Omega}+T)^{-1}(-\imath \vec{\lambda} \cdot \vec{\Omega}+T) \tag{6.50}
\end{equation*}
$$

and because these are all diagonal matrices:

$$
\begin{equation*}
(\imath \vec{\lambda} \cdot \vec{\Omega}+T)^{-1} \equiv\left((\vec{\lambda} \cdot \vec{\Omega})^{2}+T^{2}\right)^{-1}(-\imath \vec{\lambda} \cdot \vec{\Omega}+T) \tag{6.51}
\end{equation*}
$$

Writing the integral in this form lets us immediately determine which functions are odd functions of $\mu$, and are thus zero. Similarly, all terms that are linear in $\cos (\gamma)$ or $\sin (\gamma)$ or both are zero. What remains are the $1 * 1, \Omega_{x}^{2}, \Omega_{y}^{2}, \Omega_{z}^{2}, 1 * \Omega_{z}$, and $\Omega_{z} * 1$ terms. We evaluate these non-zero integrals for illustration:

$$
\begin{gather*}
\mathcal{F}_{11}=\frac{1}{4 \pi} \int_{4 \pi} d \Omega\left(|\vec{\lambda}|^{2} \mu^{2}+T^{2}\right)^{-1}(-\imath|\vec{\lambda}| \mu+T)=\frac{\arctan \left(T^{-1}|\vec{\lambda}|\right)}{|\vec{\lambda}|}  \tag{6.52}\\
\mathcal{F}_{\Omega_{z} \Omega_{z}}=\frac{1}{4 \pi} \int_{4 \pi} d \Omega\left(\mu^{2}\right)\left(|\vec{\lambda}|^{2} \mu^{2}+T^{2}\right)^{-1}(-\imath|\vec{\lambda}| \mu+T)  \tag{6.53}\\
=-\frac{T \cdot\left(T \arctan \left(T^{-1}|\lambda|\right)-|\lambda|\right)}{|\lambda|^{3}} \\
\mathcal{F}_{\Omega_{x} \Omega_{x}}=\mathcal{F}_{\Omega_{y} \Omega_{y}}=\frac{1}{4 \pi} \int_{4 \pi} d \Omega\left(1-\mu^{2}\right) \cos ^{2}(\gamma)\left(|\vec{\lambda}|^{2} \mu^{2}+T^{2}\right)^{-1}(-\imath|\vec{\lambda}| \mu+T)  \tag{6.54}\\
=\frac{1}{2} \mathcal{F}_{11}-\frac{1}{2} \mathcal{F}_{\Omega_{z} \Omega_{z}} \\
\mathcal{F}_{1 * \Omega_{z}}=\mathcal{F}_{\Omega_{z} * 1}=\frac{1}{4 \pi} \int_{4 \pi} d \Omega \mu\left(|\vec{\lambda}|^{2} \mu^{2}+T^{2}\right)^{-1}(-\imath|\vec{\lambda}| \mu+T)  \tag{6.55}\\
=-\imath|\vec{\lambda}| \mathcal{F}_{\Omega_{z} \Omega_{z}}
\end{gather*}
$$

Next we determine the spatial dependence of the two-grid operator for the same Fourier mode:

$$
\begin{equation*}
\hat{A}_{T G}=\xi\left[|\vec{\lambda}|^{2} \frac{1}{3}\left(\langle T\rangle-\langle S\rangle_{1}\right)^{-1}+\left(\langle T\rangle-\langle S\rangle_{0}\right)\right]^{-1} P S_{0, l a g} \tag{6.56}
\end{equation*}
$$

Using these expressions, we determine the eigenvalues of the operator given by Eq. (6.44) in subsection 6.4.4.

### 6.4.3 Maxwell-Boltzmann Group Structure

In the analysis that follows, we choose an energy discretization such that the population in a Maxwell-Boltzmann distribution would have a constant value by setting each energy group range to have an equal amount of neutron flux. A Maxwell-Boltzmann population distribution is given by:

$$
\begin{equation*}
N_{M}(E)=N_{0} \frac{2 \pi}{(\pi k T)^{3 / 2}} \sqrt{E} e^{-E / k T} . \tag{6.57}
\end{equation*}
$$

The non-relativistic velocity can be determined as a function of energy:

$$
\begin{equation*}
v=\sqrt{E} \sqrt{\frac{2}{m}} \tag{6.58}
\end{equation*}
$$

From the population defined above, the Maxwell-Boltzmann scalar flux distribution is given by the following equation:

$$
\begin{equation*}
\phi_{M}(E)=v N_{M}(E)=N_{0} \sqrt{\frac{2}{m}} \frac{2 \pi}{(\pi k T)^{3 / 2}} E e^{-E / k T} \tag{6.59}
\end{equation*}
$$

If we normalize the spectrum to one, the constants will cancel resulting in:

$$
\begin{equation*}
\tilde{\phi}_{M}(E)=E e^{-E / k T}, \tag{6.60}
\end{equation*}
$$

The integral of this equation over an energy range:

$$
\begin{align*}
\int_{E_{1}}^{E_{2}} d E E e^{-E / k T} & =\left[-E k T e^{-E / k T}\right]_{E_{1}}^{E_{2}}-\int_{E_{1}}^{E_{2}} d E-k T e^{-E / k T} \\
& =\left[-E k T e^{-E / k T}\right]_{E_{1}}^{E_{2}}-\left[k^{2} T^{2} e^{-E / k T}\right]_{E_{1}}^{E_{2}} \\
& =\left[-E_{2} k T e^{-E_{2} / k T}\right]-\left[-E_{1} k T e^{-E_{1} / k T}\right]-\left[k^{2} T^{2} e^{-E_{2} / k T}\right]+\left[k^{2} T^{2} e^{-E_{1} / k T}\right] \\
& =-E_{2} k T e^{-E_{2} / k T}+E_{1} k T e^{-E_{1} / k T}-k^{2} T^{2} e^{-E_{2} / k T}+k^{2} T^{2} e^{-E_{1} / k T} \\
& =k T\left(E_{1} e^{-E_{1} / k T}-E_{2} e^{-E_{2} / k T}\right)+k^{2} T^{2}\left(e^{-E_{1} / k T}-e^{-E_{2} / k T}\right) \tag{6.61}
\end{align*}
$$

The normalized flux in a group range is then given by:

$$
\begin{equation*}
\tilde{\phi}_{M}\left(E_{1}, E_{2}\right)=\left(k T E_{1}+k^{2} T^{2}\right) e^{-E_{1} / k T}-\left(k T E_{2}+k^{2} T^{2}\right) e^{-E_{2} / k T} \tag{6.62}
\end{equation*}
$$

The integral over all energies is given by:

$$
\begin{equation*}
\tilde{\phi}_{M, t o t}=\frac{\phi_{M}\left(E_{\min }, E_{\max }\right)}{C}=\left(k T E_{\min }+k^{2} T^{2}\right) e^{-E_{\min } / k T}-\left(k T E_{\max }+k^{2} T^{2}\right) e^{-E_{\max } / k T} \tag{6.63}
\end{equation*}
$$

Our goal is to obtain energy group ranges such that the particle flux is equal in each energy group:

$$
\begin{equation*}
\phi_{P G}=\frac{\phi_{M, t o t}}{G} \tag{6.64}
\end{equation*}
$$

where $G$ is the number of groups. With the flux per group defined, and the initial energy is known, we solve for $E_{2}$ :

$$
\begin{equation*}
\left(k T E_{2}+k^{2} T^{2}\right) e^{-E_{2} / k T}=\left(k T E_{1}+k^{2} T^{2}\right) e^{-E_{1} / k T}-\phi_{P G} \tag{6.65}
\end{equation*}
$$

This involves evaluation of a Lambert W function of $0^{\text {th }}$ kind, or numerical solution to obtain


Figure 6.1: Spectral Radii for Graphite at 296 K
$E_{2}$. Once obtained, the process is then repeated until all $G$ group boundaries are determined.
Using the group structure devised here gives an equal amount of neutron flux per energy group. This group structure is useful for checking analysis, which should obtain a flat spectrum for the eigenvector of the largest eigenvalue and the two-grid quantity $\xi_{g}$, and numerical tests by giving equal compute time to equal amounts of residual reduction.

### 6.4.4 Fourier Analysis of Infinite Homogeneous Graphite

We analyze the Jacobi and Gauss-Seidel operators with Isotropic and Linearly-Anisotropic scattering for graphite at 296 K using a 160 group multi-group cross section set that used the energy group structure described in the previous section. We have confirmed the largest eigenvalue occurs for all unaccelerated operators for the $|\lambda|=0$ mode, as shown in Fig. (6.1), and the spectral radii do not change significantly when including linearly anisotropic scattering.

We plot the energy eigenvalues of the mode that had the largest eigenvalue in Fig. (6.2). We see that the largest Jacobi eigenvalue is suppressed for isotropic and anisotropic scattering, but there are many more large eigenvalues which do not decrease significantly.

We plot the eigenvector associated with the largest eigenvalue of the slowest converging mode


Figure 6.2: Eigenvalues of the slowest converging mode for Graphite at 296 K
(maximum eigenvalue) in Fig. (6.3), to see the energy shape of the largest eigenvalue mode.
The largest eigenvalue's eigenvectors of the unaccelerated operators are "flat," which is a result of the Maxwell-Boltzmann energy group structure described above. We see the largest eigenvalue's eigenvector of the accelerated operators are no longer flat in energy, and the Gauss-Seidel and Jacobi operators have a different energy shape for the slowest converging mode. Additionally, the eigenvectors are zero in the linearly anisotropic region, indicating the slowest converging eigenvectors have no terms from linearly anisotropic scattering.

For the Jacobi operator with TG acceleration, although the slowest converging mode is eliminated, there are many eigenvalues that remain with large magnitude. However, our intuition of the eigenvalue distribution is that a Krylov method could solve the Jacobi+TG system effectively. Additionally, the Jacobi spectral radius could be reduced by accelerating the within-group scattering. Such a method was devised by Hanuš and Ragusa, which combines Jacobi splitting with within-group DSA and TG acceleration.

We now test the J1+wgDSA+TG method using the CDFEM operator we have devised and compare to the MIP operator that has previously been tested.


Figure 6.3: Flat-mode eigenvectors of the largest eigenvalue for Graphite at 296 K. The first 160 points correspond to $\Phi_{0}$, then remaining 160 points are for $J_{x}, J_{y}$, and $J_{z}$.

### 6.5 Numerical Results

### 6.5.1 2D Homogeneous Graphite Upscattering

Our first problem is a $20[\mathrm{~cm}] \times 20[\mathrm{~cm}]$ homogeneous graphite block that is discretized into 12 x 12 spatial cells. We use a 168 group multi-group cross section set generated with NJOY as part of a Predictive Science Academic Alliance Program (PSAAP) project at the Center for Exascale Radiation Transport (CERT) at Texas A\&M University. This cross section set has 63 groups in the fast energies, and 105 groups in the thermal energy range. We employ the $\mathrm{J} 1+\mathrm{wgDSA}+\mathrm{TG}$ method from Hanuš and Ragusa. For this method, every outer within-group-set (WGS) iteration performs 1 transport sweep and 106 diffusion solves (105 Thermal Group solves +1 TG solve). We note that the cost of the transport sweep is low compared to the cost of one diffusion solution because we chose $S_{4}$ quadrature, or 24 discrete angles.

We utilize this problem to compare effects of consistency of the CFEM solution that is part of the CDFEM low-order operator and the relative effectiveness of the CDFEM operator to MIP and unaccelerated iteration.

In Table 6.1, Rich.A solves the problem with unaccelerated Richardson iteration that per-
formed 1 transport sweep per Jacobi iteration, $P_{M I P} A$ uses the $\mathrm{J} 1+\mathrm{wgDSA}+\mathrm{TG}$ with Richardson iteration and the MIP operator, $P_{P_{1} C D F E M}$ uses the $\mathrm{J} 1+\mathrm{wgDSA}+\mathrm{TG}$ method with Richardson iteration and a CDFEM operator that uses a $P_{1}$ diffusion discretization for the global CFEM solution, and $P_{\text {StiffnessCDFEM }}$ uses the $\mathrm{J} 1+\mathrm{wgDSA}+\mathrm{TG}$ method with Richardson iteration and a CDFEM operator that uses a diffusion discretization that has a Laplacian resulting in a standard stiffness matrix for the global CFEM solution.

Table 6.1: Results from 2D Homogeneous Graphite

|  | Rich.A | $P_{M I P} A$ | $P_{P_{1} C D F E M} A$ | $P_{\text {StiffnessCDFEM }} A$ |
| :---: | :---: | :---: | :---: | :---: |
| Outer It. | 200 | 66 | 60 | 61 |
| Total Diff. It. | - | 24302 | 23173 | 23010 |
| Sweep Time [s] | 7.8 | 3.77 | 3.68 | 3.59 |
| Transport Source Calc. [s] | 24.1 | 10.1 | 9.71 | 9.52 |
| Diffusion Time [s] | - | 22 | 15.2 | 15.7 |
| Total Time [s] | 31.9 | 35.87 | 28.59 | 28.81 |

Because of the relatively low cost of transport sweeps, the largest component of unaccelerated iteration was from calculation of the scattering source, which is a cost of each outer iteration that should not be ignored. Unaccelerated Richardson iteration is a poor choice for this problem, and thus the iteration took significantly more iterations than the accelerated methods. The MIP operator is more expensive to solve, and thus took more total time than either CDFEM choice. The mesh had cells with aspect ratio of 1 , and thus the efficiency of the CDFEM operator was not degraded.

The inconsistent CFEM discretization only required one additional outer iteration, as the addition of the Discontinuous update still provided effective acceleration. The "stiffness" diffusion discretization can be a viable candidate if a code does not have $P_{1}$ diffusion discretization available. We note that it is possible to obtain the $P_{1}$ CFEM diffusion from the discontinuous update equations.


Figure 6.4: PSAAP Level 2 Problem

### 6.5.2 PSAAP Level 2 Detector-Column

The objective of this problem was to compare the CDFEM operator to the MIP operator on a real world simulation that includes complex geometry and high-aspect ratio meshes. We simulate a problem, designated as "Level 2," that was part of the PSAAP project performed by CERT at Texas A\&M. The Level 2 problem models a large block of graphite, a detector above, a source in a perpendicular direction as seen in Figure 6.4a. We modify the Level 2 by simulating only the prismatic column of meshes that includes the detector, shown by Figure 6.4b.

This problem was composed of 105 thermal groups, 128 directions, 30576 spatial cells. This problem was solved using a single core on the LLNL Quartz supercomputer, which is composed of Intel Xeon E5-2695 CPU cores. We solved this problem using the "best" algorithm from Hanuš and Ragusa, $\mathrm{J} 1+\mathrm{wgDSA}+\mathrm{TG}$. Convergence criteria and iteration settings were set to match those for the "Real World" problem in Hanuš and Ragusa's paper.[59]

To make a direct comparison, we find the time per work unit for sweeps, $U_{\text {sweep }}$, as follows:

$$
\begin{equation*}
U_{\text {sweep }}=t_{\text {sweep }} * N_{\text {processes }} / N_{\text {sweeps }} / N_{\text {groups }} / N_{\text {cells }} / N_{\text {directions }} \tag{6.66}
\end{equation*}
$$

And similarly, we find the time per work unit for diffusion, $U_{\text {diffusion }}$, as follows:

$$
\begin{equation*}
U_{\text {diffusion }}=t_{\text {diffusion }} * N_{\text {processes }} / N_{\text {sweeps }} / N_{\text {groups }} / N_{\text {cells }} \tag{6.67}
\end{equation*}
$$

A summary of iteration statistics and comparison to reference values can be found in Table 6.2.

Table 6.2: Results from 3D Level 2 full problem (Reference results) and detector-column problem (other results)

|  | $\operatorname{GMRES}(A)$ | $P_{\text {MIP }} A$ | $P_{\text {CDFEM }} A$ | Reference $P_{\text {MIP }} A$ |
| :---: | :---: | :---: | :---: | :---: |
| Outer It. | 94 | 20 | 27 | 51 |
| Total Diff. It. | - | 7590 | 14227 | 1345 |
| Sweep Time [s] | 38400 | 8930 | 12000 | 10089 |
| Transport Source Calc. [s] | 9930 | 2830 | 3500 | - |
| Diffusion Time [s] | - | 15600 | 5650 | 1253 |
| Total Time [s] | 48330 | 27360 | 21150 | 11425 |
| $U_{\text {sweep }}[\mathrm{s} / \mathrm{wu}]$ | $9.94 \mathrm{E}-7$ | $1.09 \mathrm{E}-6$ | $1.08 \mathrm{E}-6$ | $1.23 \mathrm{E}-6$ |
| $U_{\text {diffusion }}[\mathrm{s} / \mathrm{wu}]$ | - | $2.53 \mathrm{E}-4$ | $7.37 \mathrm{E}-5$ | $5.86 \mathrm{E}-4$ |

The solution times per work unit for our MIP execution was comparable to the reference MIP values. The slightly higher values of the reference times per work unit are primarily because the reference problem, which includes a larger volume of graphite and additional geometry of the surrounding room, is more difficult to solve. The reference problem was run on 3528 cores with 1 process each and may have had reduced parallel efficiency, particularly in the diffusion solution using HYPRE.

The solution using CDFEM has a factor of 3 less diffusion time per work unit. Even though the solution required significantly more iterations to converge each diffusion problem, the overall time was reduced compared to the similar MIP problem. Because the global CFEM operator has
approximately 8 times fewer degrees of freedom in 3D geometry, solution of that system has a significantly reduced cost. We find the acceleration efficiency of the CDFEM operator was not significantly reduced due to high aspect-ratio meshes, since the problem was solved in 27 thermal iterations compared to 20 using the MIP operator.

### 6.5.3 Summary

We studied linearly anisotropic neutron scattering for Gauss-Seidel and Jacobi iteration with TG acceleration. We studied infinite medium graphite problems to determine if it is necessary to accelerate linear moments of neutron flux distribution. After including linearly isotropic scattering, the spectral radius did not increase and the largest error mode remained unchanged. The eigenvectors of these largest error modes had near zero coefficients for the linearly anisotropic terms. Thus we conclude it is sufficient to accelerate only the scalar moment for problems where graphite is the primary source of difficulty when converging neutron scattering problems.

We tested the J1+wgDSA+TG method developed by Hanuš and Ragusa using the CDFEM operator instead of MIP. While using the CDFEM operator increased the number of transport sweeps, caused by degradation of acceleration in the high-aspect ratio mesh of the CERT Level 2 detector problem, the reduced degrees of freedom in the CDFEM operator result in greatly reduced diffusion time, and thus the overall solution time was reduced.

## 7. CONCLUSIONS

We have studied the three kinds of problems that have transport-driven physics: 1) $k$-eigenvalue calculation using power iteration, 2) thermal radiative transport, and 3) thermal upscattering of neutrons. Instead of accelerating the within-group scattering problems using a low-order operator, the methods we study accelerate the outermost iteration, effectively reducing the total number of high-order sweeps to converge the problem. We have devised a novel method for thermal radiative transfer that uses a linear equation for a correction, created a theoretical foundation for $k$-eigenvalue problems that use a linear equation for a correction, and tested thermal neutron upscattering iteration using the CDFEM operator we have devised.

## $7.1 k$-Eigenvalue

The use of diffusion operators as preconditioners of transport operators for scattering iterations has been widespread. We have studied the use of diffusion operators to accelerate the convergence of eigenvalue iterations. Currently the most widely used methods to accelerate eigenvalue iterations employ nonlinear functionals in the low-order operators and solve low-order problems that are themselves standard eigenvalue problems.

We have explored a family of methods, developed by Adams in 1986 and independently by Suslov in 2003, that employs a low-order eigenvalue-like problem with a fixed source to obtain an updated eigenvalue estimate and an additive correction to the eigenfunction. This method uses linear functionals and operators that were developed for scattering iterations, and has demonstrated convergence rates similar to methods with nonlinear functionals.

We have addressed several theoretical concerns regarding the multiple possible solutions that could be admitted by the eigenvalue-like problem that results from this family of methods. We have shown that the low-order linear diffusion problem becomes algebraically equivalent to the QuasiDiffusion low-order problem when the solution is close to the converged solution. Through a Fourier analysis in an infinite homogeneous medium, we have shown the iteration rapidly con-
verges to the correct eigenvalue and eigenvector and not an arbitrary solution. We have shown that for one-cell homogeneous problems the iteration procedure is convergent and converges to the correct eigenvalue if the high-order and low-order operators satisfy a mild consistency requirement, namely, that they produce eigenvalues that are within a factor of two of each other.

Finally, we add to the body of evidence that these methods work well for reactor problems, in particular in combination with the Continuous / Discontinuous finite-element diffusion operator we have developed. We have demonstrated that the method provides convergence of $k$ problems to $1 E-5$ with $\approx 15$ transport sweeps for the well-known C5G7 benchmarks in 2D and 3D, and also for a similar problem with more spatial detail and with 191 energy unknowns.

We find the family of linear eigenvalue-like methods to be robust, rapidly convergent, and easy to implement. We emphasize that if a transport code already uses a diffusion operator (or other low-order operator) as a preconditioner to accelerate convergence of scattering iterations, it is straightforward to apply the same operator to eigenvalue acceleration, using the equations described herein, without the need to develop nonlinear functionals.

### 7.2 Thermal Radiative Transfer

We have developed, analyzed, implemented, and tested iterative methods for radiative transfer iterations, in each case building on a low-order diffusion operator that we previously developed for accelerating the pseudo-scattering iteration of thermal radiative transfer. Introducing a Newton-like iteration with this low-order operator, similar to the low-order iteration used by quasi-diffusion and the local temperature iteration used by Nowak, we have obtained a linear acceleration method that uses a gray diffusion equation coupled to the matter energy equation to update both temperature and absorption-rate density.

The linear acceleration method is especially effective when the problem is highly diffusive, and when iteration error is dominated by error in the temperature field. For problems that are limited by pointwise ARD convergence, the nonlinear acceleration method quickly resolves the temperature field, and effectively becomes Richardson iteration with a grey DSA preconditioner for pseudo-scattering. For all problems studied, the linear acceleration method provides a factor of

2 improvement in solution time compared to the linear within-group preconditioning method.

### 7.3 Thermal Neutron Upscattering

We have studied linearly anisotropic neutron scattering for Gauss-Seidel and Jacobi iteration. We studied infinite medium graphite problems to determine if it is necessary to accelerate moments of neutron flux distribution other than the scalar flux. We found that the addition of linearly anisotropic scattering did not increase the spectral radius even when only the scalar flux is updated by the one-group soution. The eigenvectors of the dominant error modes had near zero coefficients for the linearly anisotropic terms. Thus we conclude it is sufficient to accelerate only the scalar moment for problems where graphite is the primary source of difficulty when converging neutron scattering problems.

We have tested the $\mathrm{J} 1+\mathrm{wgDSA}+\mathrm{TG}$ method developed by Hanuš and Ragusa using the CDFEM operator on several highly scattering problems of interest: a finite medium homogeneous graphite problem, and the PSAAP Level 2 problem developed at the CERT. While using the CDFEM operator increased the number of transport sweeps, caused by degradation of acceleration from the high-aspect ratio mesh of the Level 2 problem, the reduced degrees of freedom in the CDFEM operator result in reduced diffusion and overall solution times.

### 7.4 Future Work

A list of suggested topics for further study follows.

- Analyze $k$-Eigenvalue algorithm for non-infinite problems where low- and high-order operators are not equivalent for the fundamental mode.
- Test the $k$-eigenvalue method with more reactor designs.
- Analyze a one cell problem for thermal radiative transfer to study consistency limitations of the low-order Newton-like iteration and linear update.
- Determine if the linear HOLO methods can be derived from a linearization of QuasiDiffusion.
- Attempt to reduce degradation of CDFEM operator in high-aspect ratio geometries by improving the approximations made to the corrections for the current on interior boundaries.


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