

ACCELERATION OF PARTICLE TRANSPORT ITERATIONS WITH ‘CONSISTENT’ EDDINGTON FACTORS

Dissertation

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Abstract

In the field of computational particle transport, iterative acceleration methods are of great importance in improving convergence speed and computational performance. Acceleration methods are key to current nuclear reactor analysis, reducing the computational cost of reactor core simulations. Acceleration methods usually employ a “high-order/low-order” approach to iteratively solve the transport equation. However, current state-of-the-art techniques (such as the Coarse Mesh Finite Difference (CMFD) method) have operational limitations (such as limits on the size of the spatial grid discretization) that can lead to reduced performance or numerical instability. Another standard high-order/low-order method is the Quasidiffusion (QD) method. This method, which uses Eddington factors to correct the low-order diffusion equation, does not have such operational constraints. However, the QD method has the disadvantage of providing an approximate solution of the discrete ordinates (S_N) equations.

In this dissertation, we present a new advantageous iterative acceleration algorithm for neutron transport that reformulates and improves upon the QD method. This new method is called the *Generalized Quasidiffusion* (GQD) method. The general idea of the GQD method is to modify the Eddington factors to (i) make the accelerated solution equal to the solution of the S_N equations, and (ii) to preserve the numerical stability and speed displayed by the classical QD method. The new *consistent Eddington factors* are formulated by preserving the net neutron leakage out of each spatial cell, between the high-order and low-order

systems of equations. The new factors are calculated by solving an extra diffusion problem as an intermediate step between the high-order and low-order systems.

We present numerical GQD results for a series of fixed-source, planar-geometry, monoenergetic, and isotropically-scattering neutron transport problems. Our results confirm that the GQD method provides a solution that is equal to the S_N solution. The convergence rate and stability of the GQD method were evaluated in a series of different test problems, all of which displayed remarkable stability and convergence speed. A Fourier stability analysis was also conducted, providing theoretical validation for the numerical results. However, in some problems, the stability of the GQD method displayed sensitivity to the procedure used to obtain the consistent Eddington factors. A suggested procedure was introduced, which eliminated this issue for the presented case studies.

This dissertation sets the groundwork for the new, consistent, unconditionally stable, and rapidly-converging GQD acceleration method for neutron transport calculations. It provides a straightforward formulation that can be extended to higher dimensions and can be implemented in current core simulation software. It also allows for straightforward implementation in existing QD codes.

This work is dedicated to my parents, Simone and Alvaro, who always believed and supported me.

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List of Symbols

∇		Del operator
x, y, z		Cartesian coordinates
$\mathbf{r}$		Position vector
V		Volume
θ		Polar angle
ω		Azimuthal angle
Ω		Direction of flight vector
μ		Direction cosine
t		Time
E		Neutron energy
v		Neutron speed
Σ_f		Macroscopic fission cross-section
Σ_a		Macroscopic absorption cross-section
Σ_s		Macroscopic scattering cross-section
Σ_t		Macroscopic total cross-section
Σ_{tr}		Macroscopic transport cross-section
λ_{tr}		Transport mean free path
c		Scattering ratio
χ		Neutron fission spectrum distribution

Q		Isotropic internal source
n_d		Neutron angular density
ψ		Neutron angular flux
ϕ_0		Neutron scalar flux
ϕ_1		Neutron current
ϕ_2		Second angular moment of ψ
Φ_0		Low-order scalar flux
Φ_1		Low-order current
D		Diffusion coefficient
D^*		Modified diffusion coefficient
d		Diffusion extrapolated distance
g		Energy group index
G		Total number of energy groups
n		Discrete ordinate index
N		Total number of discrete ordinates
w_n		Quadrature weights
α_n		Angular weights
h		Discrete cell length
τ		Optical thickness
j		Discrete spatial cell index
J		Total number of discrete spatial cells
E_j		Cell-averaged Eddington factor
$\mathcal{E}_j$		Cell-averaged consistent Eddington factor
$\mathcal{J}$		Partial current

ℓ		Iteration step
ρ		Spectral radius
θ_f		Scaled Fourier parameter
ε		Convergence criterion
R		Diagonal dominance ratio

Chapter 1: Introduction

1.1 Motivation

The power produced by a nuclear reactor is determined by the neutron flux in the reactor's core. Calculating the neutron flux is essential to properly design the reactor and predict its behavior. The neutron flux is obtained as the solution of the neutron transport equation. Therefore, solving the neutron transport equation accurately and efficiently has been the objective of many research and engineering groups in the field of reactor physics [1–4]. The goal has been to develop computational methods and codes to minimize the time for the accurate simulation and modeling of the neutron flux in nuclear reactors. This enables faster and more precise simulations for both the current reactor fleet and future advanced designs [5].

The *neutron transport equation* is formally known as the *Linear Boltzmann equation* [6–12]. The equation has seven independent variables: three spatial, two angular, time, and energy. Although the equation is basically linear, nonlinearities can arise from the fact that properties of the materials, such as the cross-sections, can be temperature-dependent (while the temperature depends on the neutron flux).

The complexities due to the number of variables and possible nonlinearities provided by material properties can make it very difficult to solve the Boltzmann equation for sufficiently

large or complex problems. Other difficulties arise from the fact that the behavior of the transport equation can change from hyperbolic (in void-like regions) to elliptic (in steady-state problems) or parabolic (in time-dependent problems), depending on the nature of the physical problem [13]. This causes difficulties in choosing discretization methods that are sufficiently accurate for this wide range of operations [14].

Deterministic and *Stochastic* methods have been developed to computationally solve the transport equation. Probabilistic, or stochastic (Monte Carlo) methods are well known in the field (e.g. MCNP and SERPENT [2, 3]). In these methods, the behavior of the neutron flux is estimated by the sum of the behaviors of individual samplings in large-scale (usually millions of runs of random single-particle) simulations. Deterministic methods, on the other hand, solve an algebraic system of linear equations based on a discretization of the Linear Boltzmann equation (e.g. Spherical Harmonics (PN), Method of Characteristics (MOC), and Discrete Ordinates (S_N)) [10]. The work in this dissertation focuses on the widely-used discrete ordinates approximation and the associated methods that have been developed to solve the resulting equations iteratively. Our work also uses the Step Characteristic (SC) and multigroup (with the number of groups equal to one) approximations for spatial and energy discretization, respectively. In addition, we ignore the temperature-dependence of the cross sections. (This makes the neutron transport problems linear – although, we shall see that nonlinear iterative methods are often used to solve them.)

The *Discrete Ordinates* method simplifies the Linear Boltzmann equation by approximating the full range of direction-of-flight of neutrons into discrete angles [6, 10, 14, 15]. The *Step Characteristic* approximation, on the other hand, introduces a spatial correlation between cell-edge angular fluxes and the cell-centered angular flux. Finally, the *multigroup* approximation divides the energy spectrum into a finite number of *energy groups*, in which

the material coefficients (the cross sections) are defined as constants within each group [6, 10].

The aforementioned approximations allow the discretization of the continuous variables. More refined discretizations (e.g. more angles or energy groups) lead to greater precision, but also to more computationally expensive calculations. One can solve the resulting system of linear equations directly, but because of the typically large size of the system, this is typically very slow and costly.

Therefore, *iterative methods* have been formulated to speed up the calculations. These methods focus on achieving an approximate solution of the approximate discrete system, instead of an exact solution of the discrete system provided (in principle) by direct methods. Iterative methods provide an approximate solution significantly faster, since the number of operations to solve directly a linear system of size n are in the order of n^3 FLOPs (floating-point-operations), while iterative methods usually require a lower order of n^2 FLOPs or less [16].

In the field of neutron transport, the *Source Iteration* (SI) method is the most basic iterative method that is used to solve the discrete ordinates equations [14]. The SI method calculates the neutron flux recursively, using the generation terms (internal source and scattered neutrons) calculated from the previous recursion as a source in the subsequent iteration step. This method provides faster results compared to direct solvers, but its performance degrades significantly as the problem becomes increasingly “diffusive.” (The higher the *scattering ratio* – the ratio between scattering and total cross-sections – and the greater the optical thickness of the system, the more “diffusive” a system becomes, and the more iterations are required for the algorithm to converge.) The scattering ratio is the probability that a neutron will scatter (and therefore not be captured) upon collision. The

higher its value, the greater the probability that neutrons will experience increased numbers of collisions before being captured or leaking out of the system, thereby increasing the problem's computation time.

The dependency of the code's efficiency on the scattering ratio of the problem limits its performance and has motivated the development of newer and faster iterative methods. These newer methods, called *acceleration methods*, have faster convergence for a wide range of problems. Acceleration methods improve the convergence rate of the linear system provided by the S_N equations, increasing stability and convergence speed. In numerical methods, the convergence rate is measured by the *spectral radius* (maximum eigenvalue) of the iterative matrix operator. Reducing the spectral radius improves numerical stability and gives faster convergence.

Nonetheless, the gain in performance from acceleration methods is not “free”. These methods require more calculations per iteration than the simple S_N method. Therefore, introducing acceleration methods increases the overall computational expense per iteration. This increase per iteration is often justified by the drastic reduction of the number of iterations required for the acceleration methods to converge. A successful acceleration method would outweigh this cost per iteration by reducing the number of required iterations by many orders of magnitude. However, this does not always happen. Most acceleration methods have operational restrictions that reduce their performance and cause numerical instability as the spatial cells become more optically thick [14, 17].

1.2 Transport Acceleration – Background

Several acceleration methods have been developed during the last decades; a comprehensive review of these methods up to 2002 can be found in [14]. Some of the first practical

iterative acceleration schemes were the *Chebyshev acceleration* and the *Fine/Coarse-Mesh Rebalance* methods [14]. The Chebyshev method improved S_n calculations but still struggled with highly scattering media [18]. The Rebalance method allowed somewhat faster performance for more highly-scattering problems, but the choice of coarse mesh and cell optical thickness could cause the method to diverge [17, 19]. Other methods were developed that applied matrix preconditioning for the iterative scheme, called *preconditioning methods* (e.g. KP method). These methods worked by applying a preconditioner to the iterative transport operator, reducing its conditioning number and improving convergence speed [20].

Similar methods, called synthetic methods, were also developed, most notably the *Diffusion Synthetic Acceleration (DSA)*, which has been widely used in the transport community. The DSA method accelerates the transport iterative algorithms by solving a multi-level problem (high/low-order). The *high-order* system consists of the transport equation, and the *low-order* system is a diffusion-like problem for an additive correction term to the scalar flux [14, 21–25]. The "*synthetic*" aspect of DSA comes from the fact that the low-order system solves for a correction term, not the proper scalar flux. The DSA method displayed greater efficiency for highly-scattering problems, being a standard method for many years. However, this method is linear and cannot be directly used to solve eigenvalue problems [14].

The Nonlinear acceleration (NDA) method, introduced by Alcouffe [26], allowed easier eigenvalue calculations. The method consists of solving a high-order system (the transport equation) and a lower-order system (diffusion equation) iteratively for the neutron flux. The systems of high/low order equations are coupled by a correction term applied to either (i) the diffusion coefficient, (ii) the removal cross-section, or (iii) the source of the diffusion equation. This method is distinguished from previous synthetic acceleration methods (e.g.

DSA) by solving for the neutron flux in both the high- and low-order equations, instead of solving for a correction term in the low-order system [14].

A more general approach to NDA methods using coarse meshes in the lower-order system was introduced as the *Coarse Mesh Finite Difference* (CMFD) method [27–30]. This method increased the computational speed per iteration by employing a coarser spatial grid in the low-order system. Nonetheless, the CMFD solutions obtained by the high- and low-order systems are consistent with each other, converging to the actual solution of the Discrete Ordinates equations.

In the scope of this dissertation, we make the simplifying assumption that all high-order systems and low-order systems have the same spatial grid. Therefore, in this document, NDA and CMFD become the same method and therefore will be addressed as CMFD for simplicity.

All these methods (DSA, NDA, and CMFD) show high performance for highly-scattering media with optically thin spatial grids, improving significantly the performance of many S_N calculations. However, they have the same vulnerability to the optical thickness of the spatial grid [31–33], becoming progressively less efficient and eventually unstable as the optical widths of the spatial cells increase. Another issue is the dependence of stability on the discretization of the low-order system, i.e. it is difficult to define a preconditioner that works effectively for a wide range of problems [14]. In order to improve CMFD’s stability, newer methods – based on CMFD – were created.

The partial current-based CMFD method, called pCMFD [34–36] was developed using the partial currents for determining the correction term. This method proved to be stable for a wide range of problems with optically thicker cells. An “optimally diffusive” CMFD method (odCMFD) was introduced in [37, 38], which generalizes CMFD and pCMFD

by adding an artificial term to the diffusion coefficient. This method presented better performance (compared to both CMFD and pCMFD) for spatial cells of intermediate optical thickness, where the CMFD spectral radius tends to increase significantly. This method also is unconditionally stable in certain proposed problems [37], despite the loss of efficiency for thicker cells.

Recent work also proposed a two-level pCMFD [39–41] and a linear prolongation based CMFD (lpCMFD) [42–45] that have presented greater stability properties for a wide range of problems. A brief overview of CMFD methods can be found in [46, 47]. Other work also presented relaxation methods, in addition to CMFD variations to increase the performance of the aforementioned methods [48, 49].

A second type of acceleration method, called the *Quasidiffusion* (QD) or *Variable Eddington Factor* (VEF) method, was introduced by Gol'din in 1964 for efficiently solving the linear Boltzmann equation [50]. Further studies were conducted, expanding this line of research over the next decades, applying the method to general boundary conditions, 2-D, multigroup theory, and nonsymmetric QD diffusion equations [51–53]. Later, the QD method was also applied to strongly anisotropic scattering problems [54].

The QD method, similarly to NDA and CMFD, is a nonlinear method that solves iteratively a coupled system of the (high-order) transport equation and the (low-order) *Quasidiffusion* equation. The term *quasi-* in the QD method arises from the fact that, instead of having the regular diffusion coefficient in the classic diffusion equation, QD uses *Eddington Factors*. The lack of the consistency term (used in NDA and CMFD) causes the converged QD solution of the low-order system to not match with the converged solution of the transport equation, or the discrete ordinates solution, due to truncation errors. This

results in the high-order and low-order QD scalar flux solutions being “inconsistent.” [14, 50].

The QD method has the advantage of being highly efficient and unconditionally stable for any spatial grid. Therefore, this method has stability and performance advantages compared to other acceleration methods when simulating with coarse grids. However, the QD method is not a true acceleration method and presents some limitations to higher-fidelity algorithms, or when the diffusion equation is not a good approximation to the transport equation.

Previous work on consistent QD methods was presented by Anistratov and other authors [55, 56], which allowed the QD solution to consistently converge to the transport solution. However, these methods were complex and difficult to implement in previous QD codes. Recently, a different approach, called the *Consistent Quasidiffusion* (CQD) method, was presented in [57, 58]. The CQD method combines characteristic elements of both QD and CMFD, using both transport consistency terms (CMFD) and Eddington Factors (QD). This method presented a consistent solution, but it had the same downfall of CMFD, losing efficiency and stability with optically thick cells. The inclusion of the transport consistency term ensured the consistency of the new CQD method, but it introduced instability for optically thick cells.

This vulnerability of current state-of-the-art acceleration methods motivated the author to develop a new method that can work effectively for spatial cells with any optical thickness. *Differently from previous methods, the work in this dissertation directs its focus on redefining the Eddington Factors, to obtain consistent solutions and maintain stability.*

1.3 Objectives

This dissertation presents a new acceleration method, called the *Generalized Quasidiffusion* (GQD) method, which solves the neutron transport equation using the discrete ordinates approximation and a new consistent modification of the Quasidiffusion method. The proposed new theory utilizes *Consistent Eddington Factors*, which ensure that the high-order/low-order solutions are consistent with the unaccelerated solution (SI) upon convergence. These consistent Eddington Factors are (i) calculated in each iteration using the high-order angular flux moments' estimation and (ii) used in the low-order system to ensure consistency.

The main goal of this research is to contribute to the field of reactor physics and neutron transport acceleration methods, by developing a more stable and efficient acceleration method than the ones currently available in the literature (e.g. CMFD). As previously mentioned, the efficiency and stability of acceleration methods have been studied and tested throughout the last decades. These methods still present many challenges in terms of performance and stability for highly-scattering systems and optically thick spatial grids, which often restrict the acceleration operation and speed.

A secondary goal of this research is to provide a bridge between the inconsistent (QD) method and consistent acceleration methods. In principle, the new method developed in this dissertation can enable already-existing QD codes to have true acceleration capabilities, with straightforward modifications. This would allow QD codes to be used for higher-fidelity models (where previously QD would not be the most suitable solver method), while still preserving the fast and unconditionally stable performance of the QD method for simpler problems.

The simulation results that we have achieved have shown that GQD successfully converges to the SI solution, for spatial grids of any optical thickness. In all cases, GQD provided better performance than CMFD and CQD, showing unconditional stability for the observed range of optical thickness values and varied scattering ratio problems. So far, GQD has displayed high efficiency and stability for a wide range of problems in planar geometry. However, caution is needed when defining and calculating the consistent Eddington Factors. In deep-penetration (shielding) problems, where fluxes tend to vary rapidly in space, the method can generate *negative* corrected Eddington Factors, leading to instability. We have developed a procedure to ensure their positivity and therefore, guarantee the method's stability. All this is discussed in the remainder of this dissertation.

1.4 Outline

Here we provide a brief outline of the remainder of this dissertation.

Chapter 2 introduces key concepts of neutron transport theory, presenting the Linear Boltzmann equation. All analysis in this work is restricted to 1-D (planar geometry), steady-state, one energy group, isotropic-scattering, and fixed-source problems. Therefore, Chapter 2 also introduces these assumptions and simplifications to the transport equation. The Diffusion approximation is also presented. The remainder of this chapter focuses on computational deterministic methods, more specifically the Discrete Ordinates (S_N) method, and numerical discretizations. Finally, iterative methods are introduced with the example of the Source Iteration method.

Chapter 3 describes two commonly-used acceleration methods (QD and CMFD), providing the mathematical derivation and resulting system of equations for each method.

Chapter 4 introduces the new Generalized Quasidiffusion method – the subject of this dissertation. We provide an extensive mathematical derivation for the method. Additional details on how to calculate the new consistent Eddington factors used in the GQD are also presented. We finalize the chapter by formulating the Linearized GQD method, necessary for the application of the Fourier Stability Analysis. We emphasize here that all derivations are restricted to 1-D (planar geometry), steady-state, one energy group, isotropic-scattering, and fixed-source problems.

Chapter 5 provides a quick introduction to the convergence rate of iterative methods and proceeds with a detailed Fourier Stability Analysis of the linearized GQD method.

Chapter 6 presents numerical results and discussions obtained from applying the CMFD, QD, and GQD methods to a series of steady-state, monoenergetic, planar-geometry, isotropic-scattering, and fixed-source problems. We evaluate 5 different problems in order to stress test the GQD code and validate the consistency and stability of the method. Chapter 6 also provides an initial analysis of the diagonal dominance of each method’s low-order system.

Chapter 7 concludes the dissertation with a discussion and a description of possible future work.

Chapter 2: Neutron Transport Theory

This chapter provides an overview of the relevant topics for understanding the present dissertation. Firstly, the neutron transport equation is presented, together with the underlying physical process and equations, and standard assumptions are used to simplify it. The diffusion approximation to the neutron transport equation is also provided. Then, we discuss computational methods used to solve the neutron transport equation, including details on discretization schemes. Finally, the chapter presents some details of the most basic iterative deterministic method, called *Source Iteration*.

2.1 Neutron Transport Equation

“Neutron transport” is the process that describes collective neutron interactions with the nuclei within a physical system [6, 10]. The balance between the neutron “gain” and neutron “loss” mechanisms is described by the Linear Boltzmann equation (also called transport equation). The time-dependent transport equation (without delayed neutrons) is provided below:

$$\begin{aligned}
& \frac{1}{v} \frac{\partial \psi}{\partial t}(\mathbf{r}, \mathbf{\Omega}, E, t) + \mathbf{\Omega} \cdot \nabla \psi(\mathbf{r}, \mathbf{\Omega}, E, t) + \Sigma_t(\mathbf{r}, E) \psi(\mathbf{r}, \mathbf{\Omega}, E, t) \\
& = \int_0^\infty \int_{4\pi} \Sigma_s(\mathbf{r}, \mathbf{\Omega}' \cdot \mathbf{\Omega}, E' \rightarrow E) \psi(\mathbf{r}, \mathbf{\Omega}', E', t) d\mathbf{\Omega}' dE' \\
& \quad + \frac{\chi_p(E)}{4\pi} \int_0^\infty \int_{4\pi} v \Sigma_f(\mathbf{r}, E') \psi(\mathbf{r}, \mathbf{\Omega}', E', t) d\mathbf{\Omega}' dE' \\
& \quad + \frac{1}{4\pi} Q(\mathbf{r}, E, t), \quad \mathbf{r} \in V, \quad \mathbf{\Omega} \in 4\pi, \quad E \in [0, \infty), \quad 0 < t,
\end{aligned} \tag{2.1a}$$

$$\psi(\mathbf{r}, \mathbf{\Omega}, E, t) = \psi^b(\mathbf{r}, \mathbf{\Omega}, E), \quad \mathbf{r} \in \delta V, \quad (\mathbf{\Omega} \cdot \mathbf{n}) < 0, \quad E \in [0, \infty), \tag{2.1b}$$

$$\psi(\mathbf{r}, \mathbf{\Omega}, E, 0) = \psi^i(\mathbf{r}, \mathbf{\Omega}, E), \quad \mathbf{r} \in V, \quad \mathbf{\Omega} < 4\pi, \quad E \in [0, \infty), \tag{2.1c}$$

In Eq. (2.1), $\psi(\mathbf{r}, \mathbf{\Omega}, E, t)$ is the neutron angular flux, v is the neutron speed, t is the time variable, $\mathbf{r}$ is the spatial position vector, $\mathbf{\Omega}$ is the direction vector, E is the energy variable, and Σ is the macroscopic cross-section (the underscore s , t , and f represent the scattering, total, and fission cross-sections, respectively). The distribution $\chi_p(E)$ represents the fission spectrum, Q is the internal source, v is the average number of neutrons generated by fission, and V is the physical domain. Equation (2.1b) and Eq. (2.1c) are the boundary and initial conditions, respectively.

The spatial vector ($\mathbf{r}$) in Cartesian coordinates is described by:

$$\mathbf{r} \equiv \begin{bmatrix} x \\ y \\ z \end{bmatrix}, \tag{2.2}$$

and the direction vector ($\mathbf{\Omega}$) is defined by:

$$\mathbf{\Omega} \equiv \begin{bmatrix} \Omega_x \\ \Omega_y \\ \Omega_z \end{bmatrix} \equiv \begin{bmatrix} \sqrt{1-\mu^2} \sin \omega \\ \sqrt{1-\mu^2} \cos \omega \\ \mu \end{bmatrix}, \tag{2.3}$$

where ω and μ are the azimuthal angle and the cosine of the polar angle ($\mu = \cos \theta$), respectively. Figure 2.1 illustrates spatial vector $\mathbf{r}$ and directional vector $\mathbf{\Omega}$ in Cartesian coordinates.

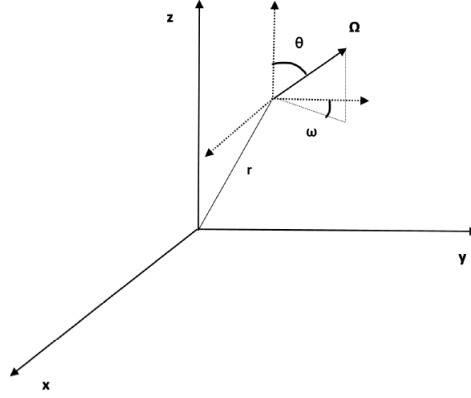


Figure 2.1: Particle Position and Angle [59]

The neutron angular flux (ψ), or *fluence rate*, is the product of the neutron angular density (n_d) and the neutron speed (v). The angular neutron density ($n_d(\mathbf{r}, \mathbf{\Omega}, E, t) dV d\mathbf{\Omega} dE$) represents the expected number of neutrons in a volume dV at $\mathbf{r}$ position, with direction of motion $d\mathbf{\Omega}$ in $\mathbf{\Omega}$, and energy level dE in E , at time t . It has the dimensions $\text{cm}^{-3} \text{sr}^{-1} \text{MeV}^{-1}$.

$$\psi(\mathbf{r}, \mathbf{\Omega}, E, t) dV d\mathbf{\Omega} dE = v n_d(\mathbf{r}, \mathbf{\Omega}, E, t) dV d\mathbf{\Omega} dE . \quad (2.4)$$

The quantity ($\psi(\mathbf{r}, \mathbf{\Omega}, E, t) dV d\mathbf{\Omega} dE$) can be interpreted as the expected rate at which path lengths are being generated by neutrons in $dV d\mathbf{\Omega} dE$ about $(\mathbf{r}, \mathbf{\Omega}, E)$, at time t . It has the dimensions $\text{cm}^{-2} \text{sr}^{-1} \text{MeV}^{-1} \text{s}^{-1}$.

The quantity that integrates all those neutron directions of flight is described as the *scalar flux*, $\phi_0(\mathbf{r}, E, t)$, also known as the zeroth angular moment:

$$\phi_0(\mathbf{r}, E, t) = \int_{4\pi} \psi(\mathbf{r}, \mathbf{\Omega}, E, t) d\mathbf{\Omega} . \quad (2.5a)$$

The scalar flux is the total distance traveled by neutrons in volume dV , energy dE about $(\mathbf{r}, E)$ at time t . It has the dimensions $\text{cm}^{-2} \text{MeV}^{-1} \text{s}^{-1}$. The first angular moment can also

be described as:

$$\phi_1(\mathbf{r}, E, t) = \int_{4\pi} \boldsymbol{\Omega} \psi(r, \boldsymbol{\Omega}, E, t) d\boldsymbol{\Omega} , \quad (2.5b)$$

which is also commonly known as the *neutron current*. This vector quantity is defined by the net number of neutrons (at energy dE in E , and time t) crossing an unit area per second along a normal direction to that surface area. It also has the dimensions $\text{cm}^{-2}\text{sr}^{-1}\text{MeV}^{-1}\text{s}^{-1}$. Other higher angular moments can be obtained, but they are generally addressed as n -th moments and lack a simple physical interpretation.

Based on their definitions, the angular flux and scalar flux are inherently non-negative. The terms in Eq. (2.1) can be physically interpreted as reaction rates. The transport equation is a "balance" equation, which describes the rate of change $\left(\frac{1}{v} \frac{\partial \psi}{\partial t}(\mathbf{r}, \boldsymbol{\Omega}, E, t)\right)$ as a sum of "gain" and "loss" mechanisms:

- Neutron loss terms:
 - Streaming $(\boldsymbol{\Omega} \cdot \nabla \psi(\mathbf{r}, \boldsymbol{\Omega}, E, t))$
 - Collision $(\Sigma_t(\mathbf{r}, E) \psi(\mathbf{r}, \boldsymbol{\Omega}, E, t))$
- Neutron gain terms:
 - In-Scattering $(\int_0^\infty \int_{4\pi} \Sigma_s(r, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, E' \rightarrow E) \psi(\mathbf{r}, \boldsymbol{\Omega}', E', t) d\boldsymbol{\Omega}' dE')$
 - Fission $(\frac{\chi_p(E)}{4\pi} \int_0^\infty \int_{4\pi} v \Sigma_f(\mathbf{r}, E') \psi(\mathbf{r}, \boldsymbol{\Omega}', E', t) d\boldsymbol{\Omega}' dE')$
 - Internal Source $(\frac{1}{4\pi} Q(\mathbf{r}, E, t))$

Equation (2.1) is a detailed balance equation for the rate of change of the angular flux in a 7-D phase space (3 spatial variables, 2 angular variables, 1 energy variable, and 1 temporal variable). Real physical systems have complicated data set structures that depend on each

variable. Therefore, several simplifications are often applied to the above Linear Boltzmann equation, to simplify the equation and improve computational performance, at the cost of some detail and accuracy.

The simplifications for the physical systems (and therefore for the transport equation) used in this dissertation are: *steady-state*, *one energy group*, *isotropic scattering*, *planar-geometry*, and *fixed-source*. Further simplifications and approximations are performed later in this document when the numerical and computational methods are presented. Instead of considering a simpler physical system, these other simplifications arise from the discretization of a continuous variable in the transport equation, such as the direction of flight vector $\mathbf{\Omega}$, space, or energy.

2.1.1 Steady-State Neutron Transport Equation

All the analysis in this work is done for steady-state problems, in which the time derivative (the rate of change) is zero. Therefore, the first term on the left-hand side of Eq. (2.1), as well as the variables' dependency on time, are removed from the equation. We obtain:

$$\begin{aligned} & \mathbf{\Omega} \cdot \nabla \psi(\mathbf{r}, \mathbf{\Omega}, E) + \Sigma_t(\mathbf{r}, E) \psi(\mathbf{r}, \mathbf{\Omega}, E) \\ &= \int_0^\infty \int_{4\pi} \Sigma_s(r, \mathbf{\Omega}' \cdot \mathbf{\Omega}, E' \rightarrow E) \psi(\mathbf{r}, \mathbf{\Omega}', E') d\mathbf{\Omega}' dE \\ &+ \frac{\chi_p(E)}{4\pi} \int_0^\infty \int_{4\pi} \nu \Sigma_f(r, E') \psi(\mathbf{r}, \mathbf{\Omega}', E') d\mathbf{\Omega}' dE + \frac{1}{4\pi} Q(r, E) . \end{aligned} \quad (2.6)$$

2.1.2 Multigroup Energy Discretization

One of the most significant simplifications to the neutron transport equations is energy discretization. The neutron energy range in a nuclear reactor varies from very low (thermal neutrons, ≈ 0.025 eV) to very high (fast neutrons, in the order of a few MeV) values [6, 10,

60], and the material properties depend highly on the incident neutron energy. The physical medium generally presents a very complex data structure of cross-sections, which vary significantly with the incident neutron energy (E).

A common approach is to apply the *multi-group* approximation in energy [6, 10, 60, 61]. This energy discretization assumes that the whole continuous energy spectrum $[0, \infty)$ is broken down into a certain finite number (G) of *energy groups*. The material properties are then calculated for each group energy range. One example of these material properties can be seen in Fig. 2.2, which displays the total cross-section for ^{235}U as a function of the continuous energy variable. This figure also presents one example of possible multi-group approximation, in red. One can see that the cross-section varies by orders of magnitude as

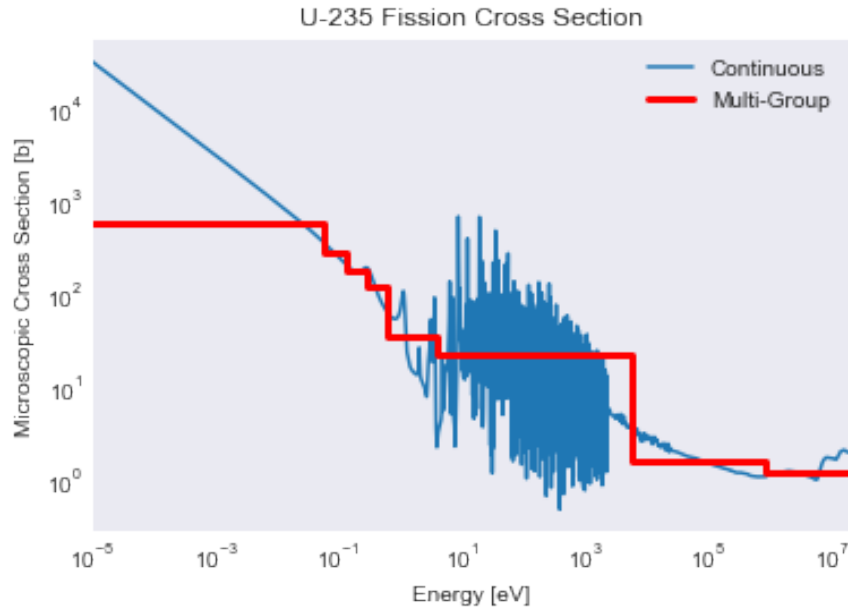


Figure 2.2: Continuous Energy Fission Cross-Section for ^{235}U and multi-group approximation [62].

it changes energy levels. The “oscillatory” behavior in the resonance region also makes it

difficult to handle the energy variable continuously. The red lines illustrate the approximated uniform energy group cross-sections for each energy range.

The multigroup approximation is widely used for deterministic methods and some Monte Carlo methods [2, 63]. The choice of how many energy groups and how they are calculated can highly impact the accuracy of the solution [64]. The number of multigroup equations is always equal to the number of energy groups, so a higher number of energy groups can considerably increase the calculation time.

The steady-state, multigroup neutron transport equation is described as:

$$\mathbf{\Omega} \cdot \nabla \psi_g(r, \mathbf{\Omega}) + \Sigma_{t,g}(r) \psi_g(r, \mathbf{\Omega}) = \sum_{g'=1}^G \int_{4\pi} \Sigma_{s,g' \rightarrow g}(r, \mathbf{\Omega}' \cdot \mathbf{\Omega}) \psi_{g'}(r, \mathbf{\Omega}') d\mathbf{\Omega}' \quad (2.7a)$$

$$+ \frac{1}{4\pi} \sum_{g'=1}^G \int_{4\pi} \chi_{g'} v \Sigma_{f,g'}(r) \psi_{g'}(\mathbf{r}, \mathbf{\Omega}') d\mathbf{\Omega}' + \frac{Q_g(r)}{4\pi}, \quad r \in V, \quad \mathbf{\Omega} \in 4\pi, \quad 1 \leq g \leq G, \\ \psi_g(r, \mathbf{\Omega}) = \psi_g^b(r, \mathbf{\Omega}), \quad r \in \delta V, \quad \mathbf{\Omega} \cdot \mathbf{n} < 0. \quad (2.7b)$$

For each energy group g , the multigroup terms in this equation are defined as:

$$\phi_{0,g'}(r) \equiv \int_{4\pi} \psi_{g'}(r, \mathbf{\Omega}) d\mathbf{\Omega}, \quad (2.8a)$$

$$\psi_g(r, \mathbf{\Omega}) = \int_{E_g}^{E_{g-1}} \psi(r, \mathbf{\Omega}, E') dE', \quad (2.8b)$$

$$\Sigma_{t,g}(r, \mathbf{\Omega}) = \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(r, E') \psi(r, \mathbf{\Omega}, E') dE'}{\psi_g(r, \mathbf{\Omega})}, \quad (2.8c)$$

$$\chi_g(r) = \int_{E_g}^{E_{g-1}} \chi(r, E') dE', \quad (2.8d)$$

$$v \Sigma_{f,g'} = \frac{\int_{E_g}^{E_{g-1}} v \Sigma_f(E') dE'}{\phi_{0,g'}(r)} \quad (2.8e)$$

$$\Sigma_{s,g' \rightarrow g}(r, \mathbf{\Omega}' \cdot \mathbf{\Omega}) = \frac{\int_{E_g}^{E_{g-1}} \int_{E_g}^{E_{g'-1}} \Sigma_s(r, \mathbf{\Omega}' \cdot \mathbf{\Omega}, E' \rightarrow E) \psi(r, \mathbf{\Omega}', E') dE' dE}{\psi_{g'}(r, \mathbf{\Omega})} \quad (2.8f)$$

$$Q_g(r) = \int_{E_g}^{E_{g-1}} Q(r, E') dE'. \quad (2.8g)$$

The energy range for group g is defined as $E_g < E < E_{g-1}$. The order g of the energy groups is defined in a decreasing manner for energy, with $(g = 1)$ the highest energy range and $g = G$ the lowest energy range.

In the specific case where there is only one energy group ($G = 1$), Eqs. (2.7) simplifies to:

$$\begin{aligned} \boldsymbol{\Omega} \cdot \nabla \psi(\mathbf{r}, \boldsymbol{\Omega}) + \Sigma_t(\mathbf{r}) \psi(\mathbf{r}, \boldsymbol{\Omega}) &= \int_{4\pi} \Sigma_s(\mathbf{r}, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}) \psi(\mathbf{r}, \boldsymbol{\Omega}') d\boldsymbol{\Omega}' \\ &+ \frac{\nu \Sigma_f(\mathbf{r})}{4\pi} \int_{4\pi} \psi(\mathbf{r}, \boldsymbol{\Omega}') d\boldsymbol{\Omega}' + \frac{Q(\mathbf{r})}{4\pi} . \end{aligned} \quad (2.9)$$

The one-group approximation may be an oversimplification of a real physical system. However, it helps reduce the complexity of the problem when analyzing newer numerical methods. When solving realistic problems, it is common to use several (sometimes hundreds of) energy groups. In this dissertation, the multigroup approximation is employed for the specific case of one group ($G = 1$).

2.1.3 Isotropic Scattering

Once a particle collides with the medium and experience a scattering event, it most likely change its direction ($\boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}$). The new direction ($\boldsymbol{\Omega}$) depends the type of particle and media material, among other variables. A common simplification used in transport problems is to assume isotropic scattering. This assumption states that neutrons have equal chance to scatter to any angle.

$$\Sigma_s(\mathbf{r}, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}) = \frac{\Sigma_s(\mathbf{r})}{4\pi} . \quad (2.10)$$

This simplifies Eq. (2.9) to:

$$\boldsymbol{\Omega} \cdot \nabla \psi(r, \boldsymbol{\Omega}) + \Sigma_t(r) \psi(r, \boldsymbol{\Omega}) = \frac{\Sigma_s(r) + \nu \Sigma_f(r)}{4\pi} \int_{4\pi} \psi(r, \boldsymbol{\Omega}') d\boldsymbol{\Omega}' + \frac{Q(r)}{4\pi} . \quad (2.11)$$

2.1.4 Planar-geometry

The next simplification used in this dissertation is the assumption of 1-D planar symmetry, also called slab geometry [61]. This simplification assumes two statements: the angular flux (i) is independent of x and y , and (ii) has azimuthal symmetry. Cross-sections, sources, and other incident boundary fluxes are also independent of x and y .

The angular flux then is described as:

$$\psi(r, \mathbf{\Omega}) = \psi(z, \mathbf{\Omega}) = \psi(z, \mu, \omega) . \quad (2.12)$$

Substituting Eq. (2.12) into Eq. (2.11) one can obtain:

$$\begin{aligned} \mu \frac{\partial \psi}{\partial z}(z, \mu, \omega) + \Sigma_t(z) \psi(z, \mu, \omega) &= \frac{\Sigma_s(z) + \nu \Sigma_f(z)}{4\pi} \int_{4\pi} \psi(z, \mu', \omega') d\mu' d\omega' \\ &+ \frac{Q(z)}{4\pi}, \quad 0 < z < Z, \quad -1 \leq \mu \leq 1, \quad 0 \leq \omega < 2\pi . \end{aligned} \quad (2.13)$$

The azimuthal angle can be eliminated from Eqs. (2.13) by defining the azimuthally-integrated angular flux:

$$\psi(z, \mu) = \int_0^{2\pi} \psi(z, \mu, \omega) d\omega , \quad (2.14)$$

and by integrating over the azimuthal angle (ω), Eqs. (2.13) simplifies to:

$$\mu \frac{d}{dz} \psi(z, \mu) + \Sigma_t(z) \psi(z, \mu) = \frac{\Sigma_s(z) + \nu \Sigma_f(z)}{2} \int_{-1}^1 \psi(z, \mu') d\mu' + \frac{Q(z)}{2} , \quad (2.15a)$$

$$\psi(0, \mu) = \psi^l(\mu), \quad 0 < \mu \leq 1 , \quad (2.15b)$$

$$\psi(Z, \mu) = \psi^r(\mu), \quad -1 \leq \mu < 0 . \quad (2.15c)$$

In these equations there are two independent variables: space (z) and angle (μ).

2.1.5 Fixed-Source Problems

The last simplification applied to the transport equation is the assumption that the problem has a fixed source. There are many cases where the neutron transport problem has a

well-defined source for a non-multiplying medium (e.g. radiation shielding or point-source calculations). These type of problems are defined as *fixed-source* problems. For other types of problems, such as *eigenvalue problems*, the neutron fission source is not known and must be calculated. These problems are somewhat more complicated.

For fixed-source problems, the fission source in Eq. (2.15) is usually assumed to be zero. As a first analysis for the proposed work in this dissertation, only fixed-source calculations are considered.

To summarize: steady-state, planar-geometry, mono-energetic, isotropically-scattering, fixed-source transport problems with $\Sigma_f = 0$, can be described as:

$$\mu \frac{d}{dz} \psi(z, \mu) + \Sigma_t(z) \psi(z, \mu) = \frac{\Sigma_s(z)}{2} \int_{-1}^1 \psi(z, \mu') d\mu' + \frac{Q(z)}{2} , \quad (2.16a)$$

$$\psi(0, \mu) = \psi^l(\mu), \quad 0 < \mu \leq 1 , \quad (2.16b)$$

$$\psi(Z, \mu) = \psi^r(\mu), \quad -1 \leq \mu < 0 . \quad (2.16c)$$

These problems are the subject of the remainder of this dissertation.

2.2 Diffusion Equation

The transport equation provides a physically accurate description of the neutron flux. However, solving this equation may require a large computation cost. A common simplification to neutron transport problems is to approximate the Linear Boltzmann equation by the *diffusion equation* (also called diffusion approximation) [60]. The diffusion equation simplifies the transport equation by assuming that the angular flux depends only weakly on the direction variable (Ω).

Instead of working with the angular flux, which (for general 3-D problems) lives in the 7-D space, the diffusion equation works with the scalar flux. Therefore, the diffusion

approximation is independent of the angular variable, reducing the complexity to just 5-D (3 space, 1 energy, and 1 time). In the specific case of planar geometry used in this work, the diffusion equation is a function of only one spatial variable (z).

The diffusion approximation uses a series of assumptions to simplify the neutron transport equation:

- Linearly anisotropic angular flux

$$\psi(z, \mu) \approx \frac{1}{4\pi} \phi_0(z) + \frac{3\mu}{4\pi} \phi_1(z) , \quad (2.17)$$

- Linearly anisotropic scattering

$$\Sigma_s(z, \mathbf{\Omega}' \cdot \mathbf{\Omega}) \approx \frac{1}{4\pi} \left(\Sigma_{s0}(z) + 3\mu_0 \Sigma_{s1}(z) \right) , \quad (2.18)$$

- Fick's Law

$$\phi_1(z) = -D(z) \frac{d\phi_0(z)}{dz} , \quad (2.19)$$

where $\mu_0 = \mathbf{\Omega}' \cdot \mathbf{\Omega}$ is the cosine of the scattering angle (θ_0). Here, Σ_{s0} and Σ_{s1} are the zeroth and first Legendre moments of the differential scattering cross-section. The term D is the *diffusion coefficient*, given by:

$$D(z) = \frac{1}{3\Sigma_{tr}(z)} = \frac{1}{3(\Sigma_t(z) - \Sigma_{s,1}(z))} . \quad (2.20)$$

The term Σ_{tr} is the *transport cross-section*. For the case of isotropic scattering, $\Sigma_{s,1}$ is equal to zero and the transport cross-section is equal to the total cross-section ($\Sigma_{tr} = \Sigma_t$).

The steady-state, mono-energetic, planar geometry neutron diffusion equation is described as:

$$-\frac{d}{dz} \left(D(z) \frac{d\phi_0(z)}{dz} \right) + \Sigma_a(z) \phi_0(z) = Q(z) , \quad (2.21)$$

where the absorption cross-section Σ_a is defined as: $\Sigma_a = \Sigma_t - \Sigma_s$.

Due to the approximations introduced, Eq. (2.21) is valid when the solution is not near a void, boundary, source, or a strong absorber. In these “transport” regions, one can expect the solution of the transport equation and the diffusion equation to differ significantly [60]. This leads to the issue of defining accurate boundary conditions for the diffusion equation, which are necessary to solve the diffusion problem.

In cases of vacuum or air boundary conditions, the general approach is that the flux tends to vanish (become zero) at a small distance (d) outside the interface (Fig. 2.3). Setting the neutron flux to zero at this *extrapolated endpoint*, although nonphysical, often gives a sufficiently close approximation to the neutron flux inside the diffusing medium. This

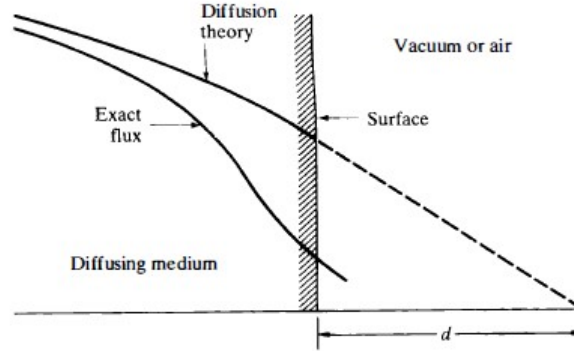


Figure 2.3: Extrapolation length for boundary condition of the diffusion approximation [60].

distance (d), known as extrapolation distance, is usually defined as:

$$d \approx 0.7104\lambda_{tr} = 2.13D , \quad (2.22)$$

where λ_{tr} is the transport mean free path of the medium and D is the diffusion coefficient as defined by Eq. (2.21).

Dealing only with the scalar flux leads to simpler equations to solve and less-complicated data structures, improving computational performance. Due to its relative simplicity, the diffusion approximation was historically used for many early nuclear reactor designs. Currently, nuclear reactor designs require a more precise approach to calculate the neutron behavior, relying on neutron transport methods that more accurately depict the physics of the problems.

The diffusion equation became mostly used as a first estimate for the neutron flux and reactor properties for more complex transport methods, or as a lower-order system for acceleration methods. In this dissertation, the diffusion equation is used in both ways: generating an initial estimation for the neutron flux, and as a low-order system of equations for the acceleration methods.

2.3 Computational Methods

The neutron transport equation is often impossible to solve analytically. Consequently, many approximate numerical methods have been developed to solve Eq. (2.1) and its simplifications [10, 60]. These numerical methods are usually separated into two types: *stochastic methods* (also known as Monte Carlo methods) and *deterministic methods*.

Monte Carlo methods work by simulating the individual histories of large numbers of neutrons. These methods allow for a continuous description of energy, angle, and space. By simulating a sufficiently large number of particles, Monte Carlo can provide high fidelity [2, 3, 63]. However, Monte Carlo methods have two major disadvantages: high computational cost and high variance in highly absorbing regions.

Firstly, Monte Carlo methods require one to simulate the histories of individual particles. To have a statistically accurate solution, one must simulate a very large number of histories,

increasing the computing time. The second issue concerns problems in which the neutron flux reduces significantly across the medium (e.g. shielding problems). The fewer the number of neutrons that reach a certain region, the higher is the statistical variance of the solution in that region. To improve confidence in the accuracy of the solution in those regions, one must increase significantly the number of particles simulated, or use more complex sorting algorithms [65, 66].

Deterministic methods, on the other hand, discretize the neutron transport equation into an algebraic system of equations and then solve this (typically large) algebraic system [14]. Deterministic solutions are not affected by the variance problems of stochastic methods. However, unlike the Monte Carlo solutions, deterministic solutions are affected by truncation errors caused by the approximate discretization of the Linear Boltzmann equation. Thus, one downside of deterministic methods comes from the approximations caused by discretization methods used, which reduce the fidelity of the solution. Another downside is the often high cost of solving the large system of discretized algebraic equations. (This cost is the motivation for the research described in this dissertation.)

Overall, the computational cost of solving deterministic neutron transport problems is often lower than that of Monte Carlo methods. Deterministic methods are used in many modern codes [1, 4, 67].

Some classical deterministic methods are: the Spherical Harmonics (PN), Simplified Spherical Harmonics (SPN), Method of Characteristics (MOC), and Discrete Ordinates (S_N). Most of these methods arise from different approaches to handle the angular variable (μ). They provide faster but approximated solution to the transport equation.

This dissertation focuses on the Discrete Ordinates method (S_N) and related iteration methods that were developed to improve its efficiency and convergence speed.

2.3.1 Discrete Ordinates

The *Discrete Ordinates* (S_N) approximation was developed in the 1960's and is widely used in many transport codes [1, 15, 68, 69]. This approximation assumes that the cosine of the angle of flight (μ) is not a continuous variable, but rather, a discrete set of N direction cosines μ_n ($n = 1, \dots, N$), where:

$$\mu_n = \cos(\theta_n) . \quad (2.23)$$

Therefore, the direction cosines μ_n have positive and negative values. This simplifies the integral aspect of angular variable μ into a discrete summation term of N directions, exemplified in Fig. 2.4. The S_N simplification of Eqs. (2.16) is a system of equations that is

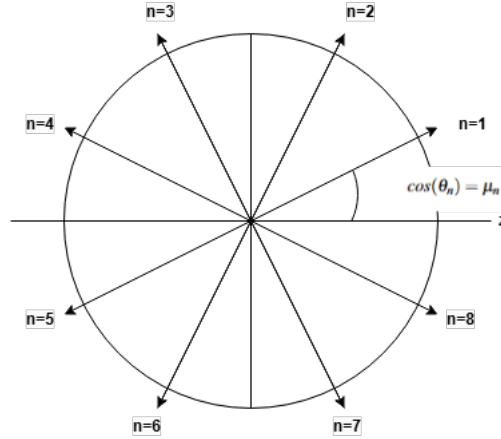


Figure 2.4: Angle discretization in Discrete Ordinates (S_N)

discrete in the angular (but not spatial) variable:

$$\mu_n \frac{\partial \psi_n}{\partial z}(z) + \Sigma_t(z) \psi_n(z) = \frac{\Sigma_s(z)}{2} \sum_{n'=1}^N \psi_{n'}(z) w_{n'} + \frac{Q(z)}{2}, \quad (2.24a)$$

$$\psi_{n,0} = \Psi_n^l, \mu_n > 0, \quad (2.24b)$$

$$\psi_{n,Z} = \Psi_n^r, \mu_n < 0. \quad (2.24c)$$

$$\phi_k(z) = \sum_{n'=1}^N (\mu_{n'})^k \psi_{n'}(z) w_{n'}, \quad z \in V. \quad (2.24d)$$

In Eqs. (2.24), the term $\phi_k(z)$ describes the discretized k -th angular moment. The Gauss-Legendre quadrature weights are represented by $w_{n'}$. Note that in this quadrature, these weights are normalized the following way:

$$\sum_{n=1}^N w_n = 2.0. \quad (2.25)$$

An example of angles and weights using the Gauss-Legendre quadrature for S_N with $N = 16$ is provided in Table 2.1. A more complete set of tables is provided in Appendix A for various values of N .

Table 2.1: Gauss-Legendre weights and angles for S_N discrete ordinates ($N = 16$).

Direction Cosine (μ_n)	Weight (w_n)
± 0.095012509837637	0.189450610455067
± 0.281603550779259	0.182603415044924
± 0.458016777657227	0.169156519395003
± 0.617876244402644	0.149595988816577
± 0.755404408355003	0.124628971255534
± 0.865631202387832	0.095158511682493
± 0.944575023073233	0.062253523938648
± 0.989400934991650	0.027152459411754

Equations (2.24) describe a system of N equations and boundary conditions. However, spatial discretization is required to fully discretize the problem, so that it can then be solved numerically.

2.3.1.1 Spatial Discretization

The planar-geometry spatial domain ($0 < z < Z$) can be discretized in J cells (see schematic in Fig. 2.5), where each individual cell (j) with width (h_j) is defined by:

$$h_j = z_{j+\frac{1}{2}} - z_{j-\frac{1}{2}}. \quad (2.26)$$

Here, $z_{j+\frac{1}{2}}$ and $z_{j-\frac{1}{2}}$ represent the position at the right and left interfaces of the cell j .

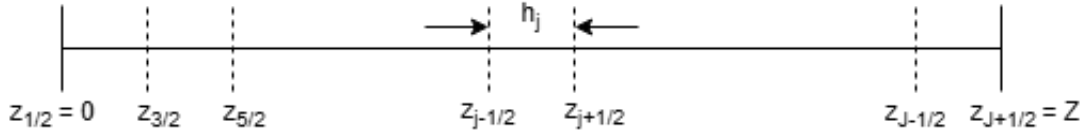


Figure 2.5: Spatial discretization of 1-D grid.

The spatially discretized system of S_N equations can be then written as:

$$\frac{\mu_n}{h_j} (\psi_{n,j+\frac{1}{2}} - \psi_{n,j-\frac{1}{2}}) + \Sigma_{t,j} \psi_{n,j} = \frac{\Sigma_{s,j}}{2} \sum_{n'=1}^N \psi_{n',j} w_{n'} + \frac{Q_j}{2}, \quad (2.27a)$$

$$\psi_{n,\frac{1}{2}} = \Psi_n^l, \mu_n > 0, \quad (2.27b)$$

$$\psi_{n,J+\frac{1}{2}} = \Psi_n^r, \mu_n < 0. \quad (2.27c)$$

These equations hold for $1 \leq j \leq J$ and $1 \leq n \leq N$, where J is the number of spatial cells, and N is the number of discrete ordinates. The terms $\psi_{n,j}$ are defined as the cell-average angular fluxes:

$$\psi_{n,j} = \frac{1}{h_j} \int_{z_{j-\frac{1}{2}}}^{z_{j+\frac{1}{2}}} \psi_n(z) dz, \quad (2.27d)$$

and the cell-edge angular fluxes are defined as:

$$\psi_{n,j\pm\frac{1}{2}} = \psi_n(z_{j\pm\frac{1}{2}}) . \quad (2.27e)$$

Equations (2.27) are derived exactly from the continuous S_N equations by integrating Eqs. (2.24) over the spatial cell j^{th} . Therefore, this new set of equations contains no spatial truncation errors.

This spatial discretization results in a system of $N(J+1)$ equations (NJ equations are from Eq. (2.27a), and N equations from Eqs. (2.27b) and (2.27c)). However, the total number of unknowns in that system is $N(2J+1)$ (NJ from the cell-average angular fluxes and $N(J+1)$ from the cell-edge angular fluxes). Therefore, it is necessary to introduce NJ extra equations (one for each spatial cell and discrete ordinates directions) to solve the S_N equations.

In recent decades, many different methods have been developed to propose these equations that are lacking [70, 71]. These differencing schemes introduce truncation errors into the formulation. The general approach used is to create a correlation between the cell-average angular flux and the cell-edge angular fluxes:

$$\psi_{n,j} = f(\psi_{n,j+\frac{1}{2}}, \psi_{n,j-\frac{1}{2}}) . \quad (2.28)$$

In principle, Equation (2.28) provides the remaining NJ equations that were lacking from Eqs. (2.27).

The simplest methods to define Eq. (2.28) are the Finite-Difference methods (which include the *Upwind*, *Diamond-Difference* (DD), and *Step Characteristic* (SC) methods). Other more sophisticated methods were later developed [71]. The algorithm developed for this dissertation includes the DD and SC capabilities, focusing mostly on the SC method.

For all three methods, Eq. (2.28), can be written as:

$$\psi_{n,j} = \left(\frac{1 + \alpha_{n,j}}{2} \right) \psi_{n,j+\frac{1}{2}} + \left(\frac{1 - \alpha_{n,j}}{2} \right) \psi_{n,j-\frac{1}{2}} , \quad 1 \leq n \leq N, \quad 1 \leq j \leq J . \quad (2.29)$$

The *angular weights* $\alpha_{n,j}$ are uniquely defined for each method. These terms are always defined so that:

$$\mu_n \alpha_{n,j} \geq 0 . \quad (2.30)$$

For the *upwind* or *Step* case:

$$\alpha_n = \frac{\mu_n}{|\mu_n|} = \begin{cases} +1, & \mu_n > 0 \\ -1, & \mu_n < 0 \end{cases} , \quad (2.31)$$

and

$$\psi_{n,j} = \begin{cases} \psi_{n,j+\frac{1}{2}}, & \mu_n > 0 \\ \psi_{n,j-\frac{1}{2}}, & \mu_n < 0 \end{cases} . \quad (2.32)$$

For the DD method, $\alpha_{n,j} = 0$. This simplifies Eq. (2.29) into:

$$\psi_{n,j} = \frac{1}{2} \left(\psi_{n,j+\frac{1}{2}} + \psi_{n,j-\frac{1}{2}} \right) . \quad (2.33)$$

Both methods were not derived from the Linear Boltzmann equation . The SC method, on the other hand, ensures that the neutron flux will be positive [72]. It is derived by assuming that Eq. (2.29) will be consistent with the transport equation for the case of constant scattering and homogeneous internal source ($S_{n,j}$) in each cell j :

$$\mu_n \frac{d\psi_n}{dz}(z) + \Sigma_t(z) \psi_n(z) = S_{n,j} \quad z_{j-\frac{1}{2}} < z < z_{j+\frac{1}{2}} \quad (2.34)$$

The complete derivation is given in Appendix B. For SC, the $\alpha_{n,j}$ are defined as:

$$\alpha_{n,j} = \alpha(\varepsilon_{n,j}) = \frac{e^{\varepsilon_{n,j}} + e^{-\varepsilon_{n,j}}}{e^{\varepsilon_{n,j}} - e^{-\varepsilon_{n,j}}} - \frac{2}{\varepsilon_{n,j}} , \quad \varepsilon_{n,j} = \frac{\Sigma_{t,j} h_j}{\mu_n} . \quad (2.35)$$

Thus, $\alpha(\varepsilon_{n,j})$ is a continuous function from $(-\infty < \varepsilon_{n,j} < \infty)$, as presented in Fig. 2.6. One can see that the SC method tends to the upwind approximation (horizontal dotted lines)

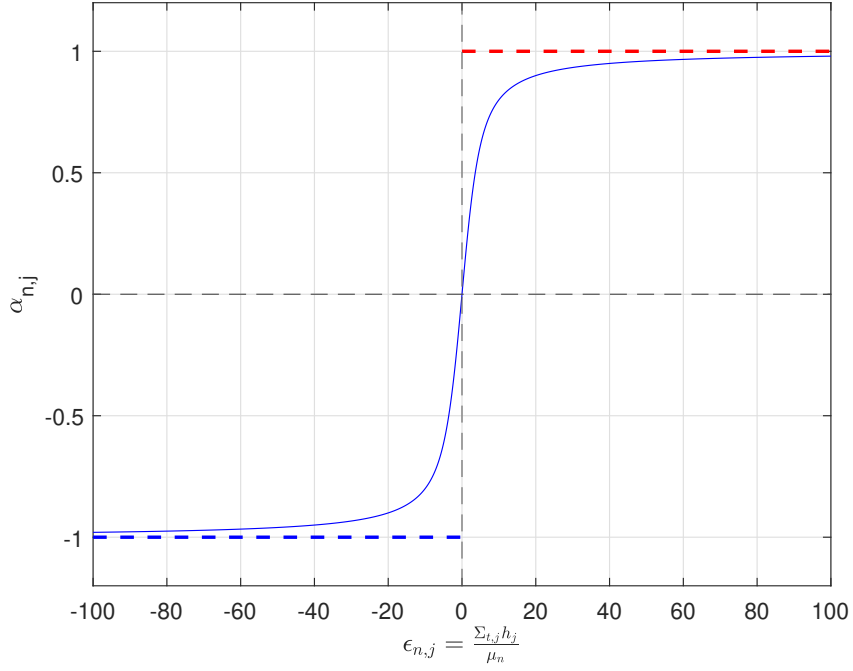


Figure 2.6: Step Characteristic $\alpha_{n,j}$ values.

when using very large (in magnitude) values of $\epsilon_{n,j}$, which happens with coarser meshes. It also approximates smoothly to the DD method when using optically thin meshes.

The SC method has been shown to be significantly more positive than the DD method. However, both SC and DD lose precision when the spatial grid becomes coarser (optically thicker) [46]. Most of the results of this dissertation were obtained using the Step Characteristic spatial discretization scheme.

The algebraic system of discrete 1-D equations that is considered in the remainder of this document, assuming the S_N approximation in angle and the SC approximation in space,

is given by:

$$\frac{\mu_n}{h_j}(\psi_{n,j+\frac{1}{2}} - \psi_{n,j-\frac{1}{2}}) + \Sigma_{t,j}\psi_{n,j} = \frac{\Sigma_{s,j}}{2} \sum_{n'=1}^N \psi_{n',j} w_{n'} + \frac{Q_j}{2}, \quad (2.36a)$$

$$\psi_{n,j} = \left(\frac{1 + \alpha_{n,j}}{2}\right) \psi_{n,j+\frac{1}{2}} + \left(\frac{1 - \alpha_{n,j}}{2}\right) \psi_{n,j-\frac{1}{2}}, \quad (2.36b)$$

$$\psi_{n,\frac{1}{2}} = \Psi_n^l, \mu_n > 0, \quad (2.36c)$$

$$\psi_{n,J+\frac{1}{2}} = \Psi_n^r, \mu_n < 0, \quad (2.36d)$$

$$\alpha_{n,j} = \frac{e^{\varepsilon_{n,j}} + e^{-\varepsilon_{n,j}}}{e^{\varepsilon_{n,j}} - e^{-\varepsilon_{n,j}}} - \frac{2}{\varepsilon_{n,j}}, \quad \varepsilon_{n,j} = \frac{\Sigma_{t,j} h_j}{\mu_n}. \quad (2.36e)$$

2.3.2 Transport Iterative Methods

In principle, the discrete S_N system described by Eqs. (2.36) can be solved directly. However, this becomes quickly unfeasible when the algebraic system becomes larger. Solving a linear system of size m by direct inversion requires $O(m^3)$ FLOPs. Meanwhile, iterative methods require a fairly lower amount, using $O(m^2)$ FLOPs [16]. Therefore, numerical schemes usually rely on iterative methods to solve larger linear systems [14].

The general approach of iterative methods is that they provide an approximate solution at each iteration. Instead of solving all equations simultaneously, they approximate some parameters for each iteration and correct those terms progressively. If the iterative method converges, the approximated solution at each iteration gets progressively closer to the actual solution.

A comparison example between solving directly and iteratively can be seen in Fig. 2.7. One can see that when solving a system directly, it must perform all the required operations ($O(m^3)$ FLOPs) to solve the system and obtain a solution with machine error precision $\varepsilon_{machine}$. For convergent iterative methods, the error between the true solution and the

approximated solution becomes progressively smaller at each iteration, reaching machine error precision at a much faster rate ($O(m^2)$ FLOPs).

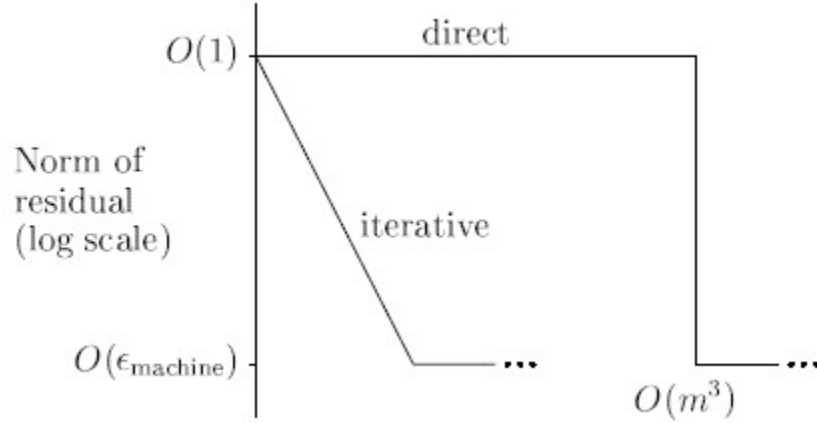


Figure 2.7: Residual error as a function of FLOPs for solving a linear system directly or iteratively [16].

2.3.2.1 Source Iteration (SI)

Source Iteration (SI) is the most basic iterative scheme and has been the basis for many other iterative methods used in neutron transport [ref]. Mathematically, the SI method applied to the continuous S_N equations can be defined by:

$$L\psi^{(l+1)} = S\psi^{(l)} + q, \quad l \geq 0, \quad (2.37a)$$

where (l) is the iteration number, L is the operator containing the leakage and collision terms:

$$L = \mu \frac{\partial}{\partial z} + \Sigma_t(z) , \quad (2.37b)$$

and S is the scattering operator:

$$S = \frac{\Sigma_s(z)}{2} \int_{-1}^1 (\cdot) d\mu'. \quad (2.37c)$$

The term $\psi^{(0)}$ is a user-defined initial guess for the neutron angular flux. The last term q is the known internal source, given by:

$$q = \frac{Q(z)}{2} . \quad (2.37d)$$

The SI method iteratively solves Eqs. (2.37) for $\psi^{(l+1)}$. The method behaves in the following way: it estimates the angular flux to compute the scattering term and then solves for the leakage and collision terms based on this estimation. The right-hand side of the equation is calculated based on an initial estimation of the neutron flux $\psi^{(0)}$, or based on the solution from the previous iteration $\psi^{(l)}$. Then Eqs. (2.37) is solved for $\psi^{(l+1)}$ by inverting the operator L , obtaining a new estimation for the angular flux. The SI method stops once the difference between consecutive neutron flux estimations (ε_l) is within a certain convergence criterion (ε_f):

$$\varepsilon_l = |\psi^{(l+1)} - \psi^{(l)}| \leq \varepsilon_f. \quad (2.38)$$

Applying this method to the discrete planar-geometry, one-group, steady-state, fixed-source problem in Eqs. (2.36), we obtain:

$$\frac{\mu_n}{h_j} \left(\psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}} \right) + \Sigma_{t,j} \psi_{n,j}^{\ell+\frac{1}{2}} = \frac{\Sigma_{s,j}}{2} \phi_{0,j}^\ell + \frac{Q_j}{2} , \quad (2.39a)$$

$$\psi_{n,j}^{\ell+\frac{1}{2}} = \left(\frac{1 + \alpha_{n,j}}{2} \right) \psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} + \left(\frac{1 - \alpha_{n,j}}{2} \right) \psi_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}} , \quad (2.39b)$$

$$\psi_{n,\frac{1}{2}} = \Psi_n^l , \mu_n > 0 , \quad (2.39c)$$

$$\psi_{n,J+\frac{1}{2}} = \Psi_n^r , \mu_n < 0 , \quad (2.39d)$$

$$\phi_{0,j}^{\ell+1} = \sum_{n=1}^N \psi_{n,j}^{\ell+\frac{1}{2}} w_n . \quad (2.39e)$$

The $\alpha_{n,j}$ values can be determined for any spatial discretization scheme. In our simulations, we generally used the SC scheme (Eq. (2.35)).

Equations (2.39) can be solved systematically from left-to-right or right-to-left direction for each angle μ_n separately. This procedure is called a *transport sweep*. The calculated values for $\psi_{n,j}^{(l+\frac{1}{2})}$ for all angles are then used to compute the newer estimate of the scalar flux $\phi_{0,j}^{(l+1)}$ for the next iteration $(l+1)$ (in Eq. (2.39c)).

The SI method converges for any choice of spatial grid used and yields the true S_N solution upon convergence. For cases where the system has significant absorption or leakage, the SI method can rapidly converge. However, this method loses efficiency when handling large systems with highly scattering media [14, 15, 68, 69]. Extensive analysis has shown that for optically thick systems with small leakage, the convergence speed of this method is strongly influenced by the scattering ratio c .

For physical systems that are "diffusive", the likelihood that neutrons will scatter and travel farther distances is higher. This leads to a higher number of iterations required for the solution to converge, increasing the computational time. For practical problems of this nature, SI can become very inefficient. Acceleration methods were developed to deal with this weakness for highly scattering media [20–26, 73]. The following chapter (Chapter 3) provides a discussion of these methods – more specifically, the Quasidiffusion (QD) method and the Coarse-Mesh-Finite-Difference (CMFD) method.

Chapter 3: Rapidly Converging Iterative Methods

The state-of-the-art acceleration methods used in the nuclear field utilize iterations that couple a “high-order” (relatively complicated) system of S_N equations to a “low-order” (relatively simpler) diffusion equation. If done properly, this speeds up the convergence of the slowly converging modes, which significantly reduces the number of iterations and thereby accelerates the iteration process [14]. Acceleration methods can be linear (e.g. DSA) or nonlinear (e.g. CMFD) [14, 21–26, 73].

Generally, acceleration methods function by (i) approximately solving the high-order system, (ii) calculating the “lagged” parameters that occur in the low-order system, and then (iii) solving the low-order system. The scalar flux solution of the low-order system is then used to estimate new scattering and fission (in cases of k-eigenvalue problems) terms for the high-order system in the subsequent iteration, thus closing the loop. A schematic in Fig. 3.1 shows how the algorithms work.

During the last decades, a wide range of acceleration methods was developed [14]. Many of these were later overshadowed by more efficient methods. However, current state-of-the-art methods also have well-known flaws that limit their applications. A desirable neutron transport iteration method would be unconditionally stable and efficient. (Unconditionally stable methods are convergent for any spatial grid.) Most methods, such as DSA and CMFD, enable efficient and fast simulations for any scattering ratio, and for problems with optically

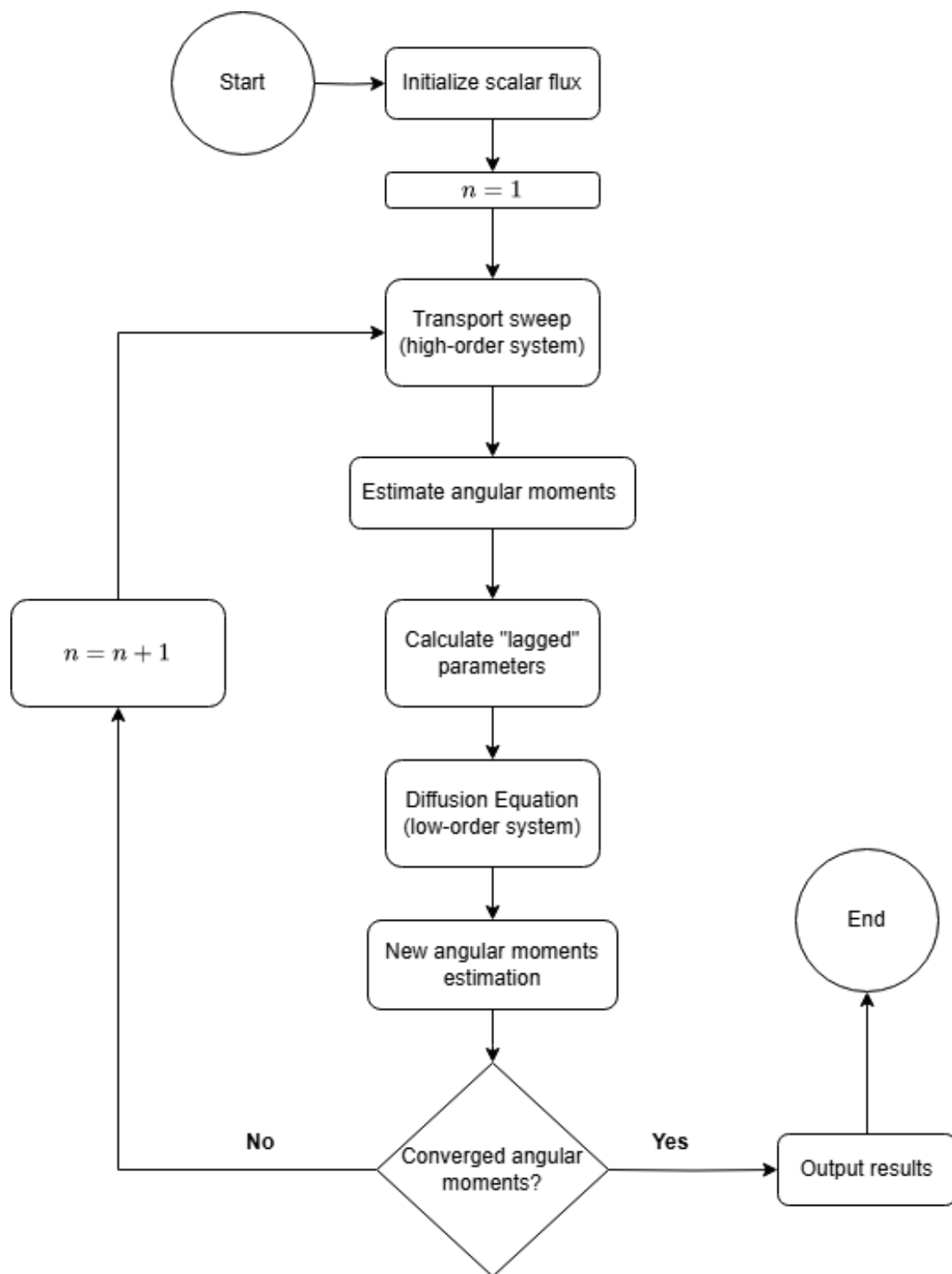


Figure 3.1: High-order/low-order schematics.

thin spatial cells [14, 17, 46]. However, these methods lose efficiency and eventually become unstable as the spatial cells become optically thicker.

A method used to generate *approximate* S_N solutions with high efficiency is the Quasidiffusion (QD) method [50–52]. This method has the advantage of being unconditionally stable and rapidly convergent for all spatial grids. However, it has the disadvantage of being *inconsistent* – upon convergence, the high-order QD scalar flux does not match the low-order QD scalar flux, and neither of these fluxes matches the S_N scalar flux. This inconsistency is caused by a truncation error in the QD equations. Therefore, the QD method is not a proper acceleration method for S_N problems – instead, it is a *rapidly-converging approximation method*. In the limiting case of optically thin cell sizes, the QD truncation errors limit to zero, and the QD solution converges to the S_N solution. (Only in the limit of optically thin cells can the QD method be considered “consistent.”)

The remarkable unconditional stability of the QD method is what led this research to consider a QD-based approach to develop a newer acceleration method. If the consistency issue of the high/low-order QD system can be resolved without impacting the method’s stability, it could lead to a significant new resource for the neutron transport community and industry.

The remainder of this chapter focuses on the detailed description of the CMFD method, which we utilize as a reference state-of-the-art algorithm. The QD method is also presented, as a basis for the newer Generalized Quasidiffusion (GQD) algorithm, developed subsequently in Chapter 4.

3.1 Coarse Mesh Finite Difference (CMFD) Derivation

In the following, we formulate the CMFD method for fixed source, planar geometry, monoenergetic, and isotropically-scattering neutron transport problems. We start this process from the S_N equations (Eqs. (2.36)):

$$\frac{\mu_n}{h_j} (\psi_{n,j+\frac{1}{2}} - \psi_{n,j-\frac{1}{2}}) + \Sigma_{t,j} \psi_{n,j} = \frac{\Sigma_{s,j}}{2} \sum_{n'=1}^N \psi_{n',j} w_{n'} + \frac{Q_j}{2}, \quad (3.1a)$$

$$\psi_{n,j} = \left(\frac{1 + \alpha_{n,j}}{2} \right) \psi_{n,j+\frac{1}{2}} + \left(\frac{1 - \alpha_{n,j}}{2} \right) \psi_{n,j-\frac{1}{2}}, \quad (3.1b)$$

$$\psi_{n,\frac{1}{2}} = \Psi_n^l, \mu_n > 0, \quad (3.1c)$$

$$\psi_{n,J+\frac{1}{2}} = \Psi_n^r, \mu_n < 0, \quad (3.1d)$$

$$\alpha_{n,j} = \frac{e^{\varepsilon_{n,j}} + e^{-\varepsilon_{n,j}}}{e^{\varepsilon_{n,j}} - e^{-\varepsilon_{n,j}}} - \frac{2}{\varepsilon_{n,j}}, \quad \varepsilon_{n,j} = \frac{\Sigma_{t,j} h_j}{\mu_n}. \quad (3.1e)$$

Here Eq. (3.1a) is the discrete ordinates approximation of the transport equation, Eq. (3.1b) and Eq. (3.1e) are the auxiliary equation and the SC differencing scheme. The boundary conditions are defined by Eqs. (3.1c) and (3.1d). These equations hold for the spatial grid $1 \leq j \leq J$ and discrete angles $1 \leq n \leq N$, with J being the total spatial cell's number in the system and N the number of discrete ordinates.

We define the cell-average and cell-edge angular flux moments from Eqs. (3.1) as:

$$\phi_{k,j} = \sum_{n=1}^N (\mu_n)^k \psi_{n,j} w_n, \quad \phi_{k,j+\frac{1}{2}} = \sum_{n=1}^N (\mu_n)^k \psi_{n,j+\frac{1}{2}} w_n. \quad (3.2)$$

These equations are the basis for the high-order CMFD system. If Eqs. (3.1) and Eq. (3.2) are solved iteratively in the manner described at the end of the previous chapter, this would directly result in the SI method. In fact, most of the high-order/low-order methods start from the SI formulation of the high-order equations, and then present a unique method for the low-order portion. The remainder of this derivation will work towards developing the low-order system particular to the CMFD method.

First, we multiply Eqs. (3.1c) and (3.1d) by $|\mu_n|w_n$ and sum each equation over the incident directions of flight, obtaining the incident partial currents:

$$\sum_{\mu_n > 0} \mu_n \psi_{n, \frac{1}{2}} w_n = \sum_{\mu_n > 0} \mu_n \Psi_n^l w_n \equiv \mathcal{J}_l^+ , \quad (3.3a)$$

$$\sum_{\mu_n < 0} |\mu_n| \psi_{n, J+\frac{1}{2}} w_n = \sum_{\mu_n < 0} |\mu_n| \Psi_n^r w_n \equiv \mathcal{J}_r^- . \quad (3.3b)$$

These partial currents attributed to the boundary conditions are fixed quantities and do not change throughout the iterations. They can be calculated and stored ahead of the iterative method. These partial currents will later be used to calculate the boundary conditions for the low-order system.

Next, we operate on Eq. (3.1a) by $\sum_{n=1}^N (\cdot) w_n$ to obtain the *neutron balance equation*:

$$\frac{1}{h_j} (\phi_{1, j+\frac{1}{2}} - \phi_{1, j-\frac{1}{2}}) + \Sigma_{a, j} \phi_{0, j} = Q_j . \quad (3.4a)$$

The neutron current $\phi_{1, j+\frac{1}{2}}$ is now defined by the discretized version of Eq. (2.19) (Fick's Law), with an additional correction term $\hat{D}_{j+\frac{1}{2}}$:

$$\phi_{1, j+\frac{1}{2}} = -D_{j+\frac{1}{2}} (\phi_{0, j+1} - \phi_{0, j}) + \hat{D}_{j+\frac{1}{2}} (\phi_{0, j+1} + \phi_{0, j}) . \quad (3.4b)$$

In this equation – which is an identity – the discretized dimensionless diffusion coefficient $D_{j+\frac{1}{2}}$ is defined as:

$$D_{j+\frac{1}{2}} = \frac{1}{3(\Sigma_t h)_{j+\frac{1}{2}}} , \quad (3.5a)$$

the term $(\Sigma_t h)_{j+\frac{1}{2}}$ is the optical thickness between the midpoints of two consecutive cells j and $j+1$:

$$(\Sigma_t h)_{j+\frac{1}{2}} = \frac{1}{2} (\Sigma_{t, j+1} h_{j+1} + \Sigma_{t, j} h_j) , \quad 1 \leq j \leq J-1 , \quad (3.5b)$$

and the last term $\hat{D}_{j+\frac{1}{2}}$ is defined as the *transport consistency factor*:

$$\hat{D}_{j+\frac{1}{2}} = \frac{\phi_{1,j+\frac{1}{2}} + \frac{1}{3(\Sigma_t h)_{j+\frac{1}{2}}} (\phi_{0,j+1} - \phi_{0,j})}{\phi_{0,j+1} + \phi_{0,j}} , \quad (3.5c)$$

which is an interface coefficient between cell j and $j+1$.

The transport consistency term ensures that upon convergence, the identity Eq. (3.5a) is satisfied by the high-order and low-order cell-average angular fluxes and cell-edge currents. This guarantees that the converged low-order scalar flux matches the scalar flux obtained by the high-order system (and the S_N solution).

Lastly, the low-order boundary conditions have to be defined. The left CMFD boundary condition is derived from Eq. (3.3a):

$$\begin{aligned} 2\mathcal{J}_l^+ &= \sum_{\mu_n > 0} 2\mu_n \psi_{n,\frac{1}{2}} w_n \\ &= \sum_{n=1}^N (\mu_n + |\mu_n|) \psi_{n,\frac{1}{2}} w_n \\ &= \sum_{n=1}^N \mu_n \psi_{n,\frac{1}{2}} w_n + \sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}} w_n \\ &= \phi_{1,\frac{1}{2}} + \left(\frac{\sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}} w_n}{\phi_{0,1}} \right) \phi_{0,1} \\ 2\mathcal{J}_l^+ &= \phi_{1,\frac{1}{2}} + B_l \phi_{0,1} , \end{aligned} \quad (3.6a)$$

where

$$B_l \equiv \frac{\sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}} w_n}{\phi_{0,1}} = \frac{\phi_{|1|,\frac{1}{2}}}{\phi_{0,\frac{1}{2}}} . \quad (3.6b)$$

This derivation can be extended to the right boundary condition (Eq. (3.3b)), yielding:

$$\begin{aligned}
2 \mathcal{J}_r^- &= \sum_{\mu_n < 0} 2|\mu_n| \psi_{n,J+\frac{1}{2}} w_n \\
&= \sum_{n=1}^N (-\mu_n + |\mu_n|) \psi_{n,J+\frac{1}{2}} w_n \\
&= - \sum_{n=1}^N \mu_n \psi_{n,J+\frac{1}{2}} w_n + \sum_{n=1}^N |\mu_n| \psi_{n,J+\frac{1}{2}} w_n \\
&= -\phi_{1,J+\frac{1}{2}} + \left(\frac{\sum_{n=1}^N |\mu_n| \psi_{n,J+\frac{1}{2}} w_n}{\phi_{0,1}} \right) \phi_{0,J} \\
2 \mathcal{J}_r^- &= -\phi_{1,J+\frac{1}{2}} + B_r \phi_{0,J} ,
\end{aligned} \tag{3.7a}$$

where

$$B_r \equiv \frac{\sum_{n=1}^N |\mu_n| \psi_{n,J+\frac{1}{2}} w_n}{\phi_{0,J}} = \frac{\phi_{|1|,J}}{\phi_{0,J}} . \tag{3.7b}$$

The aforementioned equations can now be used to build the CMFD's low-order system. Certain parameters – in particular, the transport consistency term Eq. (3.5c) and the boundary constants in Eqs. (3.6b) and (3.7b) – are assumed to be “stable.” If calculated in an iterative method, it is expected that these variables will not change significantly from one iteration to the next. (The transport consistency term have values $\hat{D}_{j+\frac{1}{2}} \approx 0$, and the boundary terms $B_{l,r} \approx \frac{1}{2}$.) Therefore, in iterative methods, these terms can be “lagged.” (A term that is “lagged” is calculated based on the estimates of the scalar flux and current obtained from the previous high-order transport sweep.)

The equations described above can now be formulated as a high-order/low-order iterative method. The iterative CMFD method starts with an estimation of the scalar flux $\phi_{0,j}^\ell$ as a known value from the previous iteration ℓ (or user defined if $\ell = 0$). This estimate is used to calculate the scattering source, which is used to solve the high-order system. The high-order S_N equations (Eqs. (3.1)) are solved through a transport sweep (identical to the SI method (Eqs. (2.39))), obtaining the $(\ell + \frac{1}{2})$ estimate for the angular flux ($\psi_{n,j}^{\ell+\frac{1}{2}}$).

Differently from the SI method, the angular flux ($\psi_{n,j}^{\ell+\frac{1}{2}}$) is used to calculate an intermediate scalar flux ($\phi_{0,j}^{\ell+\frac{1}{2}}$, instead of $\phi_{0,j}^{\ell+1}$). This intermediate estimation of the scalar flux – and the estimates of other angular flux moments – are then used to calculate the “lagged” parameters ($\hat{D}_{j+\frac{1}{2}}^{\ell+\frac{1}{2}}$, $B_l^{\ell+\frac{1}{2}}$, and $B_r^{\ell+\frac{1}{2}}$) for the low-order system.

The low-order diffusion system is then solved, using standard numerical linear algebraic methods, to obtain the next estimate of the neutron scalar flux ($\phi_{0,j}^{\ell+1}$). This completes the description of the $(\ell+1)^{st}$ CMFD iteration. If necessary, a new iteration can now begin.

A summary of CMFD’s equations with the iterative indexes is provided next.

3.1.1 Algorithm Summary (CMFD)

A CMFD iteration consists of the following two steps: (i) a high-order transport sweep, and (ii) a low-order diffusion calculation. The overview of each is described below.

(i) High-Order Transport Sweep

The CMFD iterative method starts its $(\ell+1)^{st}$ iteration with a transport sweep and the calculation of the angular flux moments by solving Eqs. (3.1), Eq. (3.2), and Eqs. (3.3):

$$\frac{\mu_n}{h_j} \left(\psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}} \right) + \Sigma_{t,j} \psi_{n,j}^{\ell+\frac{1}{2}} = \frac{\Sigma_{s,j}}{2} \phi_{0,j}^{\ell} + \frac{Q_j}{2}, \quad (3.8a)$$

$$\psi_{n,j}^{\ell+\frac{1}{2}} = \left(\frac{1 + \alpha_{n,j}}{2} \right) \psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} + \left(\frac{1 - \alpha_{n,j}}{2} \right) \psi_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}}, \quad (3.8b)$$

$$\psi_{n,\frac{1}{2}}^{\ell+\frac{1}{2}} = \Psi_n^l, \quad \mu_n > 0, \quad (3.8c)$$

$$\psi_{n,J+\frac{1}{2}}^{\ell+\frac{1}{2}} = \Psi_n^r, \quad \mu_n < 0, \quad (3.8d)$$

and:

$$\phi_{k,j}^{\ell+\frac{1}{2}} = \sum_{n=1}^N \mu_n^k \psi_{n,j}^{\ell+\frac{1}{2}} w_n \quad (k=0,2) \quad , \quad \phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} = \sum_{n=1}^N \mu_n \psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} w_n \quad , \quad (3.9a)$$

$$\phi_{|1|,\frac{1}{2}}^{\ell+\frac{1}{2}} \equiv \sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}}^{\ell+\frac{1}{2}} w_n \quad , \quad \phi_{|1|,J+\frac{1}{2}}^{\ell+\frac{1}{2}} \equiv \sum_{n=1}^N |\mu_n| \psi_{n,J+\frac{1}{2}}^{\ell+\frac{1}{2}} w_n \quad . \quad (3.9b)$$

(ii) Low-Order Diffusion Calculation

Next, we calculate certain “lagged” parameters from Eq. (3.5c), Eq. (3.6b), and Eq. (3.7b):

$$\hat{D}_{j+\frac{1}{2}}^{\ell+\frac{1}{2}} = \frac{\phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} + D_{j+\frac{1}{2}} (\phi_{0,j+1}^{\ell+\frac{1}{2}} - \phi_{0,j}^{\ell+\frac{1}{2}})}{\phi_{0,j+1}^{\ell+\frac{1}{2}} + \phi_{0,j}^{\ell+\frac{1}{2}}} \quad , \quad (3.10a)$$

$$B_l^{\ell+\frac{1}{2}} = \frac{\phi_{|1|,\frac{1}{2}}^{\ell+\frac{1}{2}}}{\phi_{0,1}^{\ell+\frac{1}{2}}} \quad , \quad B_r^{\ell+\frac{1}{2}} = \frac{\phi_{|1|,J+\frac{1}{2}}^{\ell+\frac{1}{2}}}{\phi_{0,J}^{\ell+\frac{1}{2}}} \quad . \quad (3.10b)$$

Then we introduce these “lagged” terms in Eqs. (3.4), Eqs. (3.6), and Eqs. (3.7), and solve the resulting diffusion problem (with the transport consistency term):

$$\frac{1}{h_j} (\phi_{1,j+\frac{1}{2}}^{\ell+1} - \phi_{1,j-\frac{1}{2}}^{\ell+1}) + \Sigma_{a,j} \phi_{0,j}^{\ell+1} = Q_j \quad , \quad (3.11a)$$

$$\phi_{1,j+\frac{1}{2}}^{\ell+1} = -D_{j+\frac{1}{2}} (\phi_{0,j+1}^{\ell+1} - \phi_{0,j}^{\ell+1}) + \hat{D}_{j+\frac{1}{2}}^{\ell+\frac{1}{2}} (\phi_{0,j+1}^{\ell+\frac{1}{2}} + \phi_{0,j}^{\ell+\frac{1}{2}}) \quad , \quad (3.11b)$$

$$\phi_{1,\frac{1}{2}}^{\ell+1} = 2 \mathcal{J}_l^+ - B_l^{\ell+\frac{1}{2}} \phi_{0,1}^{\ell+1} \quad , \quad (3.11c)$$

$$\phi_{1,J+\frac{1}{2}}^{\ell+1} = -2 \mathcal{J}_r^- + B_r^{\ell+\frac{1}{2}} \phi_{0,J}^{\ell+1} \quad . \quad (3.11d)$$

In Eqs. (3.11), the scalar flux $\phi_{0,j}^{\ell+1}$ in cell j is directly coupled to the adjacent scalar fluxes. In the case of planar geometry, this results in a standard tridiagonal matrix system that can be solved using the *Tridiagonal Matrix algorithm* [74] (TDMA).

The CMFD method provides rapidly converging solutions for spatial grids in which the cell’s optical thicknesses are sufficiently small. However, the CMFD method becomes

less efficient as the optical thickness of the cells increases. If a certain critical cell optical thickness is reached, the method becomes unstable and will fail to converge.

3.2 Quasidiffusion (QD) Method – Derivation

In the following, we formulate the QD method for fixed source, planar geometry, monoenergetic, and isotropically-scattering neutron transport problems. Similarly to the CMFD formulation, we start this derivation from the S_N equations (Eqs. (2.36)):

$$\frac{\mu_n}{h_j}(\psi_{n,j+\frac{1}{2}} - \psi_{n,j-\frac{1}{2}}) + \Sigma_{t,j}\psi_{n,j} = \frac{\Sigma_{s,j}}{2} \sum_{n'=1}^N \psi_{n',j} w_{n'} + \frac{Q_j}{2}, \quad (3.12a)$$

$$\psi_{n,j} = \left(\frac{1 + \alpha_{n,j}}{2}\right) \psi_{n,j+\frac{1}{2}} + \left(\frac{1 - \alpha_{n,j}}{2}\right) \psi_{n,j-\frac{1}{2}}, \quad (3.12b)$$

$$\psi_{n,\frac{1}{2}} = \Psi_n^l, \mu_n > 0, \quad (3.12c)$$

$$\psi_{n,J+\frac{1}{2}} = \Psi_n^r, \mu_n < 0, \quad (3.12d)$$

$$\alpha_{n,j} = \frac{e^{\varepsilon_{n,j}} + e^{-\varepsilon_{n,j}}}{e^{\varepsilon_{n,j}} - e^{-\varepsilon_{n,j}}} - \frac{2}{\varepsilon_{n,j}}, \quad \varepsilon_{n,j} = \frac{\Sigma_{t,j} h_j}{\mu_n}. \quad (3.12e)$$

As previously stated in the CMFD method, we opted to use the SC differencing scheme (Eq. (3.12e)). The above equations hold for the spatial grid $1 \leq j \leq J$ and discrete angles $1 \leq n \leq N$.

The cell-average and cell-edge angular flux moments are computed as in Eq. (3.2):

$$\phi_{k,j} = \sum_{n=1}^N (\mu_n)^k \psi_{n,j} w_n, \quad \phi_{k,j+\frac{1}{2}} = \sum_{n=1}^N (\mu_n)^k \psi_{n,j+\frac{1}{2}} w_n, \quad (3.13)$$

and the partial currents as in Eqs. (3.3):

$$\sum_{\mu_n > 0} \mu_n \psi_{n,\frac{1}{2}} w_n = \sum_{\mu_n > 0} \mu_n \Psi_n^l w_n \equiv \mathcal{J}_l^+, \quad (3.14a)$$

$$\sum_{\mu_n < 0} |\mu_n| \psi_{n,J+\frac{1}{2}} w_n = \sum_{\mu_n < 0} |\mu_n| \Psi_n^r w_n \equiv \mathcal{J}_r^-. \quad (3.14b)$$

This concludes the derivation of the high-order system for the QD method. Up to this point, the QD derivation is identical to the CMFD method. The remainder of this section

is focused on the derivation of the low-order QD system, which differs from the low-order CMFD system.

As we previously stated, the QD method is *inconsistent* because the high-order and low-order fluxes do not converge to the same value. This difference is caused by a truncation error in the low-order QD system. This error vanishes only when the optical cell widths $\Sigma_t h$ limit to zero.

For this reason, we present the low-order QD fluxes and currents with a different nomenclature, $\Phi_{0,j}$ and $\Phi_{1,j}$, respectively. We did this to make it clear that the converged high-order and low-order scalar fluxes and currents are not the same – they are distinct and different quantities.

To initiate the low-order derivation, we operate on the S_N equations (Eqs. (3.12)) by $\sum_{n=1}^N (\cdot) w_n$ to obtain the neutron balance equation:

$$\frac{1}{h_j} (\Phi_{1,j+\frac{1}{2}} - \Phi_{1,j-\frac{1}{2}}) + \Sigma_{a,j} \Phi_{0,j} = Q_j , \quad (3.15)$$

where the terms $\Phi_{0,j}$ and $\Phi_{1,j+\frac{1}{2}}$ are the low-order cell-average scalar flux and cell-edge current.

However, instead of using Fick's Law (plus a transport consistency term) approximation to the neutron current (Eq. (3.5a)), an approximate equation is used instead. To motivate this approximation, we operate Eq. (3.12a) by $\sum_{n=1}^N \mu_n (\cdot) w_n$ and obtain:

$$\begin{aligned} \Phi_{1,j} &= -\frac{1}{\Sigma_{t,j} h_j} (\Phi_{2,j+\frac{1}{2}} - \Phi_{2,j-\frac{1}{2}}) \\ &= -\frac{1}{\Sigma_{t,j} h_j} (E_{j+\frac{1}{2}} \Phi_{0,j+\frac{1}{2}} - E_{j-\frac{1}{2}} \Phi_{0,j-\frac{1}{2}}) , \end{aligned} \quad (3.16a)$$

which is “centered” on cell j . Equation (3.16a) uses the *cell-edge Eddington factors*, defined by:

$$E_{j+\frac{1}{2}} \equiv \frac{\phi_{2,j+\frac{1}{2}}}{\phi_{0,j+\frac{1}{2}}} . \quad (3.16b)$$

The QD method uses an approximate relationship, which is similar to Equations (3.16), but instead centered on a cell edge:

$$\Phi_{1,j+\frac{1}{2}} \approx -\frac{1}{(\Sigma_l h)_{j+\frac{1}{2}}} \left(E_{j+1} \Phi_{0,j+1} - E_j \Phi_{0,j} \right) , \quad (3.17a)$$

in which the cell-average Eddington factors are defined as:

$$E_j = \frac{\phi_{2,j}}{\phi_{0,j}} . \quad (3.17b)$$

It is important to note that Eqs. (3.16) are satisfied exactly by the converged S_N solution, but Eqs. (3.17) are not satisfied exactly. The approximation occurring in Eqs. (3.17) is the one that introduces the truncation error in the low-order QD solution.

The boundary conditions are derived the same way as is done in Eqs. (3.6), with the left QD boundary condition given as:

$$\begin{aligned} 2 \mathcal{J}_l^+ &= \sum_{\mu_n > 0} 2 \mu_n \psi_{n,\frac{1}{2}} w_n \\ &= \sum_{n=1}^N (\mu_n + |\mu_n|) \psi_{n,\frac{1}{2}} w_n \\ &= \sum_{n=1}^N \mu_n \psi_{n,\frac{1}{2}} w_n + \sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}} w_n \\ &= \Phi_{1,\frac{1}{2}} + \left(\frac{\sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}} w_n}{\phi_{0,1}} \right) \phi_{0,1} \\ 2 \mathcal{J}_l^+ &= \Phi_{1,\frac{1}{2}} + B_l \phi_{0,1} , \end{aligned} \quad (3.18a)$$

where

$$B_l \equiv \frac{\sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}} w_n}{\phi_{0,1}} = \frac{\phi_{|1|,\frac{1}{2}}}{\phi_{0,\frac{1}{2}}} . \quad (3.18b)$$

The same derivation can be extended to the right boundary condition (Eqs. (3.7)), yielding:

$$2 \mathcal{J}_r^- = -\Phi_{1,J+\frac{1}{2}} + B_r \phi_{0,J} , \quad (3.19a)$$

where

$$B_r \equiv \frac{\sum_{n=1}^N |\mu_n| \psi_{n,J+\frac{1}{2}} w_n}{\phi_{0,J}} = \frac{\phi_{|1|,J}}{\phi_{0,J}} . \quad (3.19b)$$

The equations presented so far in this section form the classical QD low-order equations. However, for future comparisons between the CMFD and GQD methods, we will slightly change the notation and redefine the Eddington factors as:

$$E_j = \frac{3\phi_{2,j}}{\phi_{0,j}} . \quad (3.20a)$$

Then, Eq. (3.17a) can be written as:

$$\Phi_{1,j+\frac{1}{2}} \approx -D_{j+\frac{1}{2}} \left(E_{j+1} \Phi_{0,j+1} - E_j \Phi_{0,j} \right) . \quad (3.20b)$$

An iterative procedure similar to that presented for CMFD can now be applied to the QD method. The iterative QD method starts with a scalar flux $\Phi_{0,j}^\ell$ estimate from the previous iteration ℓ (or assigned if $\ell = 0$). This estimate provides the scattering source for the high-order S_N equations (Eqs. (3.1)), which are solved through a transport sweep, obtaining the angular flux ($\psi_{n,j}^{\ell+\frac{1}{2}}$). As in the CMFD method, the angular flux moments obtained during the transport sweep are used to calculate the “lagged” parameters for the low-order QD system. However, the QD method uses the cell-average Eddington factors (Eq. (3.17b)), instead of the transport consistency term, as the “lagged” terms. (The Eddington factors in Eq. (3.20a) have values in the range of $E_j \approx 1$.) The low-order diffusion system (Eqs. (3.4) and Eqs. (3.5)) is then solved to obtain the next iteration estimative for the neutron scalar flux ($\Phi_{0,j}^{\ell+1}$).

The principal differences between the low-order QD equations and the low-order CMFD equations are (i) the addition of Eddington factors, and (ii) the absence of the transport consistency factor. The Eddington factors introduce a partial transport correction to the current equation, and are defined as the ratio of the second and zeroth angular flux moments. This correction only ensures consistency between the high-order, low-order, and S_N scalar fluxes when the optical thickness of the spatial cells limits to 0. For problems in which the optical thickness of the spatial cells is not zero, the converged high-order QD scalar flux, the converged low-order QD scalar flux, and the scalar flux solution of the S_N equations are all different, due to the truncation error in Eq. (3.20b) described above.

A summary of QD's equations with the iterative indexes is provided below.

3.2.1 Algorithm Summary (QD)

As in the CMFD method, each iteration of the QD method consists of two steps: (i) a high-order transport sweep, and (ii) a low-order diffusion calculation. The CMFD and QD methods have the same high-order transport sweep, changing just the low-order system and the lagged parameters. For the QD method, we have the following:

(i) High-Order Transport Sweep

The QD high-order transport sweep is the same as presented in Eq. (3.15):

$$\frac{\mu_n}{h_j} \left(\psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}} \right) + \Sigma_{t,j} \psi_{n,j}^{\ell+\frac{1}{2}} = \frac{\Sigma_{s,j}}{2} \Phi_{0,j}^{\ell} + \frac{Q_j}{2}, \quad (3.21a)$$

$$\psi_{n,j}^{\ell+\frac{1}{2}} = \left(\frac{1 + \alpha_{n,j}}{2} \right) \psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} + \left(\frac{1 - \alpha_{n,j}}{2} \right) \psi_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}}, \quad (3.21b)$$

$$\psi_{n,\frac{1}{2}}^{\ell+\frac{1}{2}} = \Psi_n^l, \quad \mu_n > 0, \quad (3.21c)$$

$$\psi_{n,J+\frac{1}{2}}^{\ell+\frac{1}{2}} = \Psi_n^r, \quad \mu_n < 0. \quad (3.21d)$$

The angular flux moments needed for the low-order calculation are calculated the same way as in Eqs. (3.9):

$$\phi_{k,j}^{\ell+\frac{1}{2}} = \sum_{n=1}^N \mu_n^k \psi_{n,j}^{\ell+\frac{1}{2}} w_n \quad (k=0,2) \quad , \quad \phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} = \sum_{n=1}^N \mu_n \psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} w_n \quad , \quad (3.22a)$$

$$\phi_{|1|,\frac{1}{2}}^{\ell+\frac{1}{2}} \equiv \sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}}^{\ell+\frac{1}{2}} w_n \quad , \quad \phi_{|1|,J+\frac{1}{2}}^{\ell+\frac{1}{2}} \equiv \sum_{n=1}^N |\mu_n| \psi_{n,J+\frac{1}{2}}^{\ell+\frac{1}{2}} w_n \quad . \quad (3.22b)$$

(ii) Low-Order Diffusion Calculation

The low-order QD system differs from the low-order CMFD system, having the Eddington factors ($E_j^{\ell+\frac{1}{2}}$) present in Eq. (3.20b) instead of a transport consistency term ($\hat{D}_{j+\frac{1}{2}}^{\ell+\frac{1}{2}}$). The Eddington factors and boundary consistency terms are calculated from the above angular flux moments by

$$E_j^{\ell+\frac{1}{2}} = \frac{3\phi_{2,j}^{\ell+\frac{1}{2}}}{\phi_{0,j}^{\ell+\frac{1}{2}}} \quad , \quad B_l^{\ell+\frac{1}{2}} = \frac{\phi_{|1|,\frac{1}{2}}^{\ell+\frac{1}{2}}}{\phi_{0,1}^{\ell+\frac{1}{2}}} \quad , \quad B_r^{\ell+\frac{1}{2}} = \frac{\phi_{|1|,J+\frac{1}{2}}^{\ell+\frac{1}{2}}}{\phi_{0,J}^{\ell+\frac{1}{2}}} \quad . \quad (3.23)$$

These lagged quantities are then introduced into the low-order equations:

$$\frac{1}{h_j} (\Phi_{1,j+\frac{1}{2}}^{\ell+1} - \Phi_{1,j-\frac{1}{2}}^{\ell+1}) + \Sigma_{a,j} \Phi_{0,j}^{\ell+1} = Q_j \quad , \quad 1 \leq j \leq J \quad , \quad (3.24a)$$

$$\Phi_{1,j+\frac{1}{2}}^{\ell+1} = -D_{j+\frac{1}{2}} (E_{j+1}^{\ell+\frac{1}{2}} \Phi_{0,j+1}^{\ell+1} - E_j^{\ell+\frac{1}{2}} \Phi_{0,j}^{\ell+1}) \quad , \quad 1 \leq j \leq J-1 \quad , \quad (3.24b)$$

$$\Phi_{1,\frac{1}{2}}^{\ell+1} = 2 \mathcal{J}_l^+ - B_l^{\ell+\frac{1}{2}} \Phi_{0,1}^{\ell+1} \quad , \quad (3.24c)$$

$$\Phi_{1,J+\frac{1}{2}}^{\ell+1} = -2 \mathcal{J}_r^- + B_r^{\ell+\frac{1}{2}} \Phi_{0,J}^{\ell+1} \quad . \quad (3.24d)$$

The system of equations in Eq. (3.24) is similar to the CMFD Eqs. (3.11). Both matrix systems can be solved using a TDMA algorithm. However, unlike the CMFD method, the low-order QD system yields a different scalar flux solution from the high-order system.

The CMFD and QD methods have certain similarities. Both methods use the same transport sweep. Both methods use the neutron balance equation for the low-order system. Their differences arise only when defining the accelerated cell-edge currents in terms of

the adjacent accelerated scalar fluxes. One method (CMFD) employs an additive consistency term ($\hat{D}_{j+\frac{1}{2}}$) (which is defined by cell-edge values), and the other (QD) introduces a “transport” scaling factor (E_j) (which is a cell-average quantity) multiplied to the scalar flux.

These different approaches cause QD and CMFD to behave differently in regard to solution and stability. The QD method is unconditionally stable but provides an inconsistent solution, and CMFD provides a consistent solution but can become unstable depending on the simulation parameters.

A Consistent Quasidiffusion (CQD) method, previously developed in [57, 58], explored the use of both CMFD and QD ideas. That method utilized both cell-average Eddington factors and cell-edge transport consistency terms. Although CQD is a consistent acceleration method, it is not unconditionally stable. (It actually has a performance similar to that of CMFD.)

This motivated the work of the present dissertation on ensuring solution consistency, by adjusting the cell-average Eddington factors (making them consistent), instead of adding a cell-edge consistency term. This idea is presented next in Chapter 4, where we introduce the new *Generalized Quasidiffusion* (GQD) method.

Chapter 4: The Generalized Quasidiffusion (GQD) Method

In Chapter 3, we presented two widely-used methods (CMFD and QD) to accelerate the iterative convergence of neutron transport calculations. These methods have advantages and disadvantages. The CMFD method yields a consistent solution but has only conditional stability. The QD method has unconditional stability but yields an inconsistent solution. A third method (CQD) uses elements of both CMFD and QD. CQD achieves a consistent solution, but unfortunately, not unconditional stability [57, 58]. The fact that CQD provides similar stability as CMFD led us to understand that although the addition of CMFD-like cell interface consistency terms is effective in ensuring consistency, it apparently also creates the loss of stability for coarser spatial grids.

In light of that, we shifted our approach away from adding cell-edge consistency terms to only using cell-average corrections. Instead of adding a *transport consistency term* at cell interfaces ($\hat{D}_{j+\frac{1}{2}}$), the new method will modify the cell-average Eddington factors (E_j) of the QD method to make them “consistent.” The new “consistent” Eddington factors would hopefully (i) ensure that the solution of the low-order system matches the high-order (S_N) solution, and (ii) avoid generating numerical instabilities for thicker spatial cells.

The new method presented in this dissertation is a variant of the classical QD method, allowing corrections of the Eddington factors to provide a consistent solution. Therefore, our new acceleration method is called the *Generalized Quasidiffusion* (GQD) method. The

key to this new method is finding a way to preserve the high- and low-order fluxes so the method is consistent, in such a way that we avoid introducing cell-edge consistency terms.

The approach that we use defines new Eddington factors that *preserve the net neutron leakage exiting from each spatial cell, between the high- and low-order systems*. This condition provides exactly one equation for each spatial cell – which is the same as the number of Eddington factors per cell. It is easily shown that this condition ensures that the converged high-order and low-order cell-averaged scalar fluxes must be identical.

In the QD method, the inconsistent Eddington factors are calculated directly from estimates of angular flux moments obtained during the previous transport sweep. In the GQD method, the new consistent Eddington factors must also be calculated during each iteration, using a slightly more expensive procedure. Thus, the new *consistent Eddington factors* are not known quantities (Eq. (3.20a)), but rather are unknowns that are obtained during the calculation.

The first major procedural difference between the GQD and QD method is that the GQD method requires one to solve an “intermediate” system of equations to obtain the consistent Eddington factors, instead of using Eq. (3.20a). The system of equations obtained for this intermediate step is singular. The Fredholm Alternative Theorem ensures that the system has **an infinite number of nontrivial solutions**, but regular linear solvers might encounter difficulties because the system is singular. However, in the special case of planar geometry (the geometry considered in this dissertation), it is possible to solve the intermediate system in closed form, without having to use an expensive algorithm. This is the approach that we followed in our numerical simulations.

The second aspect of solving the intermediate system is that it does not automatically guarantee non-negative (consistent) Eddington factors. (Negative Eddington factors will

almost certainly lead to numerical instability in the iterative method.) Fortunately, the solution of the intermediate system is not unique, and it is always possible to determine solutions that are everywhere positive. Doing this properly is key to the GQD method's success.

The third important addition to the new GQD method is the correction to the diffusion coefficient used in the low-order part of an iteration. Specifically, in its low-order diffusion calculation, the GQD method (applied to problems discretized using the Step Characteristic spatial discretization scheme) employs a slightly different diffusion coefficient, to improve the algorithm's stability for optically thick spatial cells. This formulation of the diffusion coefficient is the same as the one already proposed in [37, 38].

To summarize, the GQD formulation resembles the QD method, except for three key aspects: (i) solving the intermediate equations for the consistent Eddington factors, (ii) properly ensuring that the new Eddington factors are positive, and (iii) using the modified diffusion coefficient. The resulting formulation of the GQD method is consistent, stable, and rapidly-converging for any choice of spatial grid.

4.1 Generalized Quasidiffusion (GQD) method – Derivation

This section follows a similar structure to that of Chapter 3. We formulate the GQD method for fixed-source, planar-geometry, monoenergetic, and isotropically-scattering neutron transport problems. We opted to use SC as the differencing scheme.

The high-order system is derived from the S_N equations with SC spatial differencing (Eqs. (2.36)):

$$\frac{\mu_n}{h_j} (\psi_{n,j+\frac{1}{2}} - \psi_{n,j-\frac{1}{2}}) + \Sigma_{t,j} \psi_{n,j} = \frac{\Sigma_{s,j}}{2} \sum_{n'=1}^N \psi_{n',j} w_{n'} + \frac{Q_j}{2}, \quad (4.1a)$$

$$\psi_{n,j} = \left(\frac{1 + \alpha_{n,j}}{2} \right) \psi_{n,j+\frac{1}{2}} + \left(\frac{1 - \alpha_{n,j}}{2} \right) \psi_{n,j-\frac{1}{2}}, \quad (4.1b)$$

$$\psi_{n,\frac{1}{2}} = \Psi_n^l, \quad \mu_n > 0, \quad (4.1c)$$

$$\psi_{n,J+\frac{1}{2}} = \Psi_n^r, \quad \mu_n < 0, \quad (4.1d)$$

$$\alpha_{n,j} = \frac{e^{\varepsilon_{n,j}} + e^{-\varepsilon_{n,j}}}{e^{\varepsilon_{n,j}} - e^{-\varepsilon_{n,j}}} - \frac{2}{\varepsilon_{n,j}}, \quad \varepsilon_{n,j} = \frac{\Sigma_{t,j} h_j}{\mu_n}. \quad (4.1e)$$

The above equations hold for the spatial grid $1 \leq j \leq J$ and discrete angles $1 \leq n \leq N$.

The cell-average and cell-edge angular flux moments are computed as in Eq. (3.2):

$$\phi_{k,j} = \sum_{n=1}^N (\mu_n)^k \psi_{n,j} w_n, \quad \phi_{k,j+\frac{1}{2}} = \sum_{n=1}^N (\mu_n)^k \psi_{n,j+\frac{1}{2}} w_n, \quad (4.2)$$

and the partial currents as in Eqs. (3.3):

$$\sum_{\mu_n > 0} \mu_n \psi_{n,\frac{1}{2}} w_n = \sum_{\mu_n > 0} \mu_n \Psi_n^l w_n \equiv \mathcal{J}_l^+, \quad (4.3a)$$

$$\sum_{\mu_n < 0} |\mu_n| \psi_{n,J+\frac{1}{2}} w_n = \sum_{\mu_n < 0} |\mu_n| \Psi_n^r w_n \equiv \mathcal{J}_r^-. \quad (4.3b)$$

This concludes the high-order derivation. This *transport sweep* uses the previous scalar flux estimate to compute the scattering source. Then, it calculates a new set of angular moments that will feed the calculation of the “lagged” parameters for the low-order system.

The formulation of the low-order GQD system can be derived from the inconsistent QD method. Thus, we now consider the low-order QD system of equation:

$$E_j = \frac{3\phi_{2,j}}{\phi_{0,j}}, \quad 1 \leq j \leq J, \quad (4.4a)$$

$$B_l = \frac{\Phi_{|1|,\frac{1}{2}}}{\phi_{0,1}}, \quad B_r = \frac{\Phi_{|1|,J+\frac{1}{2}}}{\phi_{0,J}}, \quad (4.4b)$$

and:

$$\frac{1}{h_j}(\Phi_{1,j+\frac{1}{2}} - \Phi_{1,j-\frac{1}{2}}) + \Sigma_{a,j}\Phi_{0,j} = Q_j, \quad 1 \leq j \leq J, \quad (4.4c)$$

$$\Phi_{1,j+\frac{1}{2}} = -D_{j+\frac{1}{2}}(E_{j+1}\Phi_{0,j+1} - E_j\phi_{0,j}), \quad 1 \leq j \leq J-1, \quad (4.4d)$$

$$\Phi_{1,\frac{1}{2}} = 2\mathcal{J}_l^+ - B_l\Phi_{0,1}, \quad (4.4e)$$

$$\Phi_{1,J+\frac{1}{2}} = -2\mathcal{J}_r^- + B_r\Phi_{0,J}. \quad (4.4f)$$

In Eq. (4.4d), the Eddington factors are defined by the classical formulation Eq. (4.4a), and the low-order scalar fluxes ($\Phi_{0,j}$) are not consistent with the high-order scalar fluxes ($\phi_{0,j}$) because Eq. (4.4d) is not exactly satisfied by the S_N solution. The idea of the GQD method is (i) to define and calculate the cell-average Eddington factors E_j in such way that the method becomes consistent ($\phi_{0,j} = \Phi_{0,j}$), and (ii) to define diffusion coefficients D_j such that the method becomes unconditionally stable.

One difficulty in coming up with a *cell-average transport consistency term* is the lack of equations to preserve all the cell-edge currents. The CMFD method's main idea is to preserve each cell-edge current, by adding cell-edge transport consistency terms. However, the usage of cell-average terms does not provide enough equations to do this.

1-D problems with J spatial cells have a total of J Eddington factors, with a total of $J-1$ interior cell-edges. For this special 1-D geometry, there is a sufficient number of Eddington factors to “preserve” all high-order interior cell-edge currents. However, for 2-D problems with rectangular $J \times K$ cells, there are JK cells (and Eddington factors) and $K(J-1) + J(K-1) = 2JK - J - K$ interior cell edges. Thus, there are about twice as many interior cell edges as there are cells, so the number of Eddington factors is insufficient to preserve all the high-order cell-edge currents. In 3-D systems, the lack of enough Eddington factors is even more pronounced.

The GQD method does not aim to preserve the cell-edge currents. Instead, *it preserves the net neutron leakage from each cell*. (In any geometry, the number of net leakages from each cell equals the number of cells, which equals the number of Eddington factors.) Thus, for each 1-D cell j , the net high-order transport leakage out of cell j is required to equal the net low-order diffusion leakage out of cell j :

$$\boxed{\frac{1}{h_j}(\Phi_{1,j+\frac{1}{2}} - \Phi_{1,j-\frac{1}{2}}) = \frac{1}{h_j}(\phi_{1,j+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}), \quad 1 \leq j \leq J} . \quad (4.5)$$

In 2-D and 3-D problems, there would also be a similar equation for each spatial cell.

To prove that these conditions provide a consistent solution, we consider the low-order neutron balance equation Eq. (4.4c):

$$\frac{1}{h_j}(\Phi_{1,j+\frac{1}{2}} - \Phi_{1,j-\frac{1}{2}}) + \Sigma_{a,j}\Phi_{0,j} = Q_j, \quad 1 \leq j \leq J. \quad (4.6)$$

Substituting Eq. (4.6) into the high-order neutron balance equation Eq. (3.4a), we obtain:

$$\begin{aligned} \frac{1}{h_j}(\Phi_{1,j+\frac{1}{2}} - \Phi_{1,j-\frac{1}{2}}) + \Sigma_{a,j}\Phi_{0,j} &= \frac{1}{h_j}(\phi_{1,j+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}) + \Sigma_{a,j}\phi_{0,j}, \\ 1 \leq j \leq J. \end{aligned} \quad (4.7a)$$

If Eq. (4.5) is satisfied, then we immediately obtain:

$$\Phi_{j,0} = \phi_{j,0}, \quad 1 \leq j \leq J. \quad (4.7b)$$

For the boundary conditions Eqs. (4.4e) and (4.4f) can be introduced in Eqs. (3.6) and Eqs. (3.7), leading to:

$$\Phi_{1,\frac{1}{2}} + B_l\Phi_{0,1} = \phi_{1,\frac{1}{2}} + B_l\phi_{0,1}, \quad (4.7c)$$

and

$$\Phi_{1,J+\frac{1}{2}} - B_r\Phi_{0,J} = \phi_{1,J+\frac{1}{2}} - B_r\phi_{0,J}. \quad (4.7d)$$

which has the “consistent” solution $\Phi_{1,\frac{1}{2}} = \phi_{1,\frac{1}{2}}$, and $\Phi_{1,J+\frac{1}{2}} = \phi_{1,J+\frac{1}{2}}$.

Eq. (4.5) have three major implications:

- The low-order cell-average scalar fluxes must equal the high-order cell-average scalar fluxes ($\Phi_{0,j} = \phi_{0,j}$, $1 \leq j \leq J$).
- Since $\Phi_{0,1} = \phi_{0,1}$, Eq. (4.7c) implies that the current of the leftmost cell edge is preserved ($\Phi_{1,\frac{1}{2}} = \phi_{1,\frac{1}{2}}$).
- Since $\Phi_{0,J} = \phi_{0,J}$, Eq. (4.7d) implies that the current of the rightmost cell edge is preserved ($\Phi_{1,J+\frac{1}{2}} = \phi_{1,J+\frac{1}{2}}$).

Thus, the analysis performed in Equations (4.7) has a clear implication: *preserving the net leakages from each spatial cell guarantees that, upon convergence, the low-order cell-average scalar fluxes are equal to the high-order cell-average scalar fluxes.*

To proceed, we modify the low-order QD system presented in Eqs. (4.4) to account for the following changes: (i) the Eddington factors are no longer known coefficients defined by Eq. (4.4a) (thus, these equations are removed), (ii) we view the cell-average Eddington factors (E_j) as unknowns, and (iii) we introduce the net leakage balance equations (Eq. (4.5)).

Making these changes, Eqs. (4.4) and Eq. (4.5) can be written:

$$\frac{1}{h_j}(\Phi_{1,j+\frac{1}{2}} - \Phi_{1,j-\frac{1}{2}}) + \Sigma_{a,j}\phi_{0,j} = Q_j, \quad 1 \leq j \leq J, \quad (4.8a)$$

$$\frac{1}{h_j}(\Phi_{1,j+\frac{1}{2}} - \Phi_{1,j-\frac{1}{2}}) = \frac{1}{h_j}(\phi_{1,j+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}), \quad 1 \leq j \leq J, \quad (4.8b)$$

$$\Phi_{1,j+\frac{1}{2}} = -D_{j+\frac{1}{2}}(3E_{j+1}\phi_{0,j+1} - 3E_j\phi_{0,j}), \quad 1 \leq j \leq J-1, \quad (4.8c)$$

$$\Phi_{1,\frac{1}{2}} = \phi_{1,\frac{1}{2}}, \quad (4.8d)$$

$$\Phi_{1,J+\frac{1}{2}} = \phi_{1,J+\frac{1}{2}}. \quad (4.8e)$$

(The cell-averaged scalar fluxes are written as lower-case Greek letters, to emphasize that they are required to be equal to the high-order cell-averaged scalar fluxes.) The above system of $3J + 1$ equations has $3J + 1$ unknowns ($\phi_{0,j}$, E_j , and $\Phi_{1,j+\frac{1}{2}}$).

In Eq. (4.8c), we note that $D_{j+\frac{1}{2}}$ is the “classic” diffusion coefficient. *This definition of the $D_{j+\frac{1}{2}}$ can be modified without impacting the “consistency” of the solution obtained by the low-order system. If Eqs. (4.8) are satisfied, the high- and low-order neutron scalar flux will be equal (upon convergence), despite the definition of the diffusion coefficient ($D_{j+\frac{1}{2}}$) used.* However, the choice of the diffusion coefficient will impact the convergence speed and stability of the iterative method. The definition of an optimal $D_{j+\frac{1}{2}}$ will be necessary to improve the acceleration method’s stability. This will be further explored later in this section.

So far, we have derived most of the low-order GQD system. We will now focus on how the new consistent Eddington factors are derived. First, we modify the notation by defining:

$$\mathcal{E}_j \equiv 3E_j, \quad (4.9a)$$

$$F_j \equiv 3E_j\phi_{0,j} = \mathcal{E}_j\phi_{0,j}, \quad (4.9b)$$

$$D_j^* = \text{Modified Diffusion Coefficient}, \quad (4.9c)$$

where $\mathcal{E}_j$ is the new “consistent” Eddington factor. Applying these changes to Eqs. (4.8b) to (4.8e), we obtain:

$$\frac{1}{h_j}(\Phi_{1,j+\frac{1}{2}} - \Phi_{1,j-\frac{1}{2}}) = \frac{1}{h_j}(\phi_{1,j+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}), \quad 1 \leq j \leq J, \quad (4.10a)$$

$$\Phi_{1,j+\frac{1}{2}} = -D_{j+\frac{1}{2}}^*(F_{j+1} - F_j), \quad 1 \leq j \leq J-1, \quad (4.10b)$$

$$\Phi_{1,\frac{1}{2}} = \phi_{1,\frac{1}{2}}, \quad (4.10c)$$

$$\Phi_{1,J+\frac{1}{2}} = \phi_{1,J+\frac{1}{2}}. \quad (4.10d)$$

The linear system in Eqs. (4.10) has $2J + 1$ equations with $2J + 1$ unknowns ($\Phi_{1,j+\frac{1}{2}}$ and F_j). If F_j satisfies this system, the resulting scalar fluxes will be consistent, no matter how the diffusion coefficients D_j^* are defined. *Therefore, the consistency of the GQD method requires only that F_j satisfies the system Eqs. (4.10).*

In order to build a system of equations to solve for F_j , we introduce Eq. (4.10b), Eq. (4.10c), and Eq. (4.10d) into Eq. (4.10a), to algebraically eliminate the low-order cell-edge currents $\Phi_{1,j+\frac{1}{2}}$. For $j = 1$, we get:

$$\frac{1}{h_1} \left[-D_{\frac{3}{2}}(F_2 - F_1) - \phi_{1,\frac{1}{2}} \right] = \frac{1}{h_1} (\phi_{1,\frac{3}{2}} - \phi_{1,\frac{1}{2}}), \quad (4.11a)$$

for $2 \leq j \leq J - 1$, we get:

$$\frac{1}{h_j} \left[-D_{j+\frac{1}{2}}(F_{j+1} - F_j) + D_{j-\frac{1}{2}}(F_j - F_{j-1}) \right] = \frac{1}{h_j} (\phi_{1,j+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}), \quad (4.11b)$$

and for $j = J$, we get:

$$\frac{1}{h_J} \left[\phi_{1,J+\frac{1}{2}} + D_{J-\frac{1}{2}}(F_J - F_{J-1}) \right] = \frac{1}{h_J} (\phi_{1,J+\frac{1}{2}} - \phi_{1,J-\frac{1}{2}}). \quad (4.11c)$$

We can simplify Eq. (4.11a)-Eq. (4.11c) to:

$$-D_{\frac{3}{2}}(F_2 - F_1) = \phi_{1,\frac{3}{2}}, \quad j = 1, \quad (4.12a)$$

$$\begin{aligned} -D_{j+\frac{1}{2}}(F_{j+1} - F_j) + D_{j-\frac{1}{2}}(F_j - F_{j-1}) \\ = \phi_{1,j+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}, \quad 2 \leq j \leq J - 1, \end{aligned} \quad (4.12b)$$

$$D_{J-\frac{1}{2}}(F_J - F_{J-1}) = -\phi_{1,J-\frac{1}{2}}, \quad j = J. \quad (4.12c)$$

Equations (4.12) are a discrete 1-D “pure diffusion” problem for F_j , having leakage but no absorption. In these equations, F_j has the physical interpretation of being the scalar flux of the low-order diffusion system that occurs when a “pure diffusion” problem is solved, and the net low-order diffusion leakage from each cell equals the net high-order transport

leakage from that cell. In these equations, the diffusion and transport net leakages for each cell are the same, but the diffusion and transport scalar fluxes for each cell are different.

Similar formulations to Eqs. (4.12) can be obtained for higher dimensions (2-D and 3-D), but this is beyond the scope of this dissertation.

The system in Eqs. (4.12) is composed of J equations with J unknowns, and is tridiagonal and symmetric. At first glance, it seems straightforward to solve. However, the system is singular. A system is singular, if and only if the matrix that defines the left-hand side of the system (in Eqs. (4.12)) has a zero eigenvalue. This system cannot be inverted and generally does not have a solution.

We can show that the system of equations in Eqs. (4.12) is singular by setting the right sides of the equations to zero and trying to solve the resulting equations for the eigenfunction F_j . For $j = 1$:

$$-D_{\frac{3}{2}}(F_2 - F_1) = 0 \ , \quad (4.13a)$$

which leads to:

$$F_2 = F_1 \ . \quad (4.13b)$$

If we proceed through all the remaining equations $2 \leq j \leq J$:

$$-D_{j+\frac{1}{2}}(F_{j+1} - F_j) + D_{j-\frac{1}{2}}(F_j - F_{j-1}) = 0 \ , \quad (4.13c)$$

we obtain:

$$F_j = F_{j-1} \ . \quad (4.13d)$$

This leads to the final result:

$$F_1 = F_2 = F_3 = \dots = F_J \ . \quad (4.13e)$$

The results obtained in Eqs. (4.13) shows that the system does have the eigenvalue 0, and the only eigenfunction is the one corresponding to $F_j = R_f$, where R_f is any constant. Since the system is symmetric, the adjoint diffusion matrix is also singular, and its zero eigenfunction is $F_j^* = R_f^*$, where R_f^* is any constant.

Since the system in Eqs. (4.12) is singular, it appears that it does not have a solution. However, if a certain “solvability condition” is met, the Fredholm Alternative theorem states not only does this system have a solution, but it has infinitely many solutions.

If we sum the left sides of all J equations, we obtain:

$$\begin{aligned} D_{J-\frac{1}{2}}(F_J - F_{J-1}) - D_{J-\frac{1}{2}}(F_J - F_{J-1}) + D_{J-\frac{3}{2}}(F_{J-1} - F_{J-2}) \\ - D_{J-\frac{3}{2}}(F_{J-1} - F_{J-2}) + D_{J-\frac{5}{2}}(F_{J-2} - F_{J-3}) + \cdots + \\ - D_{\frac{5}{2}}(F_3 - F_2) + D_{\frac{3}{2}}(F_2 - F_1) - D_{\frac{3}{2}}(F_2 - F_1) = 0 \quad , \end{aligned} \quad (4.14)$$

because all the terms cancel out. For a solution to exist, the summation of the right-hand side of Eqs. (4.12) must also vanish. This resulting equation for the source terms is called the “solvability condition” for the system. We evaluate the sum of the right-side source terms, and we find:

$$\begin{aligned} -\phi_{1,J-\frac{1}{2}} + \phi_{1,J-\frac{1}{2}} - \phi_{1,J-\frac{3}{2}} \\ + \phi_{1,J-\frac{3}{2}} - \phi_{1,J-\frac{5}{2}} + \cdots + \\ + \phi_{1,\frac{5}{2}} - \phi_{1,\frac{3}{2}} + \phi_{1,\frac{3}{2}} = 0 \quad . \end{aligned} \quad (4.15)$$

Therefore, the “solvability condition” represented in Eq. (4.15) is automatically satisfied (the summation of the source terms results in zero). The Fredholm Alternative theorem then states that this condition is not only necessary, but also sufficient, for a solution to exist. Not only that, the theorem states that if a solution exists, it is not unique – one can add to

any “particular” solution a constant multiple of the zero-eigenvector of the original singular matrix. A more detailed discussion and application of the Fredholm Alternative Theorem is provided in Appendix B.

Therefore, because the solvability condition of the Fredholm Alternative Theorem is satisfied, the singular system Eqs. (4.12) has not only one, but infinitely many non-trivial solutions. In principle, we can then solve this system and obtain F_j that we can use to obtain the consistent Eddington factors. (The same would be true for 2-D and 3-D.)

However, solving this singular system has certain practical difficulties. The first difficulty is that standard algebraic solvers will likely experience difficulties trying to solve systems that are singular.

The second difficulty is that the existence of infinitely many solutions creates the dilemma of which solution (out of the infinite possible choices) to use for F_j .

The third difficulty is that solutions obtained by solving the singular system are not inherently guaranteed to be positive. If F_j assumes negative values, it could lead the nonlinear iterative method to become unstable. Fortunately, we developed a methodology to ensure that the values of F_j remain positive. A detailed discussion of F_j and this methodology is presented in Section 4.1.1.

After we obtain a particular solution F_j of Eqs. (4.12), we can calculate the general form of the new consistent Eddington factors $\mathcal{E}_j$ as:

$$\boxed{\mathcal{E}_j = \frac{F_j}{\phi_{0,j}} , \ 1 \leq j \leq J} . \quad (4.16)$$

The consistency of the method is guaranteed by the new consistent Eddington factors, by solving Eqs. (4.12). This consistency is not impacted by the definition of the diffusion coefficients in Eqs. (4.8). However, we will see that the stability and efficiency of the

resulting iterative method is directly impacted by the choice of a “proper” dimensionless diffusion coefficient D_j^* .

The “classic” dimensionless diffusion coefficient D_j used thus far is the one that occurs in the standard Fick’s Law (Eq. (3.5a)). However, for the SC discretization scheme, a modified definition of the diffusion coefficient $D_{j+\frac{1}{2}}^*$ has been developed [71]:

$$D_{j+\frac{1}{2}}^* = \frac{1}{3(\Sigma h)_{j+\frac{1}{2}}} + \frac{1}{4} \sum_{n=1}^N \mu_n \alpha_{n,j+\frac{1}{2}} w_n , \quad (4.17a)$$

where

$$\alpha_{n,j+\frac{1}{2}} = \frac{\alpha_{n,j+1} h_{j+1} + \alpha_{n,j} h_j}{h_{j+1} + h_j} . \quad (4.17b)$$

We note that in the SC scheme, the constants α_n limit to zero as the cell optical thickness limits to zero ($\lim_{\Sigma_t h \rightarrow 0} \alpha_n = 0$). Therefore, the value of the modified diffusion coefficient $D_{j+\frac{1}{2}}^*$ reduces to the “classic” formula for optically thin grids.

A different approach to modifying the low-order diffusion coefficient was considered in [37, 38] for the odCMFD method. In these cases – which did not employ Eddington factors – the modification of the diffusion coefficient provided an increase in stability (along with a loss of efficiency) for coarser grids. In Chapter 5, we show through the Fourier Stability Analysis that the utilization of Eqs. (4.17) helps to stabilize the GQD iterative method for optically thick cells.

Thus, we recommend using Eq. (4.17a) for the diffusion coefficient $D_{j+\frac{1}{2}}^*$ when using the SC discretization scheme. However, higher-order spatial discretization schemes (such as Linear Discontinuous or Linear Characteristics) are more accurate than SC and preserve the standard diffusion coefficients for all spatial grids [71]. In these cases, the proper diffusion coefficients is given by the “classic” form in Eq. (3.5a). (However, developing the

GQD method for these higher-order discretization schemes will not be considered in this dissertation.)

Next, we arrange all the equations in the derivation above into a sequence that will be used in the intermediate and low-order GQD equations,

First, we present the 1-D “pure diffusion” system matching the high- and low-order net leakage terms to calculate the F_j (with the introduced modified diffusion coefficients):

$$-D_{\frac{3}{2}}^*(F_2 - F_1) = \phi_{1,\frac{3}{2}}, \quad j = 1, \quad (4.18a)$$

$$\begin{aligned} -D_{j+\frac{1}{2}}^*(F_{j+1} - F_j) + D_{j-\frac{1}{2}}^*(F_j - F_{j-1}) \\ = \phi_{1,j+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}, \quad 2 \leq j \leq J-1, \end{aligned} \quad (4.18b)$$

$$D_{J-\frac{1}{2}}^*(F_J - F_{J-1}) = -\phi_{1,J-\frac{1}{2}}, \quad j = J. \quad (4.18c)$$

The consistent Eddington factors $\mathcal{E}_j$ and the boundary condition coefficients B_l and B_r are calculated in the following way:

$$B_l = \frac{\phi_{|1|,\frac{1}{2}}}{\phi_{0,1}}, \quad B_r = \frac{\phi_{|1|,J+\frac{1}{2}}}{\phi_{0,J}}, \quad (4.19a)$$

$$\mathcal{E}_j = \frac{F_j}{\phi_{0,j}}, \quad 1 \leq j \leq J. \quad (4.19b)$$

A complete description on how to obtain F_j will be provided in Section 4.1.1.

Finally, we present the low-order diffusion equations:

$$\frac{1}{h_j}(\Phi_{1,j+\frac{1}{2}} - \Phi_{1,j-\frac{1}{2}}) + \Sigma_{a,j}\Phi_{0,j} = Q_j, \quad 1 \leq j \leq J, \quad (4.20a)$$

$$\Phi_{1,j+\frac{1}{2}} = -D_{j+\frac{1}{2}}^*(\mathcal{E}_{j+1}\Phi_{0,j+1} - \mathcal{E}_j\Phi_{0,j}), \quad 1 \leq j \leq J-1, \quad (4.20b)$$

$$\Phi_{1,\frac{1}{2}} = 2\mathcal{J}_l^+ - B_l\Phi_{0,1}, \quad (4.20c)$$

$$\Phi_{1,J+\frac{1}{2}} = -2\mathcal{J}_r^- + B_r\Phi_{0,J}. \quad (4.20d)$$

Equations (4.20) employ upper-case Greek symbols ($\Phi_{0,j}$) to describe the low-order cell-average scalar fluxes. However, because the new Eddington factors are “consistent,” the

converged values of these scalar fluxes are equal to the converged values of the high-order transport scalar fluxes.

The GQD iterative method can now be explicitly formulated in a similar way as the CMFD and QD methods. We start the iteration with the previous estimate of the scalar flux $\Phi_{0,j}^\ell$ (or initial guess $\Phi_{0,j}^0$, if $\ell = 0$) for the scattering source at the high-order S_N equations. Then we obtain the new estimate for the neutron angular flux ($\psi_{0,j}^{\ell+\frac{1}{2}}$) by performing the transport sweep. Similarly to the other methods presented previously, this estimate is used to calculate the angular moments that are needed to calculate the “lagged” parameters (in Eq. (4.21)).

$$B_l^{\ell+\frac{1}{2}} = \frac{\phi_{|1|,\frac{1}{2}}^{\ell+\frac{1}{2}}}{\phi_{0,1}^{\ell+\frac{1}{2}}} , \quad B_r^{\ell+\frac{1}{2}} = \frac{\phi_{|1|,J+\frac{1}{2}}^{\ell+\frac{1}{2}}}{\phi_{0,J}^{\ell+\frac{1}{2}}} . \quad (4.21)$$

The major difference between the GQD and QD methods is that GQD requires solving an additional intermediate system for $F_j^{\ell+\frac{1}{2}}$ (Eqs. (4.22)). This step is required to calculate the consistent Eddington factors $\mathcal{E}_j$.

$$-D_{\frac{3}{2}}^*(F_2^{\ell+\frac{1}{2}} - F_1^{\ell+\frac{1}{2}}) = \phi_{1,\frac{3}{2}}^{\ell+\frac{1}{2}} , \quad j = 1 , \quad (4.22a)$$

$$\begin{aligned} -D_{j+\frac{1}{2}}^*(F_{j+1}^{\ell+\frac{1}{2}} - F_j^{\ell+\frac{1}{2}}) + D_{j-\frac{1}{2}}^*(F_j^{\ell+\frac{1}{2}} - F_{j-1}^{\ell+\frac{1}{2}}) \\ = \phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}^{\ell+\frac{1}{2}} , \quad 2 \leq j \leq J-1 , \end{aligned} \quad (4.22b)$$

$$D_{J-\frac{1}{2}}^*(F_J^{\ell+\frac{1}{2}} - F_{J-1}^{\ell+\frac{1}{2}}) = -\phi_{1,J-\frac{1}{2}}^{\ell+\frac{1}{2}} , \quad j = J . \quad (4.22c)$$

The Consistent Eddington factors are lagged and calculated by:

$$\mathcal{E}_j^{\ell+\frac{1}{2}} = \frac{F_j^{\ell+\frac{1}{2}}}{\phi_{0,j}^{\ell+\frac{1}{2}}} , \quad 1 \leq j \leq J . \quad (4.23)$$

The low-order equations [Eqs. (4.24)] are then solved to obtain a new estimate $\phi_{0,j}^{\ell+1}$ for the scalar flux:

$$\frac{1}{h_j}(\phi_{1,j+\frac{1}{2}}^{\ell+1} - \phi_{1,j-\frac{1}{2}}^{\ell+1}) + \Sigma_{a,j}\phi_{0,j}^{\ell+1} = Q_j, \quad 1 \leq j \leq J, \quad (4.24a)$$

$$\phi_{1,j+\frac{1}{2}}^{\ell+1} = -D_{j+\frac{1}{2}}^* (\mathcal{E}_{j+1}^{\ell+\frac{1}{2}} \phi_{0,j+1}^{\ell+1} - \mathcal{E}_j^{\ell+\frac{1}{2}} \phi_{0,j}^{\ell+1}), \quad 1 \leq j \leq J-1, \quad (4.24b)$$

$$\phi_{1,\frac{1}{2}}^{\ell+1} = 2\mathcal{J}_l^+ - B_l^{\ell+\frac{1}{2}} \phi_{0,1}^{\ell+1}, \quad (4.24c)$$

$$\phi_{1,J+\frac{1}{2}}^{\ell+1} = -2\mathcal{J}_r^- + B_r^{\ell+\frac{1}{2}} \phi_{0,J}^{\ell+1}. \quad (4.24d)$$

This new estimate is used to define the scattering source at the next iteration's high-order system $(\ell + 1)$. Since the GQD method is consistent, then upon convergence, the high-order scalar flux will equal the low-order scalar flux.

4.1.1 Consistent Eddington Factors $\mathcal{E}_j$

In this section, we focus on the details regarding the calculation of F_j and the consistent Eddington factors $\mathcal{E}_j$ (Eqs. (4.11) and Eq. (4.16), respectively). The motivation behind this extended discussion arises from the fact that the “pure diffusion” system that provides F_j is singular. Not only that, according to the Fredholm Alternative Theorem [75], the system has an infinite number of solutions. One can see that, if F_j satisfies Eqs. (4.11), for any constant C , the solution $F_j + C$ will also satisfy the same equations.

Solving a singular system numerically may not be straightforward. This can be avoided in 1-D problems (planar-geometry) because it is possible to reduce the discrete “second-order” Eqs. (4.12) to discrete “first-order” equations that can be solved in *closed form*. The discussion of solving the consistent singular Eddington factor equations (Eqs. (4.11)) is a required discussion for 2-D and 3-D physical systems, where a *closed form* solution is not available. However, this is not within the scope of this dissertation.

To derive the discrete first-order system, we re-introduce Eqs. (4.18):

$$-D_{\frac{3}{2}}^*(F_2 - F_1) = \phi_{1, \frac{3}{2}}, \quad j = 1, \quad (4.25a)$$

$$\begin{aligned} -D_{j+\frac{1}{2}}^*(F_{j+1} - F_j) + D_{j-\frac{1}{2}}^*(F_j - F_{j-1}) \\ = \phi_{1, j+\frac{1}{2}} - \phi_{1, j-\frac{1}{2}}, \quad 2 \leq j \leq J-1, \end{aligned} \quad (4.25b)$$

$$D_{J-\frac{1}{2}}^*(F_J - F_{J-1}) = -\phi_{1, J-\frac{1}{2}}, \quad j = J. \quad (4.25c)$$

Equation (4.25b) for $j = 2$ is:

$$-D_{\frac{5}{2}}^*(F_3 - F_2) + D_{\frac{3}{2}}^*(F_2 - F_1) = \phi_{1, \frac{5}{2}} - \phi_{1, \frac{3}{2}}.$$

This result and Eq. (4.25a) imply:

$$-D_{\frac{5}{2}}^*(F_3 - F_2) = \phi_{1, \frac{5}{2}}.$$

Continuing in this manner, the remaining “second-order” Eq. (4.25b) simplify to the following “first-order” equations:

$$\boxed{-D_{j+\frac{1}{2}}^*(F_{j+1} - F_j) = \phi_{1, j+\frac{1}{2}}, \quad 1 \leq j \leq J-1} \quad (4.26)$$

These can be written:

$$F_{j+1} - F_j = -\frac{\phi_{1, j+\frac{1}{2}}}{D_{j+\frac{1}{2}}^*}, \quad 1 \leq j \leq J-1. \quad (4.27)$$

Operating on Eq. (4.27) by $\sum_{j'=1}^{j-1}$, we obtain:

$$F_j = F_1 - \sum_{j'=1}^{j-1} \frac{\phi_{1, j'+\frac{1}{2}}}{D_{j'+\frac{1}{2}}^*}, \quad 1 \leq j \leq J. \quad (4.28)$$

Here F_1 is arbitrary, and $\sum_{j'=1}^0 \equiv 0$.

Thus, the 1-D pure diffusion problem (defined by Eqs. (4.18) and Eqs. (4.19)) has the explicit solution given by Eq. (4.28), which has the arbitrary constant F_1 . The infinite set of solutions comes from the fact that F_1 can have any value.

Equation (4.28) is obtained by summing Eq. (4.27) all over the cells to the left of the desired cell j . This process could also be formulated by summing from the right boundary, resulting in:

$$F_j = F_J + \sum_{j'=j}^{J-1} \frac{\phi_{1,j'+\frac{1}{2}}}{D_{j'+\frac{1}{2}}^*}, \quad 1 \leq j \leq J, \quad (4.29)$$

where $\sum_{j'=J}^{J-1} \equiv 0$. This time, the arbitrary constant is defined by F_J . Equation (4.29) has the same solution to Eq. (4.28), since the converged constants F_1 and F_J are correlated by:

$$F_J = F_1 - \sum_{j'=1}^{J-1} \frac{\phi_{1,j'+\frac{1}{2}}}{D_{j'+\frac{1}{2}}^*}, \quad 1 \leq j \leq J. \quad (4.30)$$

However, F_1 and F_J do not satisfy Eq. (4.30) prior to convergence.

In a more general case, one could also start from an arbitrary interior “starting” cell j^* and sum over to the cells to the left of j^* ($1 \leq j \leq j^* - 1$), obtaining:

$$F_j = F_{j^*} + \sum_{j'=j}^{j^*-1} \frac{\phi_{1,j'+\frac{1}{2}}}{D_{j'+\frac{1}{2}}^*}, \quad 1 \leq j \leq j^* - 1, \quad (4.31a)$$

and sum to the right ($j^* + 1 \leq j \leq J$), obtaining:

$$F_j = F_{j^*} - \sum_{j'=j^*}^{j-1} \frac{\phi_{1,j'+\frac{1}{2}}}{D_{j'+\frac{1}{2}}^*}, \quad j^* + 1 \leq j \leq J. \quad (4.31b)$$

In this general case, the arbitrary constant is defined as F_{j^*} . All three of the above formulations (summing to the right starting at the left edge, summing to the left starting from the right edge, and summing to the left and right starting from an interior edge) produce the same expression for F_j , module an arbitrary constant. Now, the question is: *What value should we use for this arbitrary constant?*

There are infinite possible solutions (and constants). Our only obvious requirement is that the values of the F_j must be positive. However, not any choice of F_j will provide an efficient and rapidly converging iterative method. Intuitively, basing the F_j values around

the QD method makes sense, due to its performance and stability. Therefore we believe that it could be beneficial to choose an arbitrary constant value in a way that the GQD method resembles the QD method, while still maintaining a consistent solution.

Let us consider the case in which the spatial cells are optically thin ($(\Sigma_t h)_{j+\frac{1}{2}} \approx 0$). In this case, the modified diffusion coefficient $D_{j'+\frac{1}{2}}^*$ reduces to the “classic” value $D_{j'+\frac{1}{2}}$ (Eq. (3.5a)). Equations (4.31) can be evaluated using:

$$\frac{\phi_{1,j'+\frac{1}{2}}}{D_{j'+\frac{1}{2}}} \approx 3\phi_{1,j'+\frac{1}{2}}(\Sigma_t h)_{j'+\frac{1}{2}} \approx 3 \int_{z_{j'}}^{z_{j'+1}} \phi_1(z) \Sigma_t(z) dz, \quad (4.32)$$

where $z_{j'}$ is the center of the cell j' .

The first angular moment of the neutron transport equation is:

$$\frac{d\phi_2}{dz}(z) + \Sigma_t(z)\phi_1(z) = 0. \quad (4.33)$$

Applying the definition of Eq. (4.32) and Eq. (4.33) into Eq. (4.31a), we obtain for $j < j^*$:

$$\begin{aligned} F_j &\approx F_{j^*} + 3 \sum_{j'=j}^{j^*-1} \int_{z_{j'}}^{z_{j'+1}} \Sigma_t(z) \phi_1(z) dz \\ &= F_{j^*} - 3 \int_{z_j}^{z_{j^*}} \frac{d\phi_2(z)}{dz} dz \\ &= F_{j^*} - 3 [\phi_2(z_{j^*}) - \phi_2(z_j)] \\ &\approx 3\phi_2(z_j) + [F_{j^*} - 3\phi_2(z_{j^*})]. \end{aligned} \quad (4.34)$$

The same result holds for $j^* < j$. Thus, if we choose:

$$F_{j^*} = 3\phi_{2,j^*}, \quad (4.35a)$$

then we obtain (for optically thin cells):

$$F_j = 3\phi_{2,j}, \quad 1 \leq j \leq J. \quad (4.35b)$$

This shows that for optically thin cells, with any choice of j^* , and with the above choice of F_j^* , the new consistent Eddington factors reduce to the standard QD Eddington factors (Eq. (3.17b)). As we expected, this choice in Eq. (4.35a) proved later (in Chapter 6) to be beneficial for the convergence speed of the GQD method.

This definition of the arbitrary constant F_{j^*} allows us to define simple new Eddington factors that, for optically thin cells, are positive and preserve the consistency of the solution in the low-order scalar fluxes. However, an issue arises when the spatial cells are not optically thin. The thicker the spatial grid becomes, the more difficult it becomes to ensure that the solutions (F_{j^*}) from Eqs. (4.31) remain positive.

However, one feature of the “1-D pure diffusion and singular” problem for F_j is that this problem has an infinite number of solutions. These solutions vary only by an arbitrary additive constant C . Therefore, if F_j is a solution of Eqs. (4.25), then $F_j + C$ will also do so. This ability to add C to a solution F_j enables us to ensure that $F_j + C$ remains positive, even if F_j are not positive.

Therefore, we can use this concept to adjust the value of the constant F_1 to ensure that Eq. (4.28) will have only positive F_j values. For any choice of F_1 , the low-order system will be consistent.

Assume $F_1 = 0$ and let F_j be any particular solution of Eq. (4.28). We define the cell at position j^* to be the spatial cell where the numbers F_j assume their minimum value. We can choose a new value for the constant F_1 such that:

$$F_{j^*} + F_1 = 3\phi_{2,j^*} . \quad (4.36)$$

then (i) the numerator of Eq. (4.37) is positive for all j , and (ii) the “consistent” Eddington factor for cell j^* is equal to the standard Eddington factor for that cell.

Using this logic, we have developed a methodology that ensures the method will have positive F_j values. Basically, the method developed will (i) sweep left to right, starting with the initial value $F_1 = 0$, (ii) determine the minimum value of F_{j^*} in the domain (and its position), and then (iii) add a constant to all F_j such that the minimum value F_{j^*} is equal to three times the second angular moment in that cell. In this method, we focus on ensuring that the minimum value of F_j will always be equal to $3\phi_{2,j}$.

These steps can be better described in the following way:

1. It starts by defining $F_1 = 0$.
2. Calculate all the remaining F_j by using Eq. (4.28) (sweeping left to right).
3. Find the minimum value and position of F_j in $1 \leq j \leq J$ and define it as F_{j^*} .
4. Then, recalculate the constant F_1 that $F_{j^*} + F_1 = 3\phi_{2,j^*}$.
5. Add the recalculated F_1 to all F_j .

We finalize this procedure by calculating the new consistent Eddington factors ($\mathcal{E}$):

$$\mathcal{E}_j = \frac{F_j}{\phi_{0,j}} , \quad 1 \leq j \leq J . \quad (4.37)$$

Therefore, in each iteration, we have to screen for the minimum value of F_j in order to determine the correct constant to be implemented. Since $\phi_{2,j}$ is inherently positive, all F_j are guaranteed to be positive. We note that this is not the only way to calculate the F_j . In fact, there are infinite possible ways. However, we believe that the presented method is the simplest and most intuitive way to define the F_j and its arbitrary constants.

In Chapter 6, we discuss some shortcomings of this methodology that may occur when we stress-test the method in specific problems. We also provide an alternative method that, despite working well in all problems presented, is less intuitive.

4.2 Algorithm Summary (GQD)

Each GQD iteration consists of three parts: (i) a transport sweep, followed by (ii) the calculation of consistent Eddington factors, followed by (iii) the low-order diffusion calculation of the accelerated scalar flux. The only differences between GQD and QD methods are that (i) the consistent GQD Eddington factors are calculated in an intermediate step (which does not exist in the QD method), and (ii) these new consistent Eddington factors substitute for the conventional QD's inconsistent Eddington factor in the low-order equations. Apart from these differences, the QD and GQD methods are identical. In the following, we explicitly specify the new GQD method:

Prior to initializing the iterative method, we calculate and store the incident partial currents:

$$\mathcal{J}_l^+ = \sum_{\mu_n > 0} \mu_n \psi_{n, \frac{1}{2}} w_n , \quad (4.38a)$$

$$\mathcal{J}_r^- = \sum_{\mu_n < 0} |\mu_n| \psi_{n, J+\frac{1}{2}} w_n , \quad (4.38b)$$

and the quantities:

$$\begin{aligned} (\Sigma_t h)_{j+\frac{1}{2}} &= \frac{1}{2} (\Sigma_{t,j+1} h_{j+1} + \Sigma_{t,j} h_j) , \quad 1 \leq j \leq J-1 , \\ &= \text{Optical distance between the midpoints of cells } j \text{ and } j+1 , \end{aligned} \quad (4.38c)$$

$$\begin{aligned} \alpha_{n,j+\frac{1}{2}} &= \frac{\alpha_{n,j+1} h_{j+1} + \alpha_{n,j} h_j}{h_{j+1} + h_j} , \quad 1 \leq j \leq J-1 , \\ &= \text{Cell-edge angular weights} , \end{aligned} \quad (4.38d)$$

$$\begin{aligned} D_{j+\frac{1}{2}}^* &= \frac{1}{3(\Sigma_t h)_{j+\frac{1}{2}}} + \frac{1}{4} \sum_{n=1}^N \mu_n \alpha_{n,j+\frac{1}{2}} w_n , \quad 1 \leq j \leq J-1 , \\ &= \text{Diffusion coefficient} . \end{aligned} \quad (4.38e)$$

(i) High-Order Transport Sweep

The $(\ell + 1)^{st}$ iteration begins with the transport sweep and the calculation of certain flux moments, just as before. This is described by Eqs. (4.1) and Eq. (4.2) :

$$\frac{\mu_n}{h_j} \left(\psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}} \right) + \Sigma_{t,j} \psi_{n,j}^{\ell+\frac{1}{2}} = \frac{\Sigma_{s,j}}{2} \phi_{0,j}^{\ell} + \frac{Q_j}{2}, \quad (4.39a)$$

$$\psi_{n,j}^{\ell+\frac{1}{2}} = \left(\frac{1 + \alpha_{n,j}}{2} \right) \psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} + \left(\frac{1 - \alpha_{n,j}}{2} \right) \psi_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}}, \quad (4.39b)$$

$$\psi_{n,\frac{1}{2}}^{\ell+\frac{1}{2}} = \Psi_n^l, \quad \mu_n > 0, \quad (4.39c)$$

$$\psi_{n,J+\frac{1}{2}}^{\ell+\frac{1}{2}} = \Psi_n^r, \quad \mu_n < 0, \quad (4.39d)$$

and:

$$\phi_{k,j}^{\ell+\frac{1}{2}} = \sum_{n=1}^N \mu_n^k \psi_{n,j}^{\ell+\frac{1}{2}} w_n \quad (k = 0, 2), \quad \phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} = \sum_{n=1}^N \mu_n \psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} w_n, \quad (4.40a)$$

$$\phi_{|1|,\frac{1}{2}}^{\ell+\frac{1}{2}} \equiv \sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}}^{\ell+\frac{1}{2}} w_n, \quad \phi_{|1|,J+\frac{1}{2}}^{\ell+\frac{1}{2}} \equiv \sum_{n=1}^N |\mu_n| \psi_{n,J+\frac{1}{2}}^{\ell+\frac{1}{2}} w_n. \quad (4.40b)$$

Again, this high-order system is called the *transport sweep*. This step is identical in the CMFD, QD, and GQD methods.

(ii) Calculation of Consistent Eddington Factors

This intermediate step between the high- and low-order systems is unique in the GQD method. The numerators of the consistent Eddington factors (the constants F_j) can be calculated by numerically solving Eqs. (4.18):

$$-D_{\frac{3}{2}}^* (F_2^{\ell+\frac{1}{2}} - F_1^{\ell+\frac{1}{2}}) = \phi_{1,\frac{3}{2}}^{\ell+\frac{1}{2}}, \quad j = 1, \quad (4.41a)$$

$$\begin{aligned} -D_{j+\frac{1}{2}}^* (F_{j+1}^{\ell+\frac{1}{2}} - F_j^{\ell+\frac{1}{2}}) + D_{j-\frac{1}{2}}^* (F_j^{\ell+\frac{1}{2}} - F_{j-1}^{\ell+\frac{1}{2}}) \\ = \phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}^{\ell+\frac{1}{2}}, \quad 2 \leq j \leq J-1, \end{aligned} \quad (4.41b)$$

$$D_{J-\frac{1}{2}}^* (F_J^{\ell+\frac{1}{2}} - F_{J-1}^{\ell+\frac{1}{2}}) = -\phi_{1,J-\frac{1}{2}}^{\ell+\frac{1}{2}}, \quad j = J. \quad (4.41c)$$

Alternatively, the explicit general closed-form expression for F_j is given by Eq. (4.28).

$$F_j^{\ell+\frac{1}{2}} = F_1^{\ell+\frac{1}{2}} - \sum_{j'=1}^{j-1} \frac{\phi_{1,j'+\frac{1}{2}}^{\ell+\frac{1}{2}}}{D_{j'+\frac{1}{2}}^*}, \quad 1 \leq j \leq J, \quad (4.42)$$

and the new consistent Eddington factors are defined by Eq. (4.37):

$$\mathcal{E}_j^{\ell+\frac{1}{2}} = \frac{F_j^{\ell+\frac{1}{2}}}{\phi_{0,j}^{\ell+\frac{1}{2}}}, \quad 1 \leq j \leq J. \quad (4.43)$$

The arbitrary constant $F_1^{\ell+\frac{1}{2}}$ must be defined in a way that all values of $F_j^{\ell+\frac{1}{2}}$ (in $1 \leq j \leq J$) are positive. The suggested method by the authors is to find the minimum value $F_{j^*}^{\ell+\frac{1}{2}}$ (assuming initially $F_1^{\ell+\frac{1}{2}} = 0$) and recalculate $F_1^{\ell+\frac{1}{2}}$ by:

$$F_1^{\ell+\frac{1}{2}} = 3\phi_{2,j^*}^{\ell+\frac{1}{2}} - F_{j^*}^{\ell+\frac{1}{2}}, \quad \text{where } F_{j^*}^{\ell+\frac{1}{2}} = \min F_j^{\ell+\frac{1}{2}}. \quad (4.44)$$

If this minimum value is negative, we introduce the updated constant $F_1^{\ell+\frac{1}{2}}$ into Eq. (4.42) to ensure all Eddington factors are non-negative. (Since the $F_j^{\ell+\frac{1}{2}}$ are unique to within an arbitrary additive constant, the new constants $F_j^{\ell+\frac{1}{2}}$ will still yield consistent Eddington factors.) If the minimum value is positive, the updated constant $F_1^{\ell+\frac{1}{2}}$ just scales the lowest new $F_{j^*}^{\ell+\frac{1}{2}}$ value to $3\phi_{2,j^*}^{\ell+\frac{1}{2}}$.

(iii) Low-Order Diffusion Calculation

The low-order system is very similar to the QD method (Eq. (3.23) and Eq. (3.24)). The only difference is that we use the newly defined consistent Eddington factors $\mathcal{E}_j^{\ell+\frac{1}{2}}$:

$$B_l^{\ell+\frac{1}{2}} = \frac{\phi_{|1|,\frac{1}{2}}^{\ell+\frac{1}{2}}}{\phi_{0,1}^{\ell+\frac{1}{2}}}, \quad B_r^{\ell+\frac{1}{2}} = \frac{\phi_{|1|,J+\frac{1}{2}}^{\ell+\frac{1}{2}}}{\phi_{0,J}^{\ell+\frac{1}{2}}}, \quad (4.45)$$

and:

$$\frac{1}{h_j}(\phi_{1,j+\frac{1}{2}}^{\ell+1} - \phi_{1,j-\frac{1}{2}}^{\ell+1}) + \Sigma_{a,j}\phi_{0,j}^{\ell+1} = Q_j, \quad 1 \leq j \leq J, \quad (4.46a)$$

$$\phi_{1,j+\frac{1}{2}}^{\ell+1} = -D_{j+\frac{1}{2}}^* (\mathcal{E}_{j+1}^{\ell+\frac{1}{2}} \phi_{0,j+1}^{\ell+1} - \mathcal{E}_j^{\ell+\frac{1}{2}} \phi_{0,j}^{\ell+1}), \quad 1 \leq j \leq J-1, \quad (4.46b)$$

$$\phi_{1,\frac{1}{2}}^{\ell+1} = 2\mathcal{J}_l^+ - B_l^{\ell+\frac{1}{2}} \phi_{0,1}^{\ell+1}, \quad (4.46c)$$

$$\phi_{1,J+\frac{1}{2}}^{\ell+1} = -2\mathcal{J}_r^- + B_r^{\ell+\frac{1}{2}} \phi_{0,J}^{\ell+1}. \quad (4.46d)$$

This completes the description of the GQD method.

4.3 The Linearized GQD (LGQD) Method

The GQD method formulated in the previous sections is nonlinear, due to the nonlinear definition of the consistent Eddington factors (Eq. (4.43)) and their use in the low-order equations (Eqs. (4.46)). In this section, we develop the linearized form of the GQD method. This a necessary step for the Fourier Stability Analysis, presented in Chapter 5, which requires the iterative method to be linear.

To linearize the GQD method, we must first discard the Eddington factors and modify Eq. (4.46b). In order to achieve that, lets first consider Eq. (4.46b), which upon convergence yields:

$$\phi_{1,j+\frac{1}{2}} = -D_{j+\frac{1}{2}}^* (F_{j+1} - F_j). \quad (4.47)$$

This result was obtained by: (i) rewriting Eq. (4.47) nonlinearly as:

$$\begin{aligned} \phi_{1,j+\frac{1}{2}} &= -D_{j+\frac{1}{2}}^* \left(\frac{F_{j+1}}{\phi_{0,j+1}} \phi_{0,j+1} - \frac{F_j}{\phi_{0,j}} \phi_{0,j} \right) \\ &= -D_{j+\frac{1}{2}}^* (\mathcal{E}_{j+1} \phi_{0,j+1} - \mathcal{E}_j \phi_{0,j}), \end{aligned} \quad (4.48)$$

(ii) assuming that the consistent Eddington factors are stable ($\mathcal{E}_j \approx 1$), and (iii) lagging these quantities.

One can use a similar logic to rewrite Eq. (4.47) linearly as:

$$\phi_{1,j+\frac{1}{2}} = -D_{j+\frac{1}{2}}^* \left[\phi_{0,j+1} + (F_{j+1} - \phi_{0,j+1}) - \phi_{0,j} - (F_j - \phi_{0,j}) \right]. \quad (4.49)$$

Since the additive terms $F_j - \phi_{0,j}$ are (in principle) small, they can be lagged. If Eq. (4.49) is written as part of the iterative scheme, we obtain:

$$\phi_{1,j+\frac{1}{2}}^{\ell+1} = -D_{j+\frac{1}{2}}^* \left[\phi_{0,j+1}^{\ell+1} + (F_{j+1}^{\ell+\frac{1}{2}} - \phi_{0,j+1}^{\ell+\frac{1}{2}}) - \phi_{0,j}^{\ell+1} - (F_j^{\ell+\frac{1}{2}} - \phi_{0,j}^{\ell+\frac{1}{2}}) \right]. \quad (4.50)$$

Equation (4.46b) can be then be replaced by Eq. (4.50).

The linear GQD boundary condition on the left edge of the system can be derived from the identity Eqs. (3.6):

$$2\mathcal{J}_\ell^+ = \phi_{1,\frac{1}{2}} + \sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}} w_n. \quad (4.51a)$$

This identity was rewritten nonlinearly as:

$$\begin{aligned} 2\mathcal{J}_\ell^+ &= \phi_{1,\frac{1}{2}} + \sum_{n=1}^N |\mu_n| \left(\frac{\psi_{n,\frac{1}{2}}}{\phi_{0,1}} \right) \phi_{0,1} w_n \\ &= \phi_{1,\frac{1}{2}} + \left(\frac{\sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}} w_n}{\phi_{0,1}} \right) \phi_{0,1}, \end{aligned} \quad (4.51b)$$

and it can be rewritten linearly as:

$$\begin{aligned} 2\mathcal{J}_\ell^+ &= \phi_{1,\frac{1}{2}} + \sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}} w_n \\ &= \phi_{1,\frac{1}{2}} + \sum_{n=1}^N |\mu_n| \left[\psi_{n,\frac{1}{2}} + \frac{1}{2} (\phi_{0,1} - \phi_{0,1}) \right] w_n. \end{aligned} \quad (4.51c)$$

The (nonlinear) Eq. (4.51b) leads to the following boundary condition for the nonlinear GQD method:

$$\phi_{1,\frac{1}{2}}^{\ell+1} = 2\mathcal{J}_\ell^+ - \left(\frac{\sum_{n=1}^N |\mu_n| \psi_{n,\frac{1}{2}}^{\ell+\frac{1}{2}} w_n}{\phi_{0,1}^{\ell+\frac{1}{2}}} \right) \phi_{0,1}^{\ell+1}. \quad (4.52)$$

For all iterative methods presented so far, the B_r and B_l (the quantity displayed in the large parentheses), have been assumed to be stable throughout the iterations. Therefore, these coefficients could be lagged. Similarly, the (linear) Eq. (4.51c)) leads to the following boundary condition for the linear GQD method:

$$\phi_{1,\frac{1}{2}}^{\ell+1} = 2\mathcal{J}_\ell^+ - \left(\frac{1}{2} \sum_{n=1}^N |\mu_n| w_n \right) \phi_{0,1}^{\ell+1} - \sum_{n=1}^N |\mu_n| \left(\psi_{n,\frac{1}{2}}^{\ell+\frac{1}{2}} - \frac{1}{2} \phi_{0,1}^{\ell+\frac{1}{2}} \right) w_n. \quad (4.53)$$

We can follow a similar logic for Eq. (4.53). Assuming the summation term on the rightmost side of the equation is small, and hence one should also be able to lag it. The same derivation for the right boundary conditions can also be done, resulting in:

$$\phi_{1,J+\frac{1}{2}}^{\ell+1} = -2\mathcal{J}_r^- + \left(\frac{1}{2} \sum_{n=1}^N |\mu_n| w_n \right) \phi_{0,J}^{\ell+1} + \sum_{n=1}^N |\mu_n| \left(\psi_{n,J+\frac{1}{2}}^{\ell+\frac{1}{2}} - \frac{1}{2} \phi_{0,J}^{\ell+\frac{1}{2}} \right) w_n. \quad (4.54)$$

This concludes the derivation of the linear GQD method. In summary, the new linearized method will be similar in most ways to the nonlinear one, except for:

- Equation (4.44) and Eq. (4.45) are deleted.
- Equation (4.46b) is substituted by Eq. (4.49).
- Equation (4.46c) and Eq. (4.46d) are substituted by Eq. (4.53) and Eq. (4.54), respectively.

The linear GQD methods have two conceptual advantages: (i) because the method is linear, it is unaffected by possible occurrences of negative angular fluxes, and (ii) its stability can be assessed by a Fourier stability analysis. The disadvantage is that linear methods cannot be directly used to perform eigenvalue calculations, which are inherently nonlinear.

In Chapter 5, we provide a detailed discussion of the Fourier Stability Analysis applied to the linearized GQD method.

Chapter 5: Fourier Analysis

The main objective of this work is to develop a consistent acceleration method that displays similar stability and efficiency as the QD method. So far, we have developed the GQD method and shown that it is consistent “*upon convergence*”. However, the analysis that proves that the method will be stable or rapidly convergent has not yet been presented. That task will be accomplished theoretically in the present chapter, and computationally in the subsequent chapter.

Consistent neutron transport acceleration algorithms tend to be stable and rapidly-convergent for a certain range of operational parameters (optically thin cells). However, these algorithms become inefficient or unstable if they are operated outside that range (e.g. optically thick cells). It is highly desirable that an iterative method will converge independently of operational parameters, like the inconsistent QD method.

This chapter provides a theory (Fourier Analysis) to assess the convergence properties of iterative methods. We evaluate the specific Fourier Stability Analysis for the GQD method, providing a theoretical estimation of its convergence and stability properties.

5.1 Convergence of Iterative Methods

Let us consider a simple iterative method, which, for example, could be applied to describe Source Iterations in Eq. (2.37a):

$$L\psi^{(\ell+1)} = S\psi^{(\ell)} + q, \quad \ell \geq 0, \quad (5.1)$$

where $\psi^{(\ell)}$ is the estimated solution for the iteration ℓ . The converged solution satisfies:

$$\psi = L^{-1}S\psi + q. \quad (5.2)$$

Subtracting Eq. (5.1) from Eq. (5.2), we get:

$$\psi - \psi^{(\ell+1)} = L^{-1}S(\psi - \psi^{(\ell)}). \quad (5.3)$$

Applying Eq. (5.3) recursively, we obtain:

$$\psi - \psi^{(\ell+1)} = L^{-1}S(\psi - \psi^{(\ell)}) = (L^{-1}S)^2(\psi - \psi^{(\ell-1)}) = \quad (5.4)$$

$$= \dots = (L^{-1}S)^{(\ell+1)}(\psi - \psi^{(0)}). \quad (5.5)$$

The error between the estimated solution at iteration ℓ and the converged solution is defined by:

$$e^\ell = |\psi - \psi^{(\ell)}|. \quad (5.6)$$

Therefore, Eq. (5.6) can be written as:

$$e^{(\ell+1)} = (L^{-1}S)^{(\ell+1)}e^{(0)}. \quad (5.7)$$

This provides the estimate:

$$\|e^{(\ell+1)}\| \leq \|(L^{-1}S)^{(\ell+1)}\| \|e^{(0)}\|. \quad (5.8)$$

The quantity $\|(L^{-1}S)^{(\ell+1)}\|$ can be correlated to the spectral radius (ρ) of the matrix $(L^{-1}S)$ in the following way [16]:

$$\|(L^{-1}S)^{(\ell+1)}\|_2 \leq (\rho(L^{-1}S))^{(\ell+1)} , \quad (5.9a)$$

where the spectral radius is defined by:

$$\rho(L^{-1}S) = \max\{|\lambda_1|, |\lambda_2|, \dots, |\lambda_n|\} , \quad (5.9b)$$

where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of the matrix $(L^{-1}S)$. Therefore, Eq. (5.8) becomes:

$$\|e^{(\ell+1)}\| \leq \rho^{(\ell+1)} \|e^{(0)}\| . \quad (5.10)$$

A similar discussion can be encountered in [14].

Equation (5.10) presents an important result. If the spectral radius is smaller than 1 ($\rho < 1$), the error of the iterative error reduces progressively with the number of iterations, and the method is stable. The smaller its value ($\rho \ll 1$), the faster the solution will converge to the true solution. However, if $\rho \approx 1$, the method will converge very slowly.

On the other hand, if the spectral radius is greater than 1 ($\rho > 1$), the error will increase with each iteration and the method will never converge. In this case, the method diverges and is considered unstable. In the case of $\rho = 1$, the method may not have the error increasing, but will also not converge (since the error will not reduce with the iterations).

Acceleration methods have a more complicated algorithm, making calculating the spectral radius less straightforward. The Fourier Stability Analysis provides a possible path to obtain a numerical estimate of the convergence rate. This is presented for the linear GQD method in the following section.

We can numerically estimate the spectral radius of the GQD method by calculating the difference between successive solutions:

$$\rho \approx \frac{\|\phi^{\ell+1} - \phi^\ell\|}{\|\phi^\ell - \phi^{\ell-1}\|}, \quad (5.11a)$$

where

$$\|\phi^{\ell+1} - \phi^\ell\| \equiv \left(\frac{\sum_{j=1}^J |\phi^{\ell+1} - \phi^\ell|^2 h_j}{\sum_{j=1}^J h_j} \right)^{1/2}. \quad (5.11b)$$

The GQD code developed in this dissertation uses Eqs. (5.11) to estimate numerically the spectral radius.

5.2 Fourier Stability Analysis (FSA)

The Fourier Stability Analysis (FSA) is a mathematical tool used to theoretically predict the convergence rate of iterative methods [14]. The method starts by representing these algorithms as a Fourier series in the exponential form and then analyzing its eigenvalues. As previously presented, the eigenvalues of the equation's operator are directly correlated to the performance and stability of the iterative method. The results obtained from this analysis can provide crucial insight into the method's stability and convergence speed.

The FSA makes a set of assumptions:

- The analysis is applied to an infinite spatial medium.
- The medium is homogeneous (or periodic).
- The equations being analyzed are linear.

Therefore, the method cannot be applied directly to realistic physical problems with finite boundaries. Nonetheless, the conclusions obtained from the FSA, applied to “idealized”

infinite-medium problems, have been shown to apply to realistic systems with reasonable accuracy. In other words, calculations obtained from simulating practical finite-medium reactor physics problems generally experience a similar behavior to that predicted by the infinite-medium FSA. Boundary condition effects and finite and heterogeneous media can cause deviations between the predicted and real convergence speed, and generally, these deviations are minor.

The other main requirement is for the equations in the iterative method to be linear. Thus, nonlinear methods must be linearized, in order to be Fourier-analyzed. In general, the linearized methods display similar convergence speeds to their nonlinear counterparts, and if this is true, then the FSA of the linearized methods also applies to the nonlinear methods. However, this connection between the nonlinear and linear methods must be established computationally, by testing the two methods in a computer code.

The FSA method has been widely used for neutron transport and acceleration techniques [14, 37, 38, 46]. The analysis has provided meaningful insights into increasing the stability of acceleration methods by modifying certain key parameters. Such an analysis resulted in the development of the odCMFD method [37, 38]. A similar analysis is presented in this dissertation, as the justification for the modification of the dimensionless diffusion coefficient.

Generally, the FSA has the following steps:

1. Linearize the iterative method (if the original method is nonlinear).
2. Formulate the system of equations for the error between iterations.
3. Introduce the *Fourier ansatz*.
4. Solve the system for the eigenvalues.

Next, we provide the FSA of the linearized QD and QD methods. The stability of the QD method has already been studied [76], but we use it as a reference to the new GQD method.

5.2.1 FSA of the linearized QD and GQD methods

First, we introduce the linearized QD and GQD equations for the idealized infinite homogeneous medium. The $(\ell + 1)^{\text{st}}$ iteration begins with the transport sweep (Eq. (4.39a) and Eq. (4.39b)):

$$\frac{\mu_n}{h} \left(\psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}} \right) + \Sigma_t \psi_{n,j}^{\ell+\frac{1}{2}} = \frac{\Sigma_s}{2} \phi_{0,j}^{\ell} + \frac{Q_j}{2}, \quad (5.12a)$$

$$\psi_{n,j}^{\ell+\frac{1}{2}} = \left(\frac{1 + \alpha_n}{2} \right) \psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} + \left(\frac{1 - \alpha_n}{2} \right) \psi_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}}, \quad (5.12b)$$

along with the calculation of certain angular flux moments (Eq. (4.40)):

$$\phi_{k,j}^{\ell+\frac{1}{2}} = \sum_{n=1}^N \mu_n^k \psi_{n,j}^{\ell+\frac{1}{2}} w_n, \quad k = 0, 2, \quad (5.12c)$$

$$\phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} = \sum_{n=1}^N \mu_n \psi_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} w_n. \quad (5.12d)$$

In these and subsequent equations, the spatial subscript j runs over $-\infty < j < \infty$.

Next, the numerators $F_j^{\ell+\frac{1}{2}}$ of the Eddington factors are calculated. For the linear QD method, these are explicitly given by Eq. (4.35b):

$$F_j^{\ell+\frac{1}{2}} = 3\phi_{2,j}^{\ell+\frac{1}{2}}, \quad (5.13a)$$

and for the linear GQD method, they are implicitly defined by Eq. (4.27):

$$F_{j+1}^{\ell+\frac{1}{2}} - F_j^{\ell+\frac{1}{2}} = -\frac{\phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}}}{D_{j+\frac{1}{2}}^*}. \quad (5.13b)$$

Finally, the linear low-order diffusion problem is solved for $\phi_{0,j}^{\ell+1}$. This problem is defined by the following linearized GQD equations Eq. (4.46a) and Eq. (4.49):

$$\frac{1}{h}(\phi_{1,j+\frac{1}{2}}^{\ell+1} - \phi_{1,j-\frac{1}{2}}^{\ell+1}) + \Sigma_{a,j}\phi_{0,j}^{\ell+1} = Q_j, \quad (5.13c)$$

$$\phi_{1,j+\frac{1}{2}}^{\ell+1} = -D_{j+\frac{1}{2}}^* \left[\phi_{0,j+1}^{\ell+1} + (F_{j+1}^{\ell+\frac{1}{2}} - \phi_{0,j+1}^{\ell+\frac{1}{2}}) - \phi_{0,j}^{\ell+1} - (F_j^{\ell+\frac{1}{2}} - \phi_{0,j}^{\ell+\frac{1}{2}}) \right]. \quad (5.13d)$$

For clarification, the linearized QD and GQD methods have two key differences:

- The definition of the numerator F_j of the Eddington factors in the QD and GQD methods are defined differently [Eq. (5.13a) and Eq. (5.13b), respectively].
- The QD method uses the classical definition of the dimensionless diffusion coefficient (Eq. (3.5a)), while the GQD method uses the “generalized” version of $D_{j+\frac{1}{2}}^*$ from Eq. (4.38c).

To be specific, the standard F_j for the QD method is defined by Eq. (5.13a):

$$F_j = 3\phi_{2,j}, \quad (\text{QD}) \quad (5.14a)$$

and $D_{j+\frac{1}{2}}^*$ in Eq. (5.13d) is defined by its standard, classical definition:

$$D_{j+\frac{1}{2}}^* = D_{j+\frac{1}{2}} \equiv \frac{1}{3(\Sigma_t h)_{j+\frac{1}{2}}}. \quad (\text{QD}) \quad (5.14b)$$

For the GQD method, F_j is implicitly defined by Eq. (5.13b):

$$F_{j+1}^{\ell+\frac{1}{2}} - F_j^{\ell+\frac{1}{2}} = -\frac{\phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}}}{D_{j+\frac{1}{2}}^*}, \quad (\text{GQD}) \quad (5.15a)$$

and we show below that $D_{j+\frac{1}{2}}^*$ in Eq. (5.13d) should be defined by Eq. (4.38c):

$$D_{j+\frac{1}{2}}^* = \frac{1}{3(\Sigma_t h)_{j+\frac{1}{2}}} + \frac{1}{4} \sum_{n=1}^N \mu_n \alpha_n w_n. \quad (\text{GQD}) \quad (5.15b)$$

The rate of convergence of Eqs. (5.12) and Eqs. (5.13) can now be analyzed by subtracting the solution of two consecutive iterations ($\ell - 1$ from ℓ iteration). The following system of equations defines the difference between successive iterations, or *iteration errors* (ϵ). The high-order system can be rewritten as:

$$\frac{\mu_n}{h} \left(\iota_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \iota_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}} \right) + \Sigma_t \iota_{n,j}^{\ell+\frac{1}{2}} = \frac{\Sigma_s}{2} \iota_{0,j}^{\ell} , \quad (5.16a)$$

$$\iota_{n,j}^{\ell+\frac{1}{2}} = \left(\frac{1+\alpha_n}{2} \right) \iota_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} + \left(\frac{1-\alpha_n}{2} \right) \iota_{n,j-\frac{1}{2}}^{\ell+\frac{1}{2}} , \quad (5.16b)$$

where $\iota_{n,j+\frac{1}{2}}$ is the iteration error for the high-order system. The necessary angular moments of the high-order iteration error are defined by:

$$I_{k,j}^{\ell+\frac{1}{2}} = \sum_{n=1}^N \mu_n^k \iota_{n,j}^{\ell+\frac{1}{2}} w_n , \quad k=0,2 , \quad (5.16c)$$

$$I_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} = \sum_{n=1}^N \mu_n \iota_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} w_n . \quad (5.16d)$$

The low-order system is then defined by:

$$F_j^{\ell+\frac{1}{2}} = 3I_{2,j}^{\ell+\frac{1}{2}} \quad (\text{QD}) , \quad (5.16e)$$

$$F_{j+1}^{\ell+\frac{1}{2}} - F_j^{\ell+\frac{1}{2}} = -\frac{I_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}}}{D_{j+\frac{1}{2}}^*} \quad (\text{GQD}) . \quad (5.16f)$$

$$\frac{1}{h} \left(I_{1,j+\frac{1}{2}}^{\ell+1} - I_{1,j-\frac{1}{2}}^{\ell+1} \right) + \Sigma_{a,j} I_{0,j}^{\ell+1} = 0 , \quad (5.16g)$$

$$I_{1,j+\frac{1}{2}}^{\ell+1} = -D_{j+\frac{1}{2}}^* \left[I_{0,j+1}^{\ell+1} + \left(F_{j+1}^{\ell+\frac{1}{2}} - I_{0,j+1}^{\ell+\frac{1}{2}} \right) - I_{0,j}^{\ell+1} - \left(F_j^{\ell+\frac{1}{2}} - I_{0,j}^{\ell+\frac{1}{2}} \right) \right] . \quad (5.16h)$$

Since these equations are linear, the resulting system Eqs. (5.16) yields identical equations to Eqs. (5.12) and Eqs. (5.13), except that the external sources are now zero ($Q_j = 0$). The convergence rate of the iterative method can be obtained now by determining how rapidly the *iteration errors* limit to zero. We do this by examining the different Fourier components of

the equation Eqs. (5.16), i.e. by applying the *Fourier ansatz* and assuming that the unknowns all have the same single Fourier-mode spatial dependence. This dependence has the form $e^{i\lambda\Sigma_t z}$, where the Fourier frequency λ is arbitrary.

Specifically, we apply the standard *Fourier ansatz* for a single Fourier error mode of Eqs. (5.16):

$$I_{0,j}^\ell = \omega^\ell e^{i\lambda\Sigma_t z_j}, \quad (5.17a)$$

$$I_{n,j}^{\ell+\frac{1}{2}} = \omega^\ell a_n e^{i\lambda\Sigma_t z_j}, \quad (5.17b)$$

$$I_{n,j+\frac{1}{2}}^{\ell+\frac{1}{2}} = \omega^\ell b_n e^{i\lambda\Sigma_t z_{j+\frac{1}{2}}}, \quad (5.17c)$$

$$I_{k,j}^{\ell+\frac{1}{2}} = \omega^\ell A_k e^{i\lambda\Sigma_t z_j}, \quad k = 0, 2, \quad (5.17d)$$

$$I_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} = \omega^\ell B_1 e^{i\lambda\Sigma_t z_{j+\frac{1}{2}}}, \quad (5.17e)$$

$$F_j^{\ell+\frac{1}{2}} = \omega^\ell f e^{i\lambda\Sigma_t z_j}, \quad (5.17f)$$

$$I_{1,j+\frac{1}{2}}^{\ell+1} = \omega^\ell \chi e^{i\lambda\Sigma_t z_{j+\frac{1}{2}}}, \quad (5.17g)$$

$$I_{0,j}^{\ell+1} = \omega^{\ell+1} e^{i\lambda\Sigma_t z_j}. \quad (5.17h)$$

In Eqs. (5.17), the Fourier parameter λ is arbitrary, taking any real value ($-\infty < \lambda < \infty$). The constants $a_n, b_n, A_k, B_1, f, \chi$, and ω are to be calculated. All the unknowns in Eqs. (5.17) have the same spatial distribution (shape) from one iteration to the next. The only difference between iterations is a multiplicative factor of ω , which occurs from one iteration to the next. The constant $\omega = \omega(\lambda)$ is defined as the “eigenvalue” of this system. As the iterative method proceeds, the spatial shape of the above Fourier modes remains the same, but their amplitudes are multiplied by a factor of ω^ℓ .

The value of $\omega(\lambda)$ dictates if the Fourier mode will decrease or increase as the iteration number ℓ increases. If $|\omega| < 1$ the amplitude of the Fourier mode decreases, and the opposite happens if $|\omega| \geq 1$. As stated in the previous section, the convergence of iterative methods

can be tied to the spectral radius of the iterative operator. Therefore, the slowest converging mode in the Fourier modes is tied to the largest value of $|\omega(\lambda)|$. The spectral radius of the iterative system can be defined as:

$$\rho = \sup_{-\infty < \lambda < \infty} |\omega(\lambda)| . \quad (5.18)$$

As previously stated, if $\rho < 1$, the method is stable. If $\rho \ll 1$, the method converges rapidly. If $\rho < 1$ and $\rho \approx 1$, the method converges slowly. If $\rho \geq 1$, the method diverges. In this way, the stability of the iterative method is measured by the spectral radius ρ .

Introducing the *Fourier ansatz* definitions from Eqs. (5.17) into Eqs. (5.16), we obtain:

$$\frac{i\mu_n}{\tau} b_n \sin \theta_f + a_n = \frac{c}{2} , \quad (5.19a)$$

$$a_n = b_n (\cos \theta_f + i\alpha_n \sin \theta_f) , \quad (5.19b)$$

$$A_m = \sum_{n=1}^N \mu_n^m a_n w_n , \quad (m = 0, 2) , \quad (5.19c)$$

$$B_1 = \sum_{n=1}^N \mu_n b_n w_n , \quad (5.19d)$$

$$f = 3A_2 \quad (\text{QD}) , \quad (5.19e)$$

$$f(2i \sin \theta_f) = -\frac{B_1}{D^*} \quad (\text{GQD}) , \quad (5.19f)$$

$$\frac{i\chi}{\tau} \sin \theta_f + (1 - c)\omega = 0 , \quad (5.19g)$$

$$\chi = -D^*(\omega + f - A_0)(2i \sin \theta_f) . \quad (5.19h)$$

For simplicity in Eqs. (5.19), we define the following quantities:

$$c = \frac{\Sigma_s}{\Sigma_t} = \text{scattering ratio} , \quad (5.20a)$$

$$\tau = \frac{\Sigma_t h}{2} = \frac{1}{2} (\text{cell optical thickness}) , \quad (5.20b)$$

$$\theta_f = \lambda \tau = \text{scaled Fourier parameter} , \quad (5.20c)$$

Solving Eq. (5.19a) and Eq. (5.19b) for a_n and b_n , we obtain:

$$b_n = \frac{c}{2} \left(\frac{1}{\cos \theta_f + i \left(\alpha_n + \frac{\mu_n}{\tau} \right) \sin \theta_f} \right), \quad (5.21a)$$

$$a_n = \frac{c}{2} \left(\frac{\cos \theta_f + i \alpha_n \sin \theta_f}{\cos \theta_f + i \left(\alpha_n + \frac{\mu_n}{\tau} \right) \sin \theta_f} \right). \quad (5.21b)$$

Introducing these results into Eq. (5.19c) and Eq. (5.19d), we obtain:

$$A_m = \left(\frac{c}{2} \right) \sum_{n=1}^N \mu_n^m \left(\frac{\cos^2 \theta_f + \alpha_n \left(\alpha_n + \frac{\mu_n}{\tau} \right) \sin^2 \theta_f}{\cos^2 \theta_f + \left(\alpha_n + \frac{\mu_n}{\tau} \right)^2 \sin^2 \theta_f} \right) w_n, \quad (m = 0, 2), \quad (5.21c)$$

$$B_1 = -i \left(\frac{c}{2} \right) \sum_{n=1}^N \left(\frac{\mu_n \left(\alpha_n + \frac{\mu_n}{\tau} \right) \sin \theta_f}{\cos^2 \theta_f + \left(\alpha_n + \frac{\mu_n}{\tau} \right)^2 \sin^2 \theta_f} \right) w_n. \quad (5.21d)$$

Introducing these results into Eq. (5.19e) and Eq. (5.19f), we obtain:

$$f = \frac{c}{2} \sum_{n=1}^N (3\mu_n^2) \left(\frac{\cos^2 \theta_f + \alpha_n \left(\alpha_n + \frac{\mu_n}{\tau} \right) \sin^2 \theta_f}{\cos^2 \theta_f + \left(\alpha_n + \frac{\mu_n}{\tau} \right)^2 \sin^2 \theta_f} \right) w_n, \quad (\text{Linear QD}), \quad (5.21e)$$

$$f = \frac{c}{4D^*} \sum_{n=1}^N \left(\frac{\mu_n \left(\alpha_n + \frac{\mu_n}{\tau} \right)}{\cos^2 \theta_f + \left(\alpha_n + \frac{\mu_n}{\tau} \right)^2 \sin^2 \theta_f} \right) w_n, \quad (\text{Linear GQD}). \quad (5.21f)$$

Finally, we eliminate χ between Eq. (5.19g) and Eq. (5.19h) to obtain the following explicit formula for ω :

$$\omega = \left(\frac{\frac{2D^*}{\tau} \sin^2 \theta_f}{\frac{2D^*}{\tau} \sin^2 \theta_f + 1 - c} \right) (A_0 - f). \quad (5.21g)$$

We emphasize that the D and f are defined differently for the linear QD and GQD methods. [For the QD method, D and f are defined by Eq. (5.14b) and Eq. (5.21e). For the GQD method, D and f are defined by Eq. (5.15b) and Eq. (5.21f).]

Combining Eq. (5.21g), Eq. (5.21c), Eq. (5.21e), and Eq. (5.16b), we obtain the following result for the linear QD (sometimes called the ‘‘Second Moment’’) method:

$$\omega = \frac{c}{2} \left(\frac{\frac{2D}{\tau} \sin^2 \theta_f}{\frac{2D}{\tau} \sin^2 \theta_f + 1 - c} \right) \sum_{n=1}^N (1 - 3\mu_n^2) \left(\frac{\cos^2 \theta_f + \alpha_n \left(\alpha_n + \frac{\mu_n}{\tau} \right) \sin^2 \theta_f}{\cos^2 \theta_f + \left(\alpha_n + \frac{\mu_n}{\tau} \right)^2 \sin^2 \theta_f} \right) w_n. \quad (5.22a)$$

Similarly, we obtain the following result for the linear GQD method:

$$\omega = \frac{c}{2} \left(\frac{\frac{2D^*}{\tau} \sin^2 \theta_f}{\frac{2D^*}{\tau} \sin^2 \theta_f + 1 - c} \right) \sum_{n=1}^N \left(\frac{\cos^2 \theta_f + \alpha_n \left(\alpha_n + \frac{\mu_n}{\tau} \right) \sin^2 \theta_f - \frac{\mu_n}{2D^*} \left(\alpha_n + \frac{\mu_n}{\tau} \right)}{\cos^2 \theta_f + \left(\alpha_n + \frac{\mu_n}{\tau} \right)^2 \sin^2 \theta_f} \right) w_n . \quad (5.22b)$$

Eqs. (5.22) define the eigenvalue ω for the linearized QD and GQD iterative methods. The scaled Fourier parameter θ_f in Eqs. (5.22) is defined in the range $-\infty < \theta_f < \infty$. However, we note that these equations are periodic functions in θ_f , and have a period of $\pi/2$. Therefore, we can evaluate the spectral radius based on the maximum value of $\omega(\theta_f)$ in the range $0 \leq \theta_f \leq \frac{\pi}{2}$:

$$\rho = \sup_{0 \leq \theta_f \leq \frac{\pi}{2}} |\omega(\theta_f)| . \quad (5.23)$$

The eigenvalue ω in Eq. (5.22a) is the classical result for the QD method [76]. We can evaluate this result for the “worst” case in which the scattering ratio is maximum ($c = 1$), and the spatial modes are “flat” ($\theta_f = 0$) to obtain:

$$\omega|_{c=1, \theta_f=0} = \frac{1}{2} \sum_{n=1}^N (1 - 3\mu_n^2) w_n = 0 . \quad (5.24)$$

Thus, the “flat” QD error modes converge instantly.

For the GQD method, we obtain for $c = 1$ and the “flat” error modes:

$$\begin{aligned} \omega|_{c=1, \theta_f=0} &= \frac{1}{2} \sum_{n=1}^N \left[1 - \frac{\mu_n}{2D^*} \left(\alpha_n + \frac{\mu_n}{\tau} \right) \right] w_n \\ &= 1 - \frac{1}{D^*} \left(\frac{1}{4} \sum_{n=1}^N \mu_n \alpha_n w_n + \frac{1}{3\Sigma_t h} \right) . \end{aligned} \quad (5.25)$$

If we apply the classical definition of the dimensionless diffusion coefficient D^* (Eq. (5.15b)), we obtain:

$$\omega|_{c=1, \theta_f=0} = - \left(\frac{3\Sigma_t h}{4} \right) \sum_{n=1}^N \mu_n \alpha_n w_n . \quad (5.26)$$

Equation (5.26) shows that the flat error modes converge only for optical thin spatial grids. For thicker grids, the numerator of Eq. (5.26) can become larger than 1, causing the iterative method to diverge. However, if we apply the modified dimensionless diffusion coefficient defined in Eq. (5.15b):

$$D^* = \frac{1}{3\Sigma_t h} + \frac{1}{4} \sum_{n=1}^N \mu_n \alpha_n w_n, \quad (5.27)$$

then the flat error modes limit to zero ($\omega|_{\theta_f=0} = 0$). These error modes, like those in the linear QD method, converge “instantly” for spatial cells of any optical thickness. *The use of the modified dimensionless diffusion coefficient causes the flat LGQD error modes (obtained from the FSA) to vanish in the worst case of $c = 1$.*

For optically thin spatial grids ($\Sigma_t h \approx 0$), we can simplify both formulas in Eq. (5.24) to:

$$\omega(\lambda)|_{\Sigma_t h \approx 0} \approx \frac{1}{2} \left(\sum_{n=1}^N \frac{1 - 3\mu_n^2}{1 + \lambda^2 \mu_n^2} w_n \right), \quad (5.28)$$

since $\alpha_n \approx 0$. We note that, for optically thin cells, both linearized QD and GQD formulas agree with the FSA for the continuous S_N equations with standard diffusion acceleration. The maximum value obtained by Eq. (5.28) is $\omega(\lambda) = 0.2247$, which matches the optimal CMFD’s spectral radius [29]. This confirms theoretically that the GQD method should perform well and efficiently for optically thin spatial grids.

The other extreme case can also be verified, by evaluating Eqs. (5.22) when $\Sigma_t h \rightarrow \infty$. For optically thick grids, $\alpha \approx \text{sign}(\mu_n)$, leading to:

$$\omega(\lambda)|_{\Sigma_t h \approx \infty} \approx 0. \quad (5.29)$$

This implies that for optically thick grids, and for all Fourier modes, the iterative scheme will converge “instantly”.

In summary, by performing the FSA, we have provided a theoretical evaluation of the spectral radius of the linearized GQD acceleration method. This method should behave

well for both optically thin ($\Sigma_t h \approx 0$) and optically thick ($\Sigma_t h \approx \infty$) spatial grids. However, we have not yet evaluated the formulas for intermediate optical thickness. This analysis is performed numerically in Chapter 6, where we show that the GQD method is stable and rapidly convergent for any $0 \leq c \leq 1$ and any $0 < \Sigma_t h < \infty$.

The general validation of the spectral radius of the nonlinear GQD method is presented next in Chapter 6, where the theoretical estimation of the spectral radius for the linearized GQD method is evaluated and compared to the numerically-estimated spectral radius [defined by Eqs. (5.12)] for a series of test problems that employ a wide range of spatial grids.

Chapter 6: Numerical Results

In this chapter, we present a series of numerical results obtained using a `C++` code developed by the author. Our results have the following objectives: validate the numerical code, and show that the GQD method is consistent and (iii) unconditionally stable. The objectives are verified, based on the results of 5 different test problems described below.

The code has implemented the S_N , CMFD, QD, and GQD algorithms for fixed-source, planar-geometry, monoenergetic, and isotropically-scattering neutron transport problems. It has the option to simulate using the DD and SC spatial discretization schemes. The code allows for heterogeneous media and nonuniform spatial grids.

For all test cases, we used the standard S_{16} Gauss-Legendre quadrature set and the convergence criterion $\epsilon = 10^{-12}$.

6.1 Problem 1: Heterogeneous Medium

Test problem 1 is designed to check if the GQD method provides consistent solutions. In this test, the physical system is defined by a slab $0 < z < 25$ [cm] with vacuum boundaries. The system has five subregions, each 5 cm thick. Going from left to right, subregions 1, 3, and 5 have the following properties: $\Sigma_t = 1.0$ [cm⁻¹], $\Sigma_s = 0.9$ [cm⁻¹], and $Q = 0$ [cm⁻³sec⁻¹] (material 1). Subregions 2 and 4 have: $\Sigma_t = 1.0$ [cm⁻¹], $\Sigma_s = 0.99$ [cm⁻¹], and $Q = 1.0$ [cm⁻³sec⁻¹] (material 2). A schematic of the system is presented on Fig. 6.1.

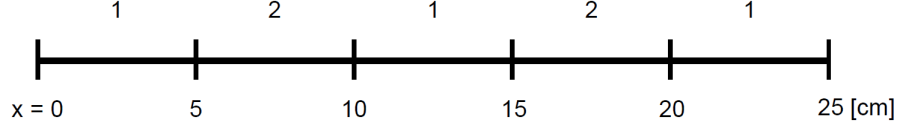


Figure 6.1: Problem 1: physical system schematic.

In this figure, (1) and (2) stand for the material and property types (1 or 2). We initially defined the cell size as $h = 0.5 \text{ [cm]}$. The diffusion version of this problem is solved ahead of the iterative method to provide the initial guess for the transport scalar flux ($\phi_{0,j}^0$).

The converged transport scalar flux, calculated using different iterative methods (SI, CMFD, QD, and GQD) is provided in Fig. 6.2. (A detailed table with the results is presented in Appendix C.) These results show that the GQD method provides a solution that matches both the SI and CMFD methods. It was already known that the CMFD method provided a consistent solution to the SI method. However, we have now presented evidence that the new GQD method is, in fact, also consistent with the SI solution. The QD method, on the other hand, provides just an approximate solution, which is visibly different in the source regions.

The consistency of the converged GQD solution between the high-order and low-order scalar fluxes was also verified. The difference between the high-order and low-order solution (called H.O/L.O error) is presented in detail in Fig. 6.3. One can see that the difference between the high-order and low-order GQD converged scalar fluxes is in the range of 10^{-13} , which is smaller than the defined convergence criterion (10^{-12}). This demonstrates the GQD method's consistency. Meanwhile, the QD method shows a significant difference between

the solutions of the high-order and low-order systems (in the range of 10^{-1}). These results were also expected, due to the inconsistency of the QD method.

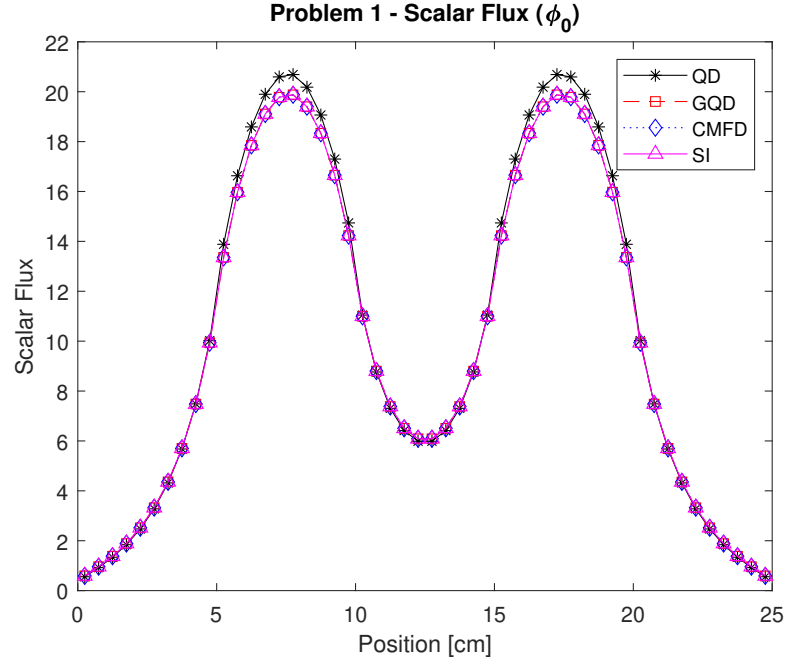


Figure 6.2: Problem 1: Scalar Flux versus Position ($\sum_i h = 0.5$)

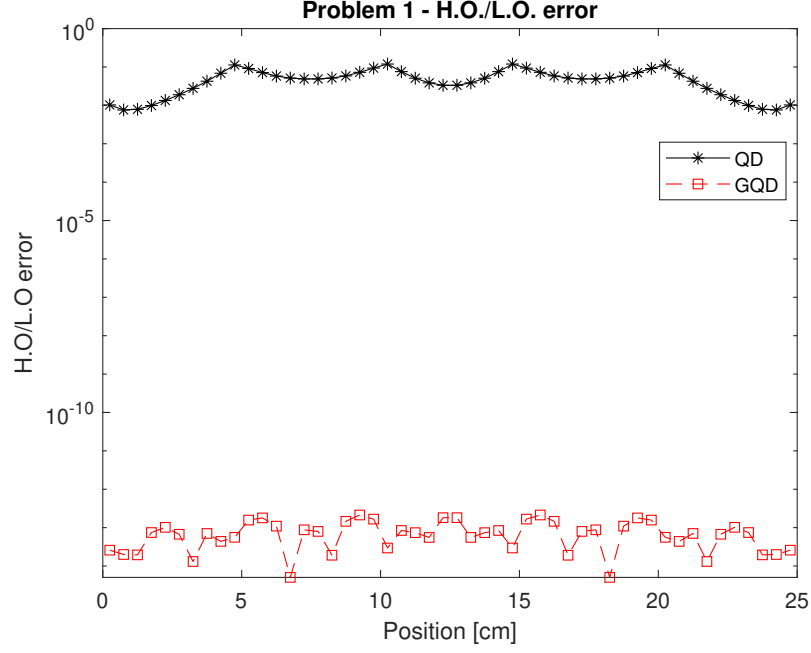


Figure 6.3: Problem 1: High-order/Low-order scalar flux error ($\Sigma_t h = 0.5$)

The iteration errors ($\|\phi_0^{\ell+1} - \phi_0^\ell\|_2$) are depicted in Fig. 6.4. As expected, all methods (besides SI) presented a rapidly-converging behavior. For this problem, the CMFD method presented the fastest convergence rate, with 13 iterations. The GQD method completed the calculations with 14 iterations, and the QD and SI methods required 17 and 458 iterations, respectively.

(These results demonstrate the extraordinary value of efficient transport acceleration schemes. Because of the included diffusion calculation, each accelerated iteration is slightly more expensive than a single SI transport sweep. However, the acceleration method reduces the number of iterations so drastically that the overall cost of the simulation is greatly reduced.)

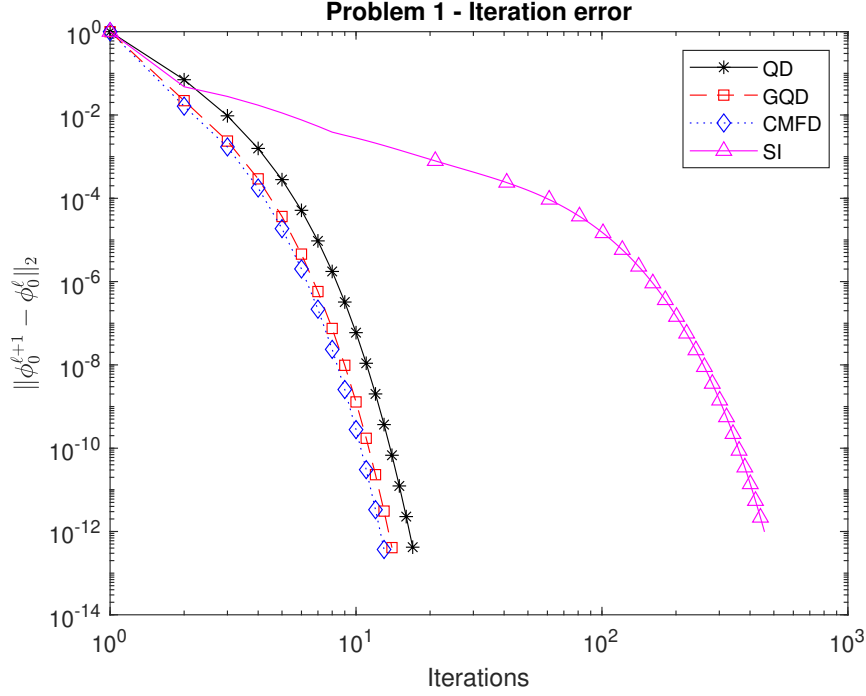


Figure 6.4: Problem 1: Iteration error ($\Sigma_t h = 0.5$).

One question may arise: *what happens if we change the optical thickness $\Sigma_t h$ of the spatial cells?* To explore the effect of varying $\Sigma_t h$, we simulated problem 1 with different cell sizes h_j (from 0.125 cm up to 5 cm), without changing the physical system. Thus, each simulation will have a different number of total cells.

Table 6.1 displays the spectral radius of each method with different cell optical thicknesses ($\Sigma_t h$). The values in between parentheses in the first column represent the total number of cells in the simulation (J). We note that the SI method has, in all cases, a very high spectral radius value, showing very slow convergence compared to the other methods. The CMFD, QD, and GQD, as expected, presented a small spectral radius for fine grids. For

optically thicker cells, the CMFD method loses efficiency as the QD and GQD methods become faster. (These behaviors are predicted by the Fourier Stability analysis).

Table 6.1: Spectral Radius (ρ) for different methods and $\Sigma_t h$.

$\Sigma_t h$ (J)	Spectral Radius (ρ)			
	SI	CMFD	QD	GQD
0.125 (200)	0.9556	0.1943	0.2008	0.1962
0.25 (100)	0.9554	0.1757	0.1957	0.1797
0.5 (50)	0.9548	0.1105	0.1853	0.1317
1.0 (25)	0.9528	0.1395	0.1747	0.0604
2.5 (10)	0.9467	0.7224	0.1225	0.1771
5.0 (5)	0.9417	0.9326	0.0747	0.0869

The converged scalar fluxes for the GQD simulations are presented in Fig. 6.5, for different spatial grids. (Some results for other optical thicknesses ($\Sigma_t h = 0.25$ and $\Sigma_t h = 5.0$) are omitted for clarity and better visualization). For coarser grids, the converged solution (even if consistent) is not accurate. However, as the grid becomes optically thinner, the solution tends to approximate better to the true solution of the system. A similar trend happens when we analyze the converged F_j values (in Fig. 6.6). It is also visible that, as expected, F_j has similar behavior to the scalar flux ($\phi_{0,j}$).

We further explore these similarities in Fig. 6.7. Here, we can see the converged scalar $\phi_{0,j}$, F_j , and $3\phi_{2,j}$ for the specific case $\Sigma_t h = 0.5$ in problem 1. The values of these three variables are nearly the same across the whole domain. Fig. 6.8 was added to provide a closer look at their differences.

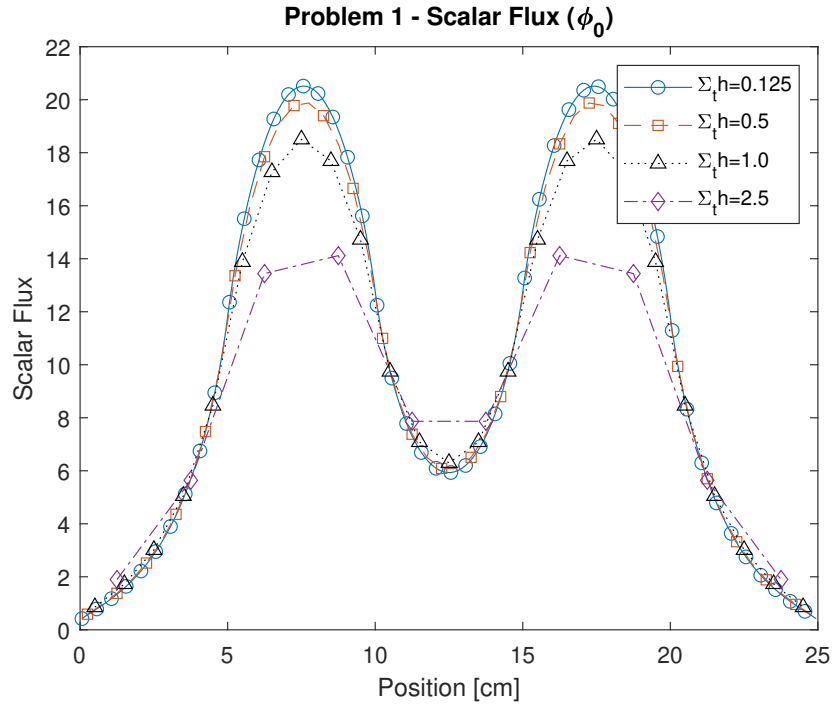


Figure 6.5: Problem 1: Scalar Flux for different $\Sigma_t h$.

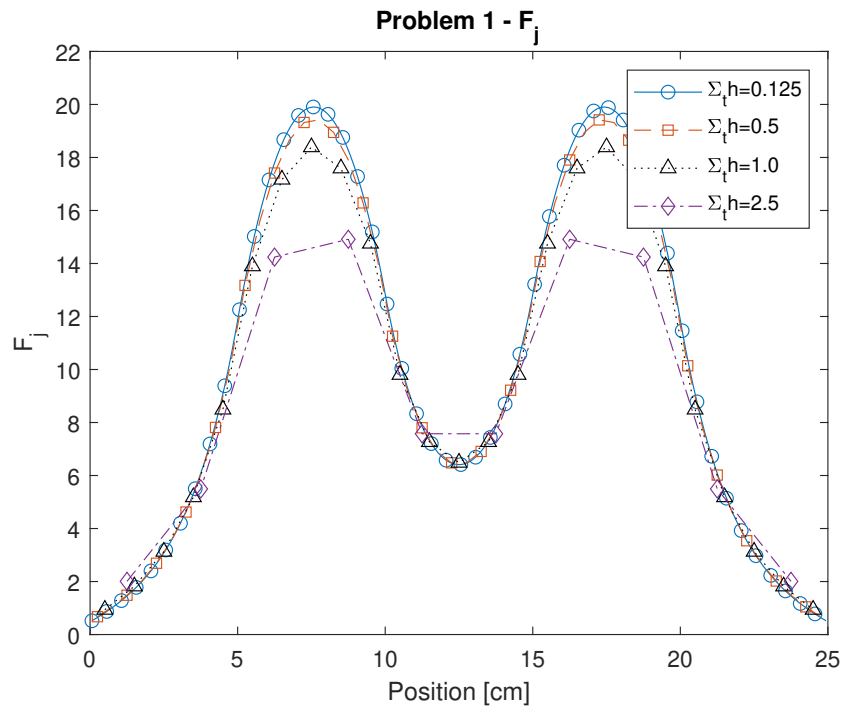


Figure 6.6: Problem 1: F_j for different $\Sigma_t h$.

In Fig. 6.8, we see that $\phi_{0,j}$ and F_j are slightly smaller than $3\phi_{2,j}$ in the non-source regions, and larger in the source regions. This result illustrates the small but meaningful difference between the QD and GQD methods: the quantities $3\phi_{2,j}$ and F_j are the numerators of the classic (QD) and the consistent (GQD) Eddington factors, respectively. Thus, Fig. 6.8 shows that (in this case) the QD method slightly underestimates the consistent Eddington factors in source regions, and slightly overestimates them in the non-source regions.

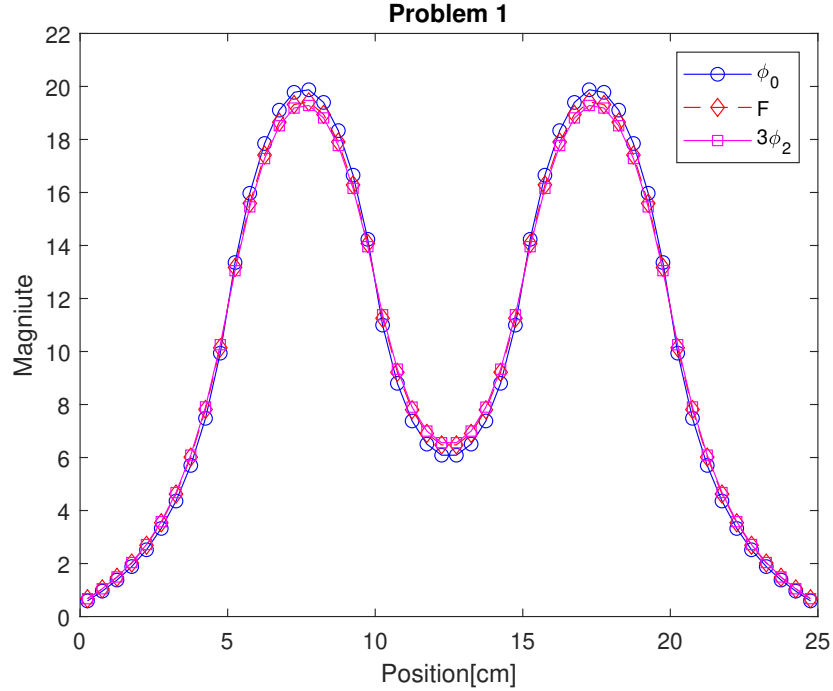


Figure 6.7: Problem 1: $\phi_{0,j}$, F_j , and $3\phi_{2,j}$ for $\Sigma_t h = 0.5$.

This is better observed by analyzing the classic and consistent Eddington factors directly, in Fig. 6.9 (obtained by Eq. (3.20a) and Eq. (4.16), respectively). In this test case, the two Eddington factors have the same described behavior: (i) the classic Eddington factors are larger than the consistent Eddington factors in non-source regions and (ii) larger in

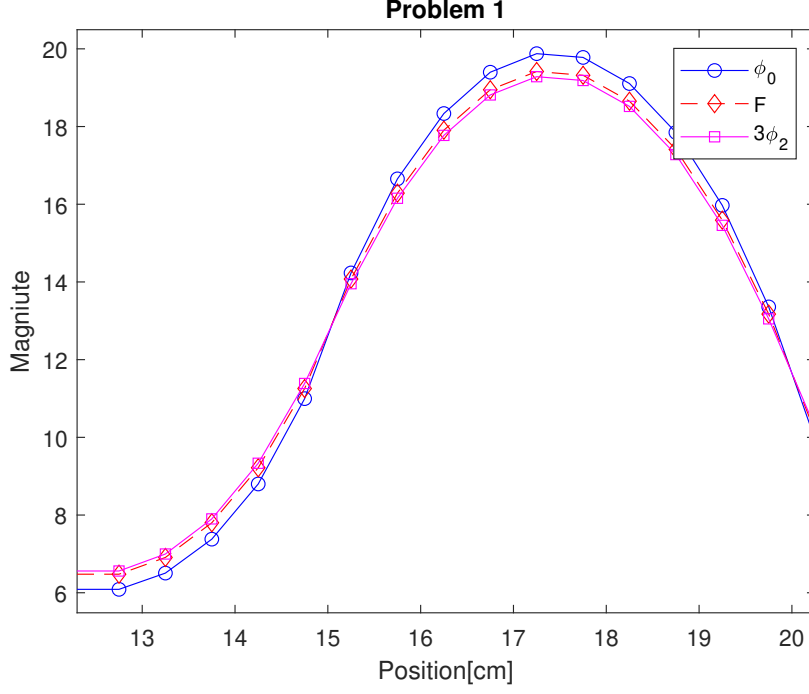


Figure 6.8: Problem 1: $\phi_{0,j}$, F_j , and $3\phi_{2,j}$ for $\Sigma_t h = 0.5$ (zoomed in for detail).

non-source regions. (In this problem, the consistent Eddington factors are “flatter” than the classic Eddington factors.)

We note that the more “diffusive” the physical system is, the closer the classic and consistent Eddington factors values are to 1. In this problem, the consistent Eddington factors are closer to unity than the classic ones. The consistency transport correction introduced into the Eddington factors (in the GQD method) fixes the overestimation of the QD method in the source regions and the underestimation in the non-source regions (observed in Fig. 6.2). This pattern may change with different test problems, and we will discuss that in the following cases.

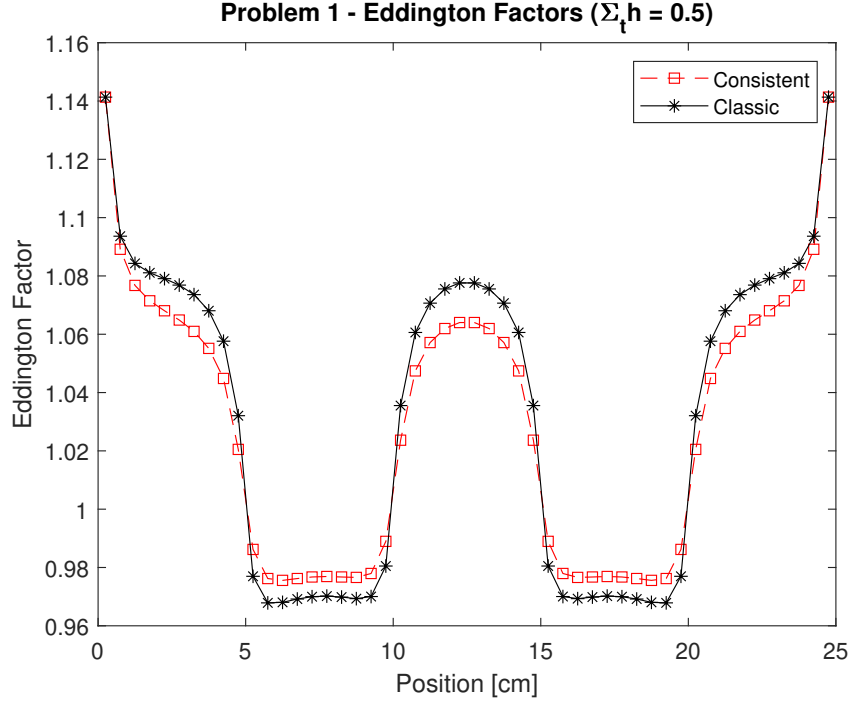


Figure 6.9: Problem 1: Classic and Consistent Eddington Factors ($\Sigma_t h = 0.5$).

The difference between the Eddington factors is visible for an intermediate spatial grid size ($\Sigma_t h = 0.5$), but this difference becomes progressively smaller as we reduce the cell size. This can be seen in Fig. 6.10, for $\Sigma_t h = 0.125$. In this figure the classic and consistent Eddington factors at the outmost cells match perfectly. This is not a coincidence. Since the problem is spatially symmetric and these cells display the smallest F_j , the method presented in Chapter 4 uses them as the F_{j^*} reference point, and defines them to be equal to $3\phi_{2,j}$. So, by definition, it is expected that the two Eddington factors have at least one shared value. Moreover, our analysis has shown that the F_j should, in the limit of small $\Sigma_t h$, limit to $3\phi_{2,j}$. Fig. 6.10 confirms that for optically thin spatial grids, the classic and consistent

Eddington factors are nearly identical. (In this figure, the two Eddington factors are almost indistinguishable to the naked eye.)

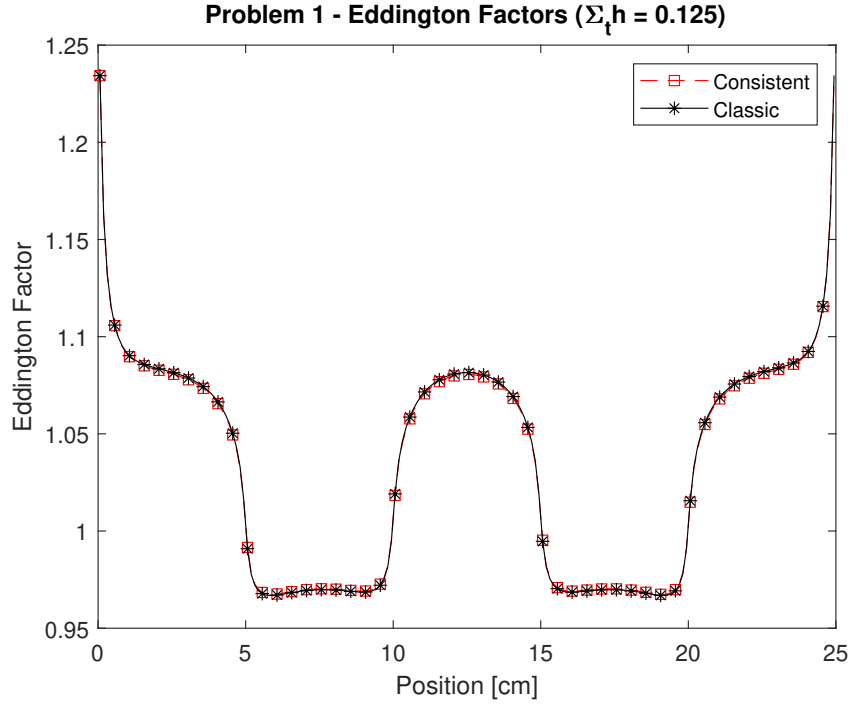


Figure 6.10: Problem 1: Classic and Consistent Eddington Factors ($\Sigma_t h = 0.125$).

Again, the outcome depicted in Fig. 6.10 is expected for two reasons: (i) the GQD method was formulated to converge to the QD method in the limit $\Sigma_t h \rightarrow 0$, and (ii) the QD method becomes consistent at the limit $\Sigma_t h \rightarrow 0$. Therefore, the results obtained in Fig. 6.10 agree with the GQD derivation. Another interesting characteristic of both Eddington factors is the significant increase or decrease of the Eddington factors in boundary regions. With little doubt, this is due to the more highly anisotropic character of the angular flux in the boundary layer regions adjoining the outer boundaries. (Away from these boundaries, the

angular flux is more isotropic.) Thinner spatial grids allow both methods to describe more accurately the boundary effects.

Finally, in Fig. 6.11, we analyze the behavior of the consistent Eddington factors as we vary the spatial grid discretization. The Eddington factors tend to increase in the non-source regions and decrease in the source regions as the grid becomes optically thinner. The opposite happens when the cells become too coarse. For $\Sigma_t h = 2.5$, the behavior is reversed, which can be expected due to the low accuracy of the method for such large spatial grids.

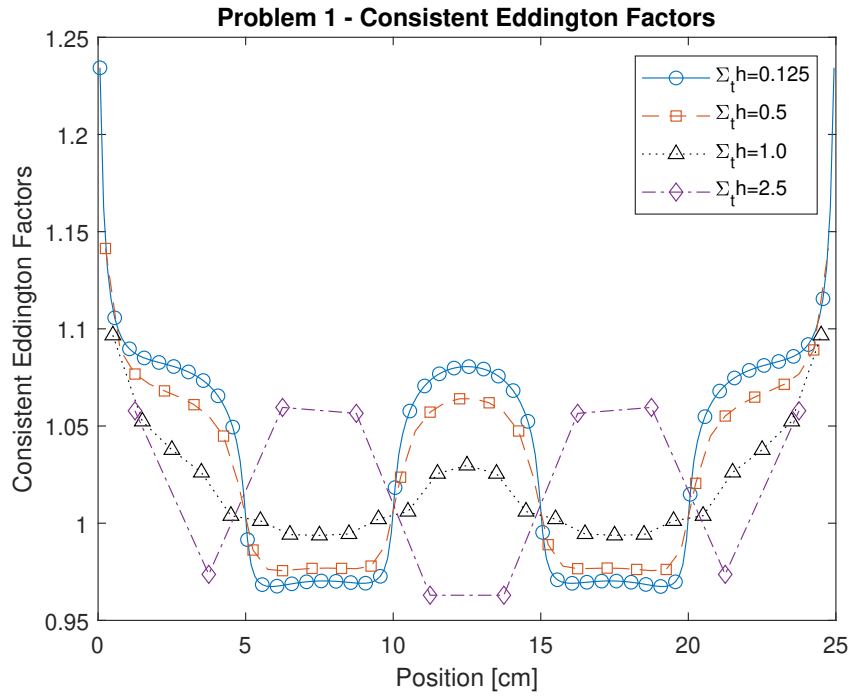


Figure 6.11: Problem 1: Consistent Eddington factors for different $\Sigma_t h$.

We note that a fully discretized method's accuracy is highly influenced by the choice of spatial grid. Likewise, the consistent Eddington factors can also be strongly influenced

by the choice of spatial grid. However, at least in this problem, the consistent Eddington factors for coarser grids are not “unreasonable,” and they still lead to fast convergence.

For an initial assessment of the GQD method, the most relevant questions to answer are: *is the method (i) consistent and (ii) stable for any spatial grid?* For problem 1, the answer to these two questions is “Yes.” The following test cases provide a deeper analysis of the GQD method’s stability.

6.2 Problem 2: Uniform Internal Source

In the following test (Problem 2), we evaluate the scalar flux for a homogeneous slab of variable thickness ($0 \leq z \leq Z = 100h$), where h is the (variable) width of each spatial cell. The domain is always $J = 100$ cells thick. The outer boundaries are vacuum, and the system materials have the following properties: $\Sigma_t = 1.0 [cm^{-1}]$, $\Sigma_s = 0.99 [cm^{-1}]$, and $Q = 0.01 [cm^{-3}sec^{-1}]$. By varying the width h of the spatial cells, we can study the performance of the QD, CMFD, and GQD methods as the optical width of the spatial cells $\Sigma_t h$ varies by small amounts.

In Fig. 6.12, we present the converged scalar flux for the QD and GQD methods, in the case of $h = 0.5$ ($Z = 50 cm$). One can see that these methods produce very similar solutions. This behavior is expected, since the problem is simple, it has a somewhat “diffusive” behavior, and $\Sigma_t h$ is not large. The QD method has more accurate solutions when the physical system is well-approximated by the diffusion equation. This is the case for problem 2, which has constant uniform internal source and materials properties.

We also evaluated the classic and consistent Eddington factors for the case of $\Sigma_t h = 1.0$ ($c = 0.99$). The results are displayed in Fig. 6.13. Here we see that the classic Eddington factors tend to the estimated “diffusive value” of $3\phi_{2,j} \approx 1.0$, except closer to the boundaries,

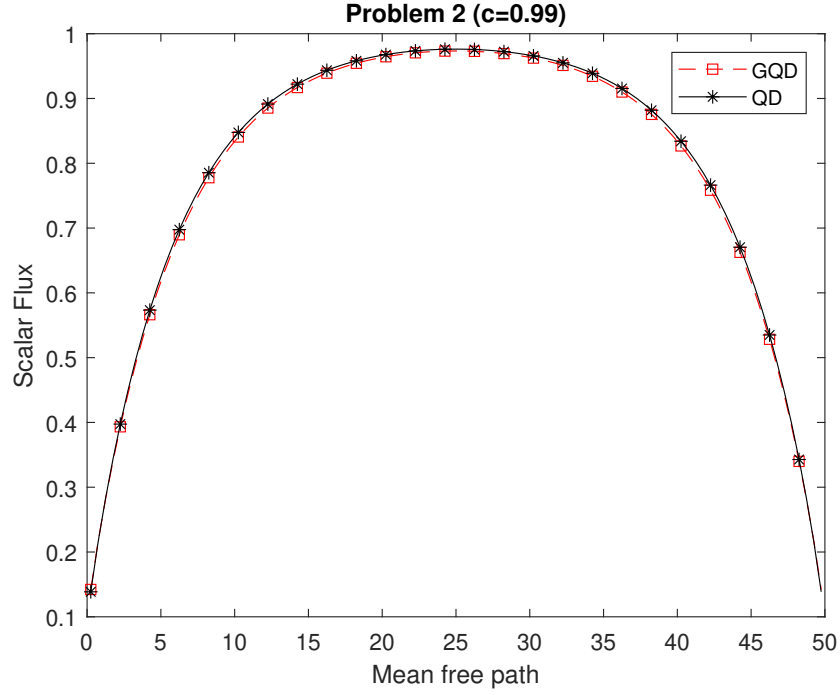


Figure 6.12: Problem 2: QD and GQD Scalar flux for $\Sigma_t h = 0.5$ ($c = 0.99$).

where the angular flux is highly anisotropic. A similar shape is observed by the consistent Eddington factors, although the values are slightly smaller than the classic ones. Both the classic and consistent Eddington factors have the same values at the outermost cells, where F_j has its minimum value. However, their values differ immediately after the boundary cells.

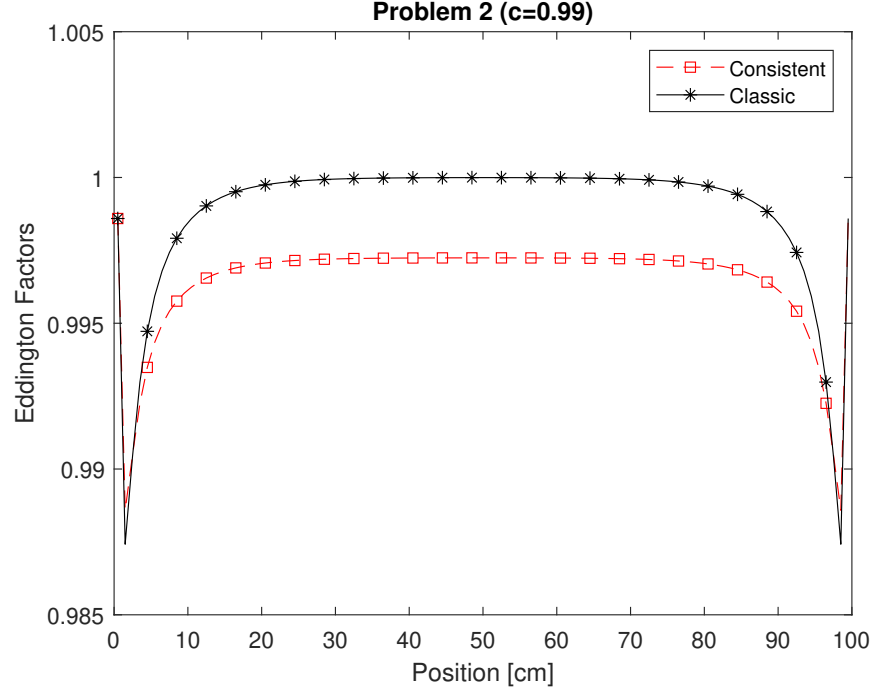


Figure 6.13: Problem 2: Classic and consistent Eddington factors for $\Sigma_t h = 1.0$ ($c = 0.99$).

The change of the consistent Eddington factors for different $\Sigma_t h$ is depicted in Fig. 6.14. Similarly to Fig. 6.11, the effects at the boundaries are more pronounced in thinner meshes. For the specific case $\Sigma_t h = 2.5$, the outermost cell's Eddington factors do not display the previously observed increase, decreasing its value instead.

We proceed with the evaluation of the numerical spectral radius (ρ_{num}) of the GQD method. In this test, We simulate problem 2 for a series of different h values (and therefore $Z = 100h$). The range studied is $0.01 \leq h \leq 10 \text{ cm}$ ($1 \leq Z \leq 1000 \text{ cm}$). The numerical spectral radius is then estimated by Eq. (5.12a) for the GQD, QD, and CMFD methods and then displayed in Fig. 6.15.

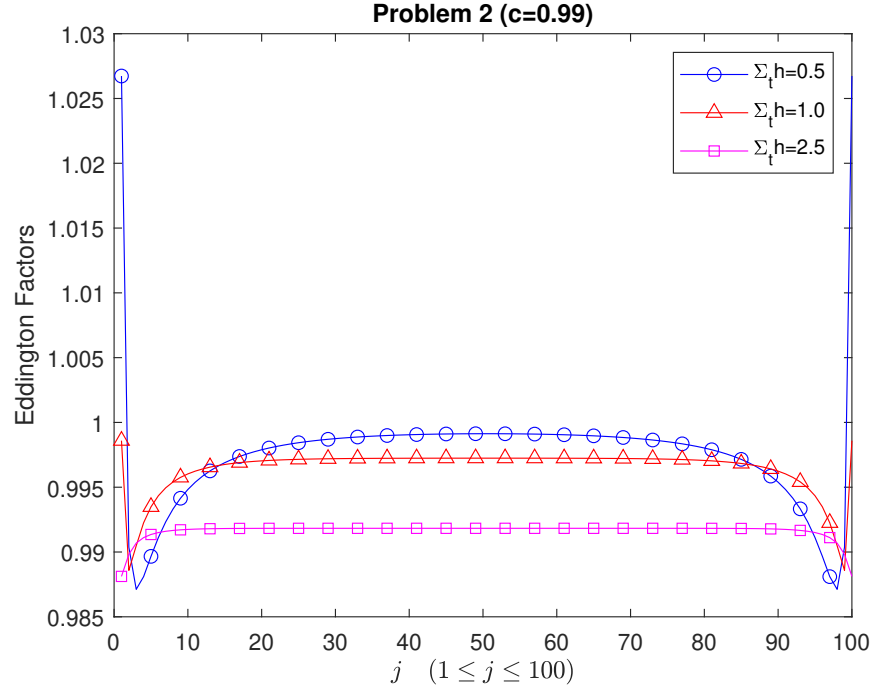


Figure 6.14: Problem 2: Consistent Eddington factors for different $\Sigma_t h$ ($c = 0.99$).

The CMFD method shows a rapidly-converging behavior ($\rho \ll 1$) for optically thin cells. However, as the spatial grid becomes thicker, CMFD quickly starts losing efficiency, in the range $1.0 < \Sigma_t h < 2.3$. The CMFD method becomes unstable for $\Sigma_t h > 2.3$. These results are expected and well-known in the field of neutron transport. Overall, CMFD is only conditionally stable.

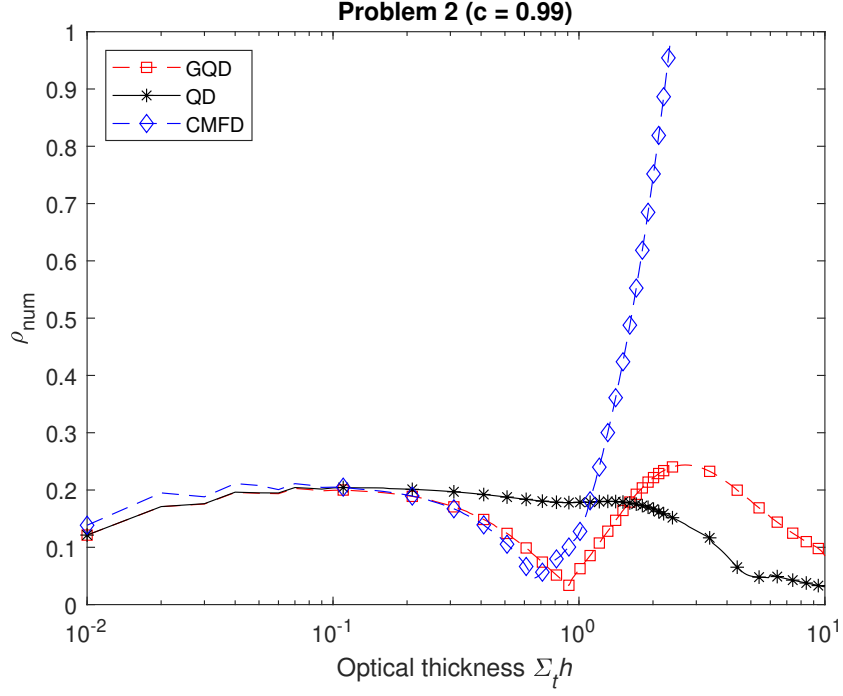


Figure 6.15: Problem 2: ρ vs $\Sigma_t h$ ($c = 0.99$).

The QD method, another well-understood method, also behaves as predicted. In this test, the QD results show rapidly-converging behavior for all spatial grids, displaying unconditional stability. The method agrees with theoretical prediction in Eq. (5.29), as it tends to increase its convergence speed at higher values of $\Sigma_t h$.

The new results presented in Fig. 6.15 are the behavior of the GQD method, introduced in this dissertation. We see that the GQD method is stable and rapidly-converging for all values of $\Sigma_t h$. For thin spatial grids, the method converges very fast, showing similar performance to the QD and CMFD methods. In the range of $0.1 \leq h \leq 0.7$ cm, the GQD method behaves closer to the CMFD method, showing a reduction in the numerical spectral radius. However, for the optically thicker spatial grids, the GQD method behaves differently than the other

two methods. Instead of increasing its spectral radius and becoming unstable (in CMFD) or decreasing progressively (in QD), the GQD method first shows a small increase in the spectral radius in the range of $\Sigma_t h \approx 3$. After that, GQD then proceeds to reduce its spectral radius monotonically for larger cells (similar to QD), which agrees with the prediction in Eq. (5.29). The biggest difference between QD and GQD is the behavior in intermediate-size cells. In spite of these differences, the GQD method is stable and rapidly-converging for all tested values of $\Sigma_t h$.

To validate these results, we also provide a comparison with the Fourier Stability Analysis (FSA) estimate of the spectral radius, obtained from Eqs. (5.22). In Fig. 6.16, the numerical spectral radius obtained from the numerical C++ code is compared with the theoretical estimate obtained by solving Eqs. (5.22). The FSA is only presented in test problems 2 and 3 for the following reason: *the proposed physical systems (in problems 2 and 3) are the closest possible to the assumptions required for the FSA method.*

In Fig. 6.16, different spectral radii are presented as a function of $\Sigma_t h$ for the case of $c = 0.99$. In this figure, we present the QD and GQD numerical estimations calculated by the numerical algorithm in C++, and the linearized QD and GQD spectral radii estimated from the FSA (Eq. (5.29)). In general, the numerical results presented for both methods agree closely with the shape of the Fourier analysis. There is a small discrepancy in the amplitude for optically thin cells, for which the physical system becomes optically thinner. This difference is most likely caused by two reasons: (i) the leakage in the finite physical system reduces the spectral radius (which is not accounted for in the infinite medium in the FSA); and (ii) the fact that the method converges very quickly, and may have some noise in the estimations of the numerical spectral radius.

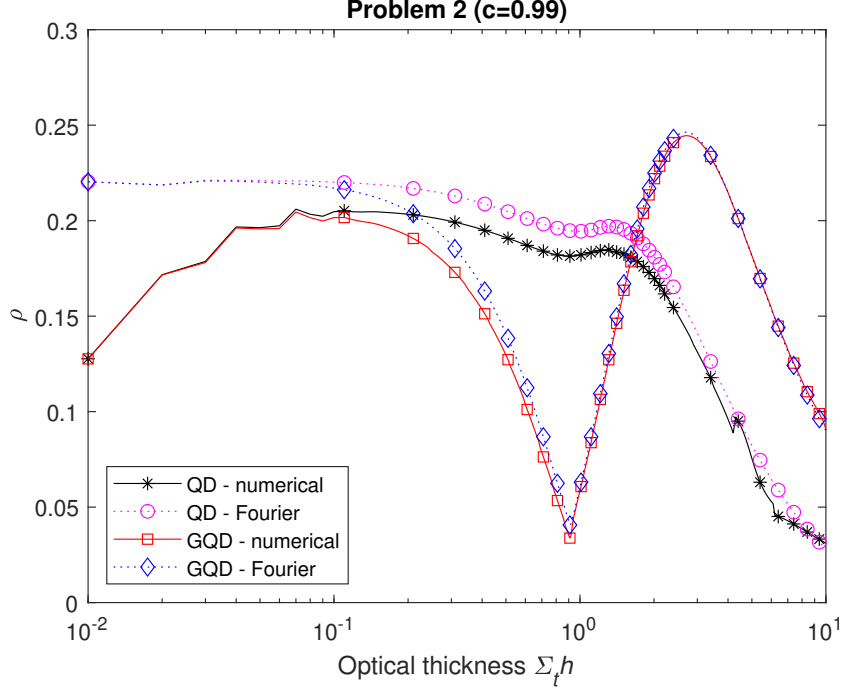


Figure 6.16: Problem 2: Fourier Analysis – ρ vs $\Sigma_t h$ ($c = 0.99$).

Overall, the behavior presented in Fig. 6.16 provides strong theoretical evidence that the GQD method is unconditionally stable and rapidly-converging for any spatial grid thickness.

6.3 Problem 3: “Purely” Diffusive Medium

Problem 3 is similar to Problem 2. Again, we evaluate the scalar flux for a homogeneous slab of variable thickness ($0 \leq z \leq Z = 100h$), where h is the (variable) width of each spatial cell (with the domain 100 cells thick). We also assume vacuum boundary conditions. However, for problem 3, we define:

$$\Sigma_t = \Sigma_s = 1.0 [cm^{-1}] \text{ which implies } c = 1.0, \quad (6.1)$$

and

$$Q = \frac{8h}{Z^2} D^* = \frac{8}{Z^2} \left(\frac{1}{3\Sigma_t} + \frac{h}{4} \sum_{n=1}^N \mu_n \alpha_n w_n \right). \quad (6.2)$$

[This definition of Q causes the continuous diffusion approximation of the transport problem, using zero-flux boundary conditions, to have a scalar flux maximum value of 1.0 at the center of the system.] This choice of Q should lead to a transport scalar flux having a nearly parabolic shape, with a theoretical maximum close to $\phi_{max} = 1.0$ [$cm^{-2}sec^{-1}$] for thick systems.

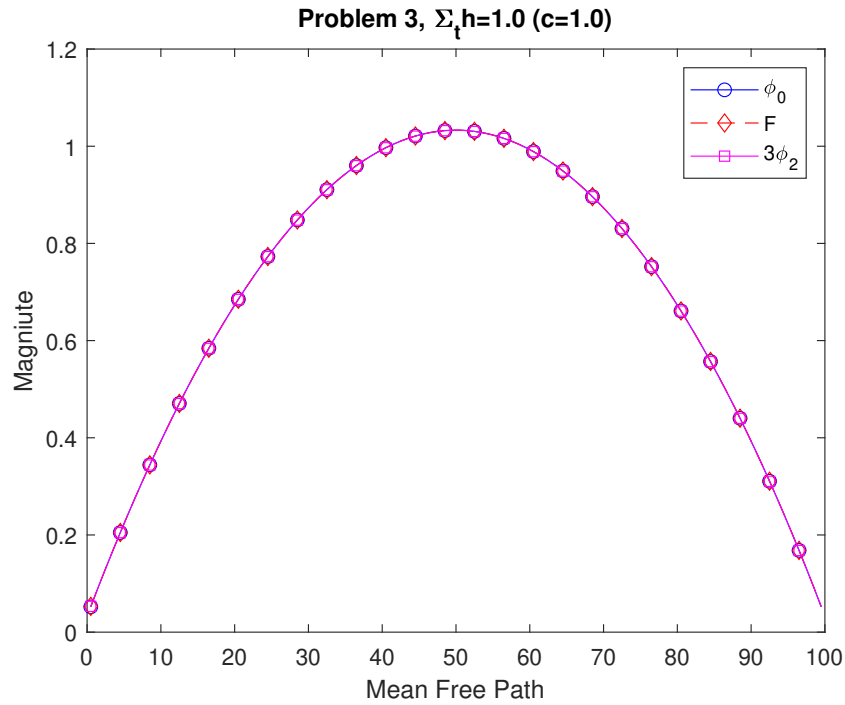


Figure 6.17: Problem 3: $\phi_{0,j}$, F_j , and $3\phi_{2,j}$ for $\Sigma_t h = 1.0$ ($c = 1.0$).

The values of $\phi_{0,j}$, F_j , and $3\phi_{2,j}$ are displayed in figure Fig. 6.17 for the case $\Sigma_t h = 1.0$. The scalar flux, as expected, has a parabolic shape with the maximum value close to the

predicted value (1.0). Since the system is not thick enough, there is still a minor discrepancy between the simulation and the theoretical prediction.

As expected, “diffusive” systems display a good agreement between F_j and $3\phi_{2,j}$ (the small difference is barely visible without any zoom). This difference can be better analyzed by inspecting the classic and consistent Eddington factors directly. Figure 6.18 shows that, in this test case, the consistent Eddington factors are equal to 1.0 except close to the boundaries. The classic Eddington factors, on the other hand, tend to have a value slightly smaller than 1.0. Once again, the consistent Eddington factors displayed a less abrupt change closer to the boundaries (compared to the classic Eddington factors).

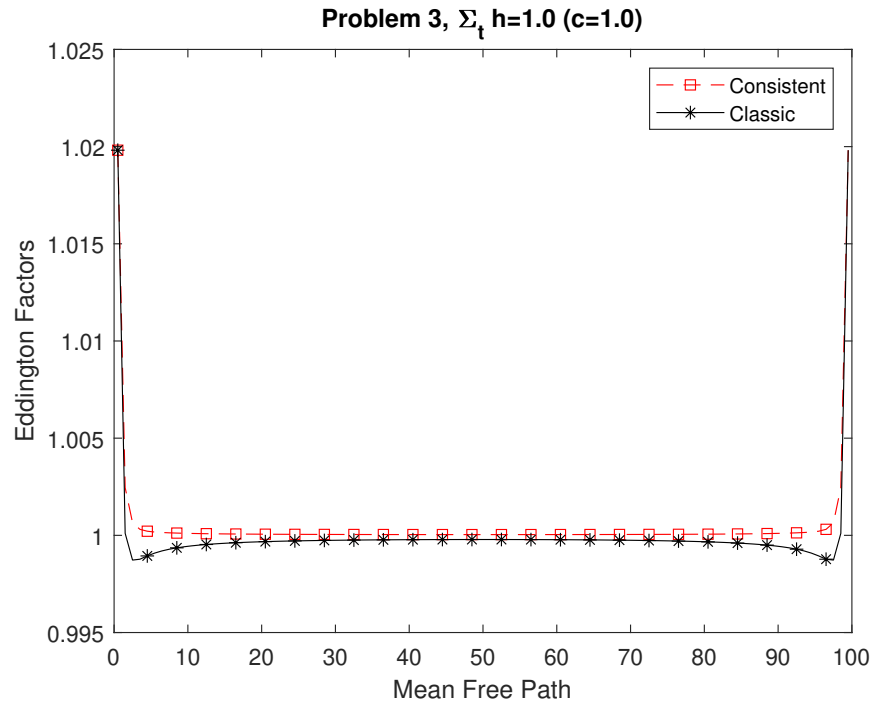


Figure 6.18: Problem 3: Classic and consistent Eddington factors for $\Sigma_t h = 1.0$ ($c = 1.0$).

The behavior of the consistent Eddington factors for different $\Sigma_t h$ is shown in Fig. 6.19. Once again, the coarser the cells, the less the boundary effects are captured by the Eddington factors.

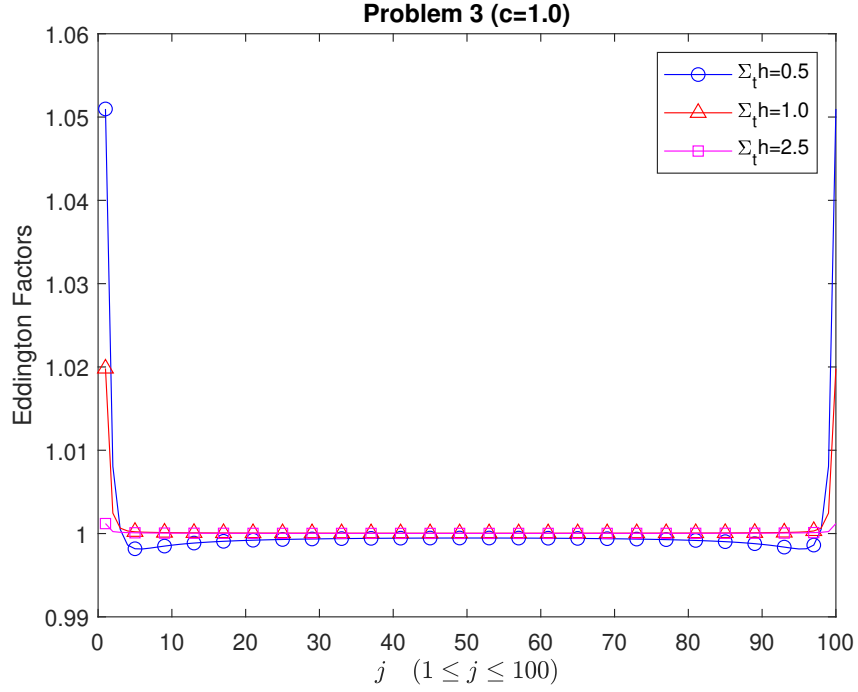


Figure 6.19: Problem 3: Consistent Eddington factors for different $\Sigma_t h$ ($c = 1.0$).

One aspect of problem 3 is that the neutron absorption of the system is zero. The only way for the neutrons to vanish from the domain is by leakage at the outer boundaries. The lack of neutron absorption as a neutron removal mechanism could increase the stress on the iterative method, requiring more iterations to converge. This would lead to a higher spectral radius, and therefore, a slower convergence rate. However, as we see in Fig. 6.20, the GQD method is unconditionally stable, showing a convergence rate very similar to Problem 2.

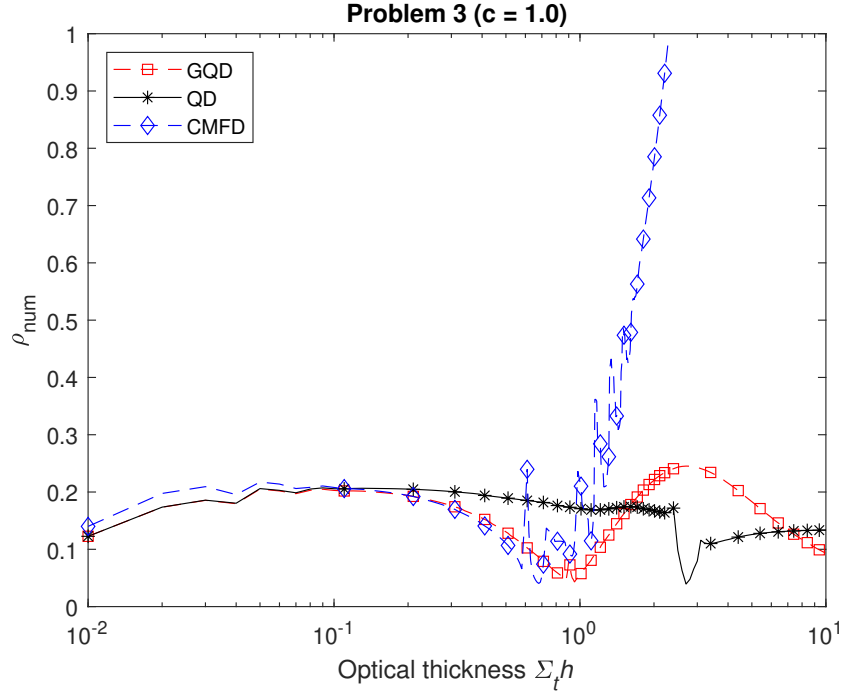


Figure 6.20: Problem 3: ρ vs $\Sigma_t h$ ($c = 1.0$).

To further validate these results, we provide a comparison with the Fourier Stability Analysis (FSA) estimate of the spectral radius, obtained from Eqs. (5.22). In Fig. 6.21, the numerical spectral radii obtained from the numerical $C++$ code (for the QD and GQD method) are compared with the theoretical estimates obtained by solving Eqs. (5.22).

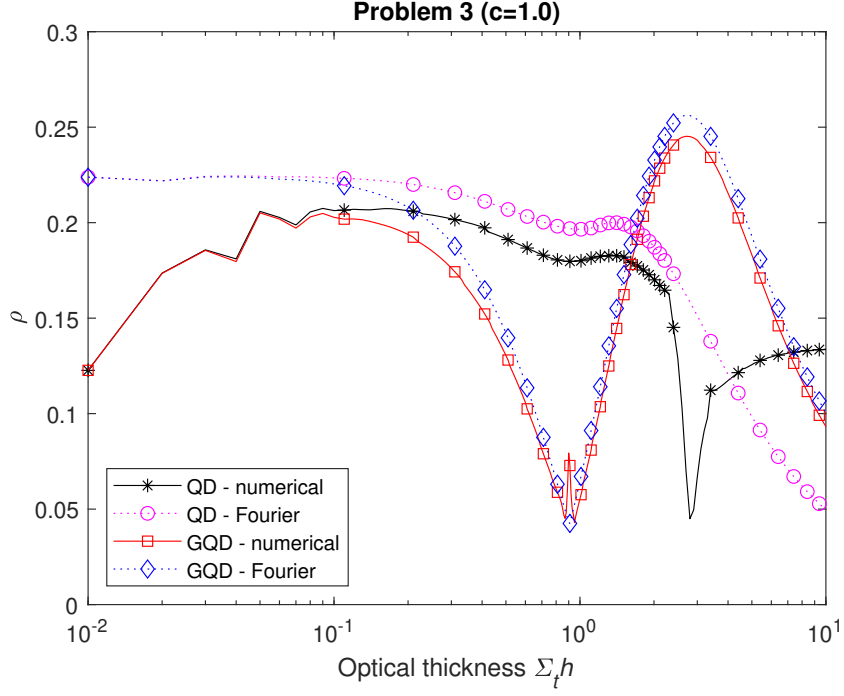


Figure 6.21: Problem 3: Fourier Analysis – ρ vs $\Sigma_t h$ ($c = 1.0$).

We can see that the numerically estimated spectral radius for the GQD method matches closely the behavior of the theoretically predicted spectral radius from the Fourier Stability Analysis (FSA). At the same time, the QD method displays a small discrepancy for coarser meshes. (We believe that this minor discrepancy is an artifact, caused by the extremely rapid convergence of the method, causing an error in the estimate of the spectral radius.)

Besides the discrepancy in the QD solution for very coarse meshes. Both methods match closely with the FSA solution. Again, there is a small difference in overall values for the spectral radii, most likely caused by (i) leakage from a finite physical system and (ii) numerical estimation of the spectral radius in the $C++$ code (based on Eqs. (5.22)).

This concludes the tests regarding homogeneous media with uniform internal sources.

6.4 Problem 4: Step Internal Source

The test case of problem 4 is another variant of problem 2. We use the same physical system of a homogeneous slab of variable thickness ($0 \leq z \leq Z = 100h$), where h is the (variable) width of each spatial cell and vacuum boundary conditions. The material properties in this case are defined the following way: $\Sigma_t = 1.0 [cm^{-1}]$ and $\Sigma_s = 0.999 [cm^{-1}]$. However, instead of using a uniform internal source, we define Q as a histogram:

$$Q(z) = \begin{cases} 0 & , \ 0 < z < \frac{Z}{2} , \\ 0.001 & , \ \frac{Z}{2} < z < Z . \end{cases} \quad (6.3)$$

Therefore, Q is a step function, with its discontinuity at the middle of the system.

In the specific case of $\Sigma_t h = 1.0$ and $c = 0.999$, the GQD algorithm developed provided the following results for $\phi_{0,j}$, F_j , and $3\phi_{2,j}$ in Fig. 6.22. In this figure, all variables behave similarly and show a significant decrease as one moves away from the source region, leading to a very small flux at the left boundary of the system. This behavior becomes more pronounced as we increase the values of $\Sigma_t h$.

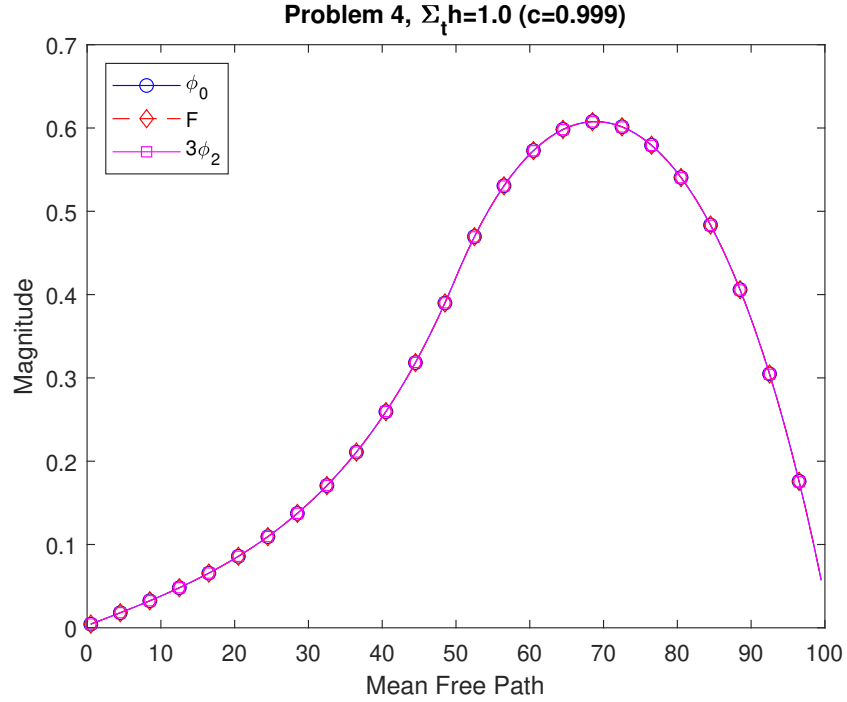


Figure 6.22: Problem 4: $\phi_{0,j}$, F_j , and $3\phi_{2,j}$ for $\Sigma_t h = 1.0$ ($c = 0.999$).

The classic and consistent Eddington factors are depicted in Fig. 6.23. The behavior of the consistent Eddington factors for different optical thicknesses is provided in Fig. 6.24. In both cases, the results obtained agreed with the previous analysis obtained from previous tests. The classic Eddington factor tends to vary considerably closer to the outer boundaries; and in optically thicker grids, these boundary effects on the consistent Eddington factors are underestimated compared to thinner cells. A significant difference between this case and previous tests is that the system in problem 4 is not symmetric. Because of that, the classic and consistent Eddington factors do not have the same values at the right-most and left-most cells (in Fig. 6.23).

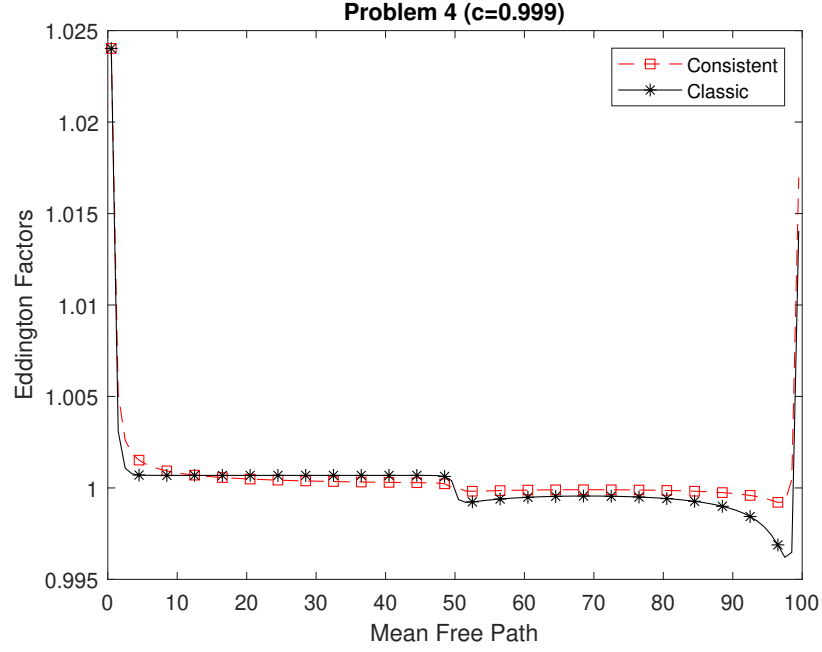


Figure 6.23: Problem 4: Classic and consistent Eddington factors for $\Sigma_t h = 1.0$ ($c = 0.999$).

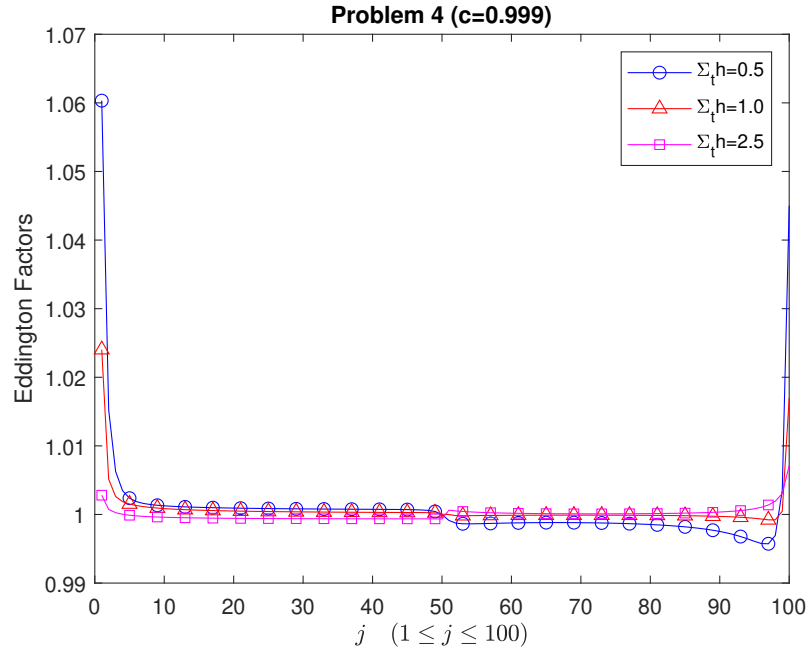


Figure 6.24: Problem 4: Consistent Eddington factors for different $\Sigma_t h$ ($c = 0.999$).

The numerical evaluation of the spectral radius is presented in Fig. 6.25. Similar to the previous tests, the GQD algorithm displayed unconditional stability and rapid convergence for all spatial grid discretizations. At coarser grids, the GQD method tends to converge to similar spectral radii obtained from the QD method, which also shows unconditional stability for this problem. The CMFD method, on the other hand, loses efficiency at the intermediate cell size range and quickly becomes unstable (which was already expected).

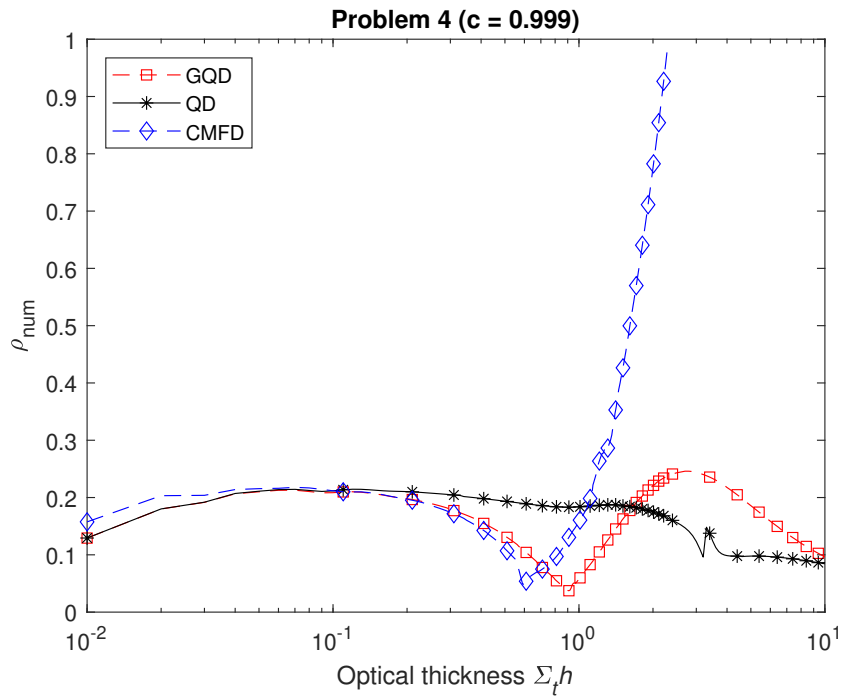


Figure 6.25: Problem 4: ρ vs $\Sigma_t h$ ($c = 0.999$).

This test case is particularly interesting because as we increase the cell sizes, the domain expands and the non-source region progressively becomes larger. This leads to smaller scalar fluxes on the left side of the system. This scalar flux could potentially become very close to zero. And the question is: *why would this matter?*

In our work, we have defined the F_j in a way that guarantees that they all will remain positive so that the resulting consistent Eddington factors will be guaranteed to be positive. However, let us, for the moment, relax this constraint. Then, “deep penetration” regions (where the fluxes tend to very small values) might lead to negative values for F_j from Eq. (5.29). For example, let us consider the case that we decide to solve this problem with Eq. (4.29) (summing from the right boundary) and use the expected $F_J = 3\phi_{2,J}$ value as the initial arbitrary constant. If in this case, we do not recalculate the arbitrary constant F_J according to the method defined in Section 4.1.1, this procedure could potentially lead to negative F_j values, which would destabilize the iterative method. One numerical example of how this can happen is provided in Fig. 6.26.

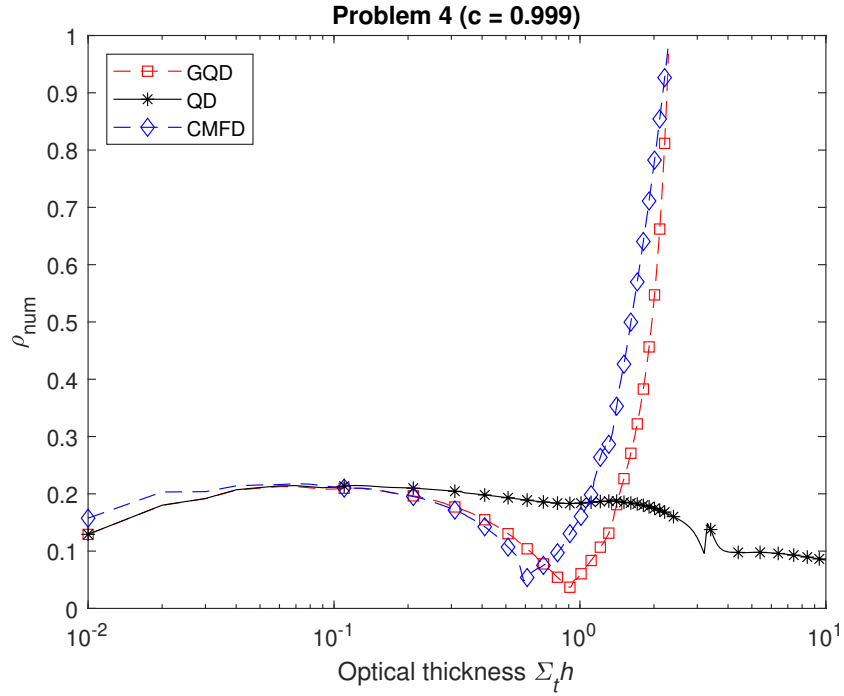


Figure 6.26: Problem 4: ρ vs $\Sigma_t h$ ($c = 0.999$) – conditionally stable.

Potential culprits for this problem could be (i) the rough estimate of the consistent Eddington factors for coarse meshes (especially in regions with small scalar fluxes, such as in “shielding” problems or close to boundaries), (ii) the fact that Eq. (4.29) does not guarantee that the F_j would be inherently positive, and (iii) roundoff errors that may appear in very low flux regions.

Fortunately, the method presented in Chapter 4 (Section 4.1.1) mitigates these difficulties from Eq. (4.28) and Eq. (4.29). Instead of choosing an arbitrary point to define the arbitrary constant $F_{j^*} = 3\phi_{2,j^*}$, we let the algorithm calculate all $F_j^{\ell+\frac{1}{2}}$ and choose the smallest value as reference point j^* to calculate the arbitrary constant ($F_1^{\ell+\frac{1}{2}}$). The constant is then added to all values of $F_j^{\ell+\frac{1}{2}}$. This way, the algorithm always chooses the minimal F_{j^*} obtainable in the iteration $\ell + \frac{1}{2}$ and define it as a positive value. All remaining F_j will, therefore, be larger and positive.

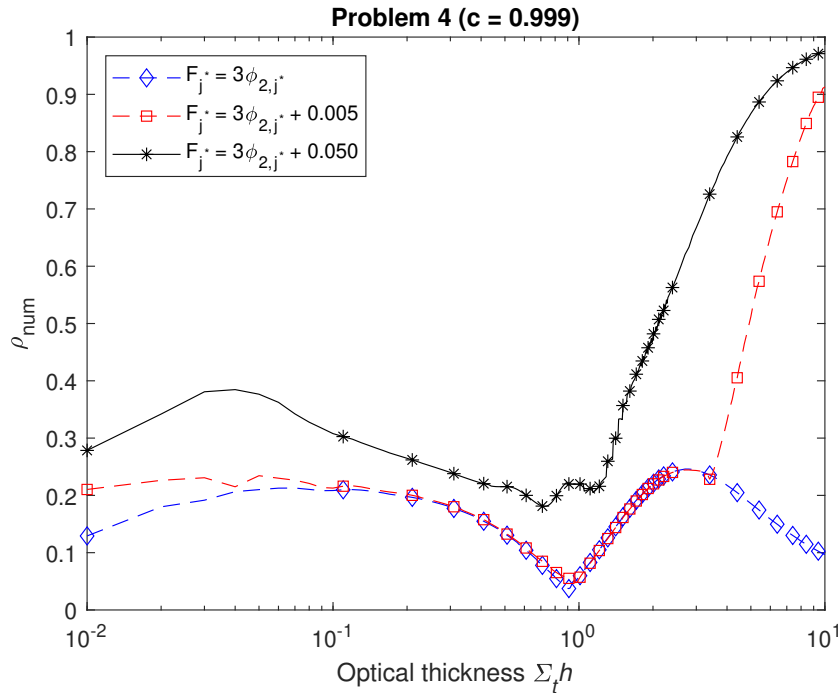


Figure 6.27: Problem 4: ρ vs $\Sigma_t h$ ($c = 0.999$) – using additional constants.

The ability to choose the arbitrary constant can impact the convergence speed, even if it does not affect the consistency of the method and its solution. Unnecessarily large constants F_1 that increase the consistent Eddington factors values can have unpredictable effects on the spectral radius. In Fig. 6.27, we present the numerically estimated spectral radius for problem 4 when an additional constant is introduced to F_1 . In these simulations, the value of F_1 is defined by:

$$F_1 = 3\phi_{2,j^*} - F_{j^*} + C , \quad (6.4)$$

where C can be 0, 0.005, or 0.005. One can observe that, in these simulations, including additional constants into the consistent Eddington factors generally leads to larger spectral radii values and loss of efficiency for coarser spatial grids.

We initially defined the ideal case for $F_{j^*} = 3\phi_{2,j^*}$ so that the GQD method limits to the QD method when the cells are optically thin. In Fig. 6.28 we present the comparison using $F_{j^*} = 3\phi_{2,j^*}$ and the case a different reference value ($F_{j^*} = 1.5\phi_{2,j^*}$ or $F_{j^*} = 6\phi_{2,j^*}$). In this case, we show that the current definition $F_{j^*} = 3\phi_{2,j^*}$ is more efficient than other scaling factors.

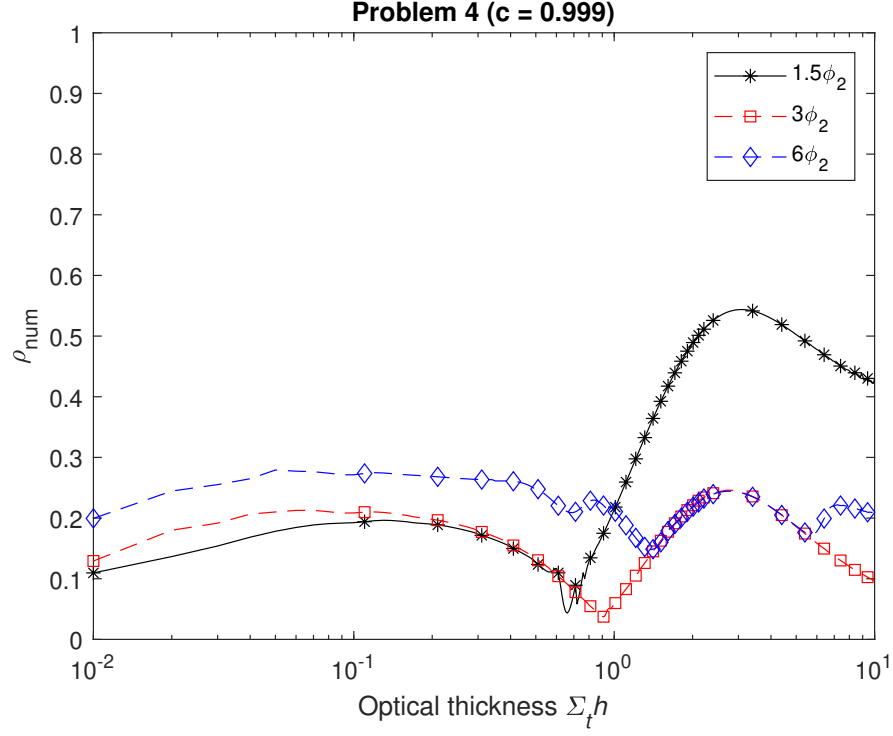


Figure 6.28: Problem 4: ρ vs $\Sigma_t h$ for different F_{j*} values ($c = 0.999$).

Therefore, numerical results have shown that the method's choice presented the most stable and efficient solutions (to our knowledge).

The fortunate property of the system of equations in Eqs. (4.12) to have infinite solutions allows us to define new Eddington factors that make the GQD consistent. However, the effect of the arbitrary constant F_1 on the method's stability has yet to be fully understood. At this stage, we do not have a theoretical explanation to justify the procedure that we have developed for determining F_1 . The procedure that we have developed seems to be optimal, but this may not be the case.

6.5 Problem 5: Shielding

Similarly to problems 2-4, we use the same physical system of a homogeneous slab of variable thickness ($0 \leq z \leq Z = 100h$), where h is the (variable) width of each spatial cell. However, in this test case, we assume an incident isotropic flux at the left boundary and a vacuum (zero incident flux) condition at the right boundary. The material properties are $\Sigma_t = 1.0 [cm^{-1}]$ and $\Sigma_s = 0.9999 [cm^{-1}]$, with no internal source $Q = 0 [cm^{-3}sec^{-1}]$.

Figure 6.29 displays the $\phi_{0,j}$, F_j , and $3\phi_{2,j}$ versus mean free paths across the domain, where $\Sigma_t h = 1.0$. In this figure, these variables have their maximum at the left boundary and their minimum at the rightmost cell. This behavior is expected since all neutrons in the system originally come from the incident flux at the left boundary. Then, the neutrons are progressively scattered as they travel through the medium, reducing gradually as they either leak out or are captured.

For the initial case in which $c = 0.9999$, the difference between the classic and consistent Eddington factors is displayed in Fig. 6.30. These results show that both Eddington factors agree very closely throughout most of the system, having just a small difference closer to both boundaries. At the left boundary, where there is an incident flux, the Eddington factors have a value similar to 1. The right boundary, where there is vacuum (and a small scalar flux), displays a rapid increase in the Eddington factors.

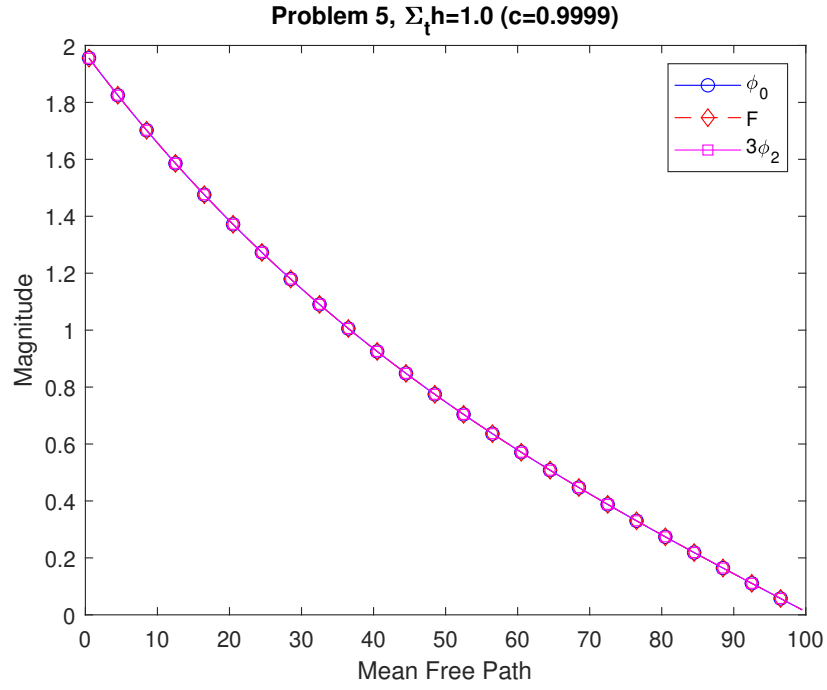


Figure 6.29: Problem 5: $\phi_{0,j}$, F_j , and $3\phi_{2,j}$ for $\Sigma_t h = 1.0$ ($c = 0.9999$).

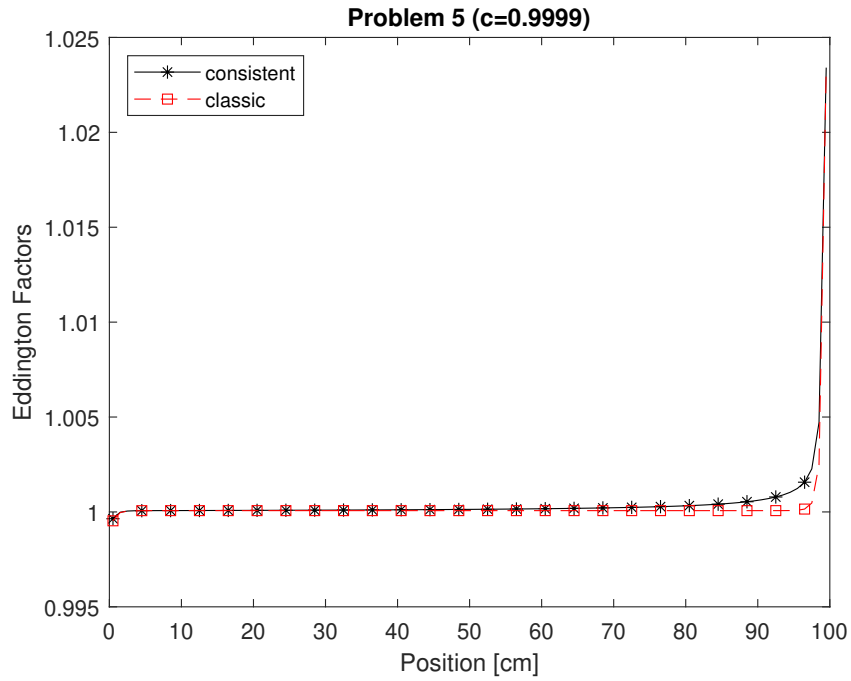


Figure 6.30: Problem 5: Classic and consistent Eddington factors for $\Sigma_t h = 1.0$ ($c = 0.9999$).

Finally, we analyze the spectral radius of the GQD method for this boundary condition-driven problem. We execute the same procedure used for generating Fig. 6.15, Fig. 6.20, and Fig. 6.25. We vary the value of $\Sigma_t h$ from 0.01 up to 10 and calculate the numerical estimate for the spectral radius (ρ_{num}). The results for problem 5 ($c = 0.9999$) are presented in Fig. 6.31.

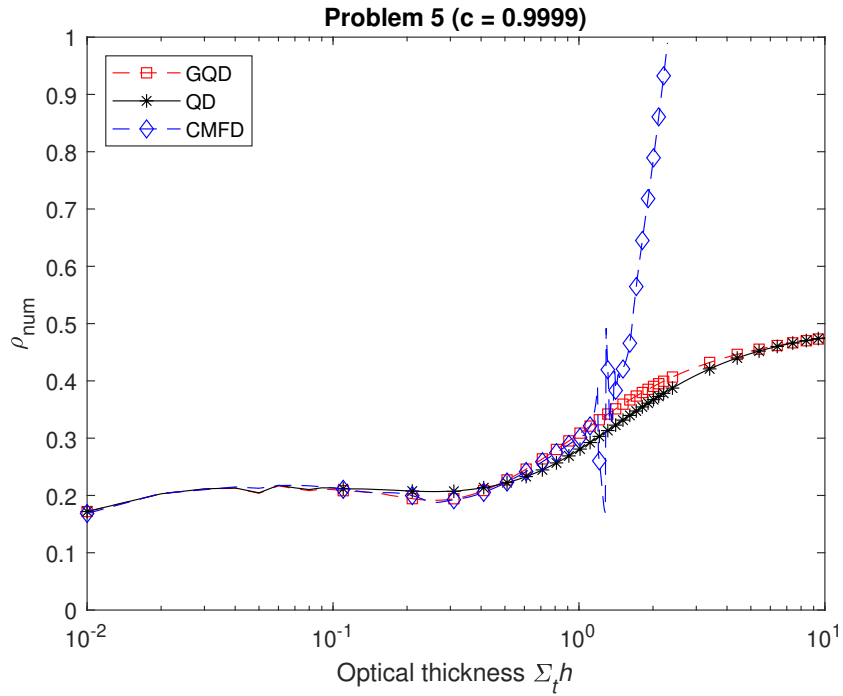


Figure 6.31: Problem 5: ρ vs $\Sigma_t h$ ($c = 0.9999$).

In this case, the numerical spectral radius behaved differently from problems 2-4. In previous tests, $\rho_{num} \rightarrow 0$ as $\Sigma_t h \rightarrow \infty$. However, in problem 5, the QD and GQD methods presented the following behavior: $\rho_{num} \rightarrow 0.5$ as $\Sigma_t h \rightarrow \infty$. The CMFD method, as expected, lost efficiency and eventually became unstable around $\Sigma_t h \approx 2.3$. Nonetheless, this test

shows that the GQD method remains unconditionally stable for prescribed boundary flux shielding problems.

However, if we decrease the scattering ratio, the GQD method starts having difficulties converging within the prescribed convergence criteria (10^{-12}). In “deep penetration” problems, the order of magnitude of the scalar flux varies significantly. The lower the scattering ratio, the more the scalar flux changes over the domain. The size of the domain also dictates how small the scalar flux will be at the opposite edge of the system (from the incident source).

Therefore, it is expected that we will encounter nearly zero scalar fluxes. Which, as in problem 4, could result in negative F_j values in Eq. (4.28). The methodology presented in Chapter 4, however, struggles to converge for certain cases due to roundoff errors. Even using *long double* (10^{-18}) precision, the scalar flux quickly reaches values close to machine precision before the right boundary of the system.

The method proposed calculates the minimum value and position of F_j within each iteration, and the system oscillates the solution due to a lack of more digit precision. These oscillations on the lower range of the scalar flux cascade to the region where the flux is not negligible, causing larger errors and fluctuations in the solution, which causes the method to not converge within the requested criteria.

Therefore, the methodology used has encountered some difficulties when stressed by “deep penetration” (shielding) problems due to numerical precision. The methodology itself should work if provided a large enough digit representation. Since this may not always be available or desired, we explored other options to circumvent this situation.

Luckily, the choice of how to define the F_j is not unique. For problem 5 in a less scattering medium, we changed the approach slightly to define F_j :

1. We define the reference point j^* and $F_{j^*}^{\ell+\frac{1}{2}}$ based on the previous iteration j^* . (if $\ell = 0$, we check the minimum value of $\phi_{2,j^*}^{\frac{1}{2}}$)
2. We set $F_{j^*}^{\ell+\frac{1}{2}} = 3\phi_{2,j^*}^{\ell+\frac{1}{2}}$.
3. Instead of using Eq. (4.28), we choose Eqs. (4.31) and sweep both directions from the reference point j^* .

We can verify the performance of this method by checking the case for $c = 0.9$, in Fig. 6.32.

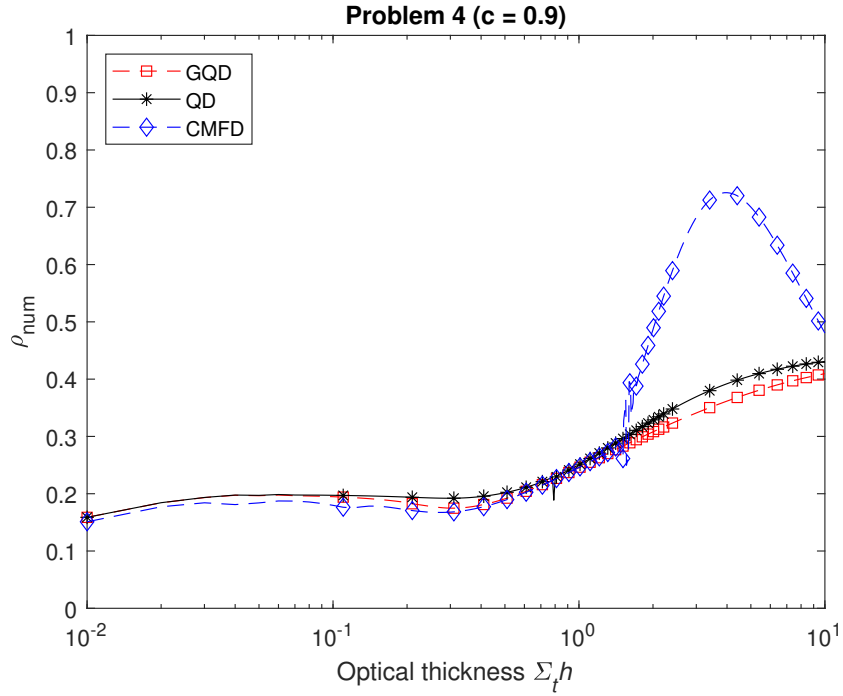


Figure 6.32: Problem 5: ρ vs $\Sigma_t h$ ($c = 0.9$).

So far, the GQD method with this new methodology described has (experimentally) (i) oscillated less the position j^* of the minimum value F_{j^*} , (ii) converged to the SI solution with a similar spectral radius to the QD method. In this case, the CMFD method is also

presented to be stable between 0.01 and 10, having a peak around $\Sigma_t h = 4.0$. The fact that this new methodology for defining F_j works shows that the method is susceptible to roundoff error and machine precision for severe shielding problems with optically thick grids.

We can further investigate this claim by showing how the scalar flux can quickly reach the range of machine precision in Fig. 6.33, for $c = 0.9$ and $\Sigma_t h = 1.0$.

In Fig. 6.33b (where the scalar flux is represented in logarithmic scale), we can see that after $j = 90$, the solution is already below 10^{-18} , causing the system to consider it zero. This shows that the roundoff errors are most likely taking effect.

The different methodology presented in this chapter to define F_j is not necessarily “bulletproof,” but in this case, it behaved more stably than the one suggested in Chapter 4. The formulation in Chapter 4 is more intuitive and has fewer procedural restrictions, but it encountered more difficulty when stressed by problems that change the scalar flux by many orders of magnitude (such as shielding problems).

To emphasize, this numerical stability observed in certain cases of Problem 5 is most likely caused by the numerical precision of the hardware. Assuming infinite precision, both methods should work. In the cases that the F_j is properly defined to avoid roundoff errors, the method is shown to be unconditionally stable for any choice of optical thickness.

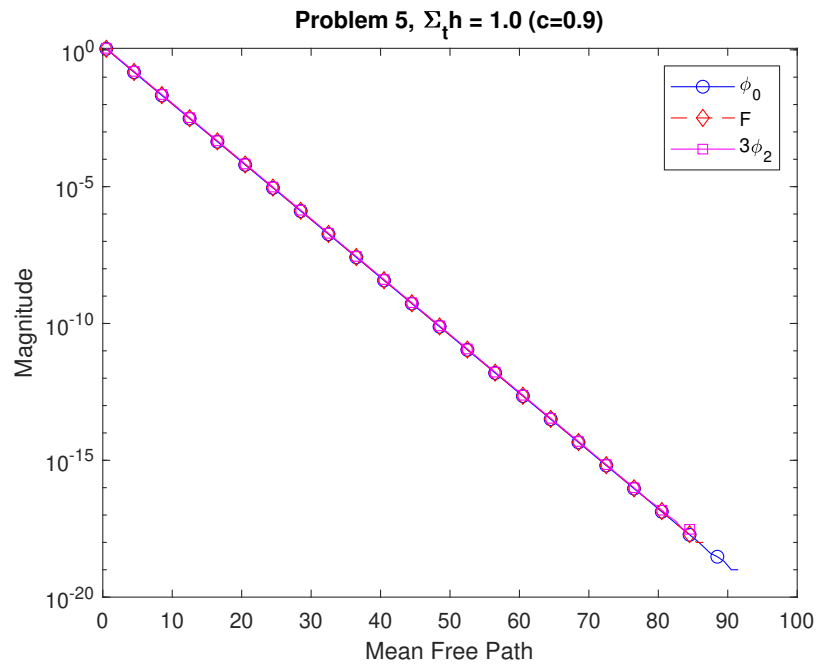
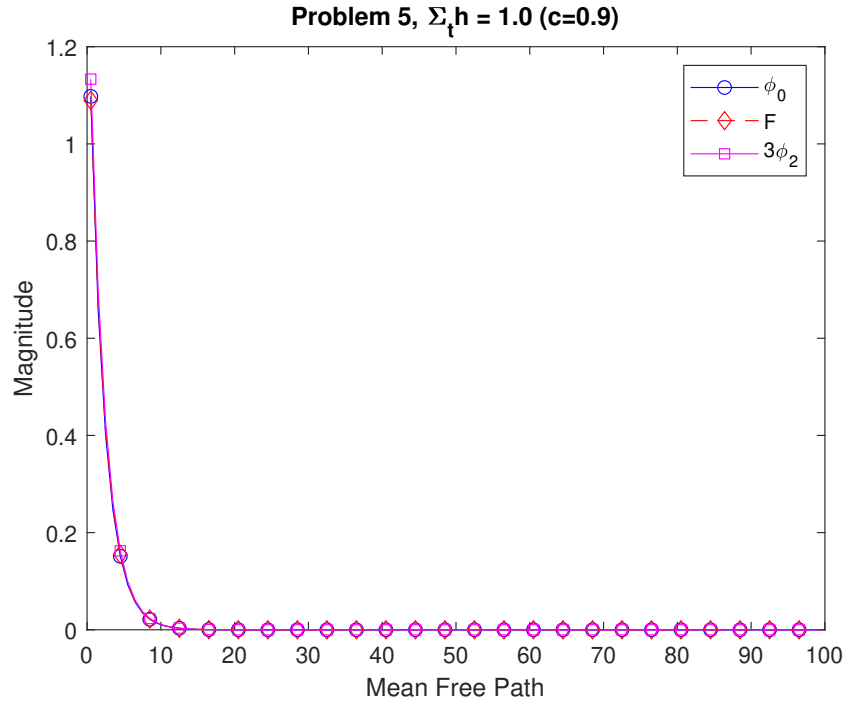


Figure 6.33: Problem 5: $\phi_{0,j}$, F_j , and $3\phi_{2,j}$ for $\Sigma_t h = 1.0$ ($c = 0.9$).

6.6 Diagonal dominance

We conclude Chapter 6 by providing additional insight into the stability of the QD and GQD methods. In iterative methods, often one can correlate or prove the stability of the method by evaluating the diagonal dominance of the iteration matrix $\mathbf{A}_{J \times J}(\cdot)$ that operates iterative over the estimated solution (ϕ_0) [77].

A matrix $\mathbf{A}_{J \times J}$ is said to be diagonally dominant if, for every row $1 \leq i \leq J$, it has the following property:

$$A_{i,i} \geq \sum_{j \neq i} |A_{i,j}|, \quad (6.5)$$

where $A_{i,j}$ is the elements of the matrix $\mathbf{A}$ at the row i and column j . In other words, if all diagonal entries of the matrix $\mathbf{A}$ are larger than the sum of the magnitudes of the other non-diagonal components in their respective row, the matrix is diagonally dominant.

We can evaluate the diagonal dominance of a matrix by checking the ratio between the right-hand side and the left-hand side of Eq. (6.5). If this ratio is below 1 for all rows of $\mathbf{A}$, it is defined as diagonally dominant. This quantity, that we will opt to call the *diagonal dominance ratio* (R) in this dissertation, is expressed by:

$$R = \max_{1 \leq i \leq J} R_i = \max_{1 \leq i \leq J} \frac{\sum_{j \neq i} |A_{i,j}|}{A_{i,i}}. \quad (6.6)$$

If $R < 1$, the matrix is diagonally dominant, and if $R > 1$, the matrix is not diagonally dominant. Diagonally dominant matrices have certain desirable properties. For example, these matrices are invertible. Diagonal dominance is often a sufficient condition for iterative systems to be convergent [77].

Therefore, we considered evaluating if any of the presented methods are diagonally dominant in the low-order diffusion systems, where they differ. Since the QD and GQD

methods displayed unconditional stability for any optical thickness, we expect that the formulation of these methods could lead to diagonally dominant low-order systems. The opposite prediction was made for the CMFD method. We note that this assumption also arises from the fact that the Eddington factors are defined as cell-average values that tend to have smaller fluctuations for coarser meshes. On the other hand, the *transport consistency terms*, presented in CMFD and CQD methods are cell-edge defined quantities that have the behavior of increasing their values for larger cells [57, 58].

Here we define the low-order diffusion matrix $\mathbf{A}$ for QD, CMFD, and GQD in Eqs. (6.7).

For row $i = 1$:

$$A_{1,1} = \frac{1}{h_1} \left[\frac{E_1^{\ell+\frac{1}{2}}}{(\Sigma_t h)_{\frac{3}{2}}} + \hat{D}_{\frac{3}{2}}^{\ell+\frac{1}{2}} + B_\ell^{\ell+\frac{1}{2}} \right] + \Sigma_{a,1}, \quad (6.7a)$$

$$A_{1,2} = -\frac{1}{h_1} \left[\frac{E_2^{\ell+\frac{1}{2}}}{(\Sigma_t h)_{\frac{3}{2}}} + \hat{D}_{\frac{3}{2}}^{\ell+\frac{1}{2}} \right], \quad (6.7b)$$

with the other elements of the first row being 0. For rows $2 \leq i \leq J-1$:

$$A_{i,i-1} = \frac{1}{h_i} \left[-\frac{E_{i-1}^{\ell+\frac{1}{2}}}{(\Sigma_t h)_{i-\frac{1}{2}}} - \hat{D}_{i-\frac{1}{2}}^{\ell+\frac{1}{2}} \right], \quad (6.7c)$$

$$A_{i,i} = \frac{1}{h_i} \left[\frac{E_i^{\ell+\frac{1}{2}}}{(\Sigma_t h)_{i+\frac{1}{2}}} + \frac{E_i^{\ell+\frac{1}{2}}}{(\Sigma_t h)_{i-\frac{1}{2}}} + \hat{D}_{i+\frac{1}{2}}^{\ell+\frac{1}{2}} - \hat{D}_{i-\frac{1}{2}}^{\ell+\frac{1}{2}} \right] + \Sigma_{a,i}, \quad (6.7d)$$

$$A_{i,i+1} = \frac{1}{h_i} \left[-\frac{E_{i+1}^{\ell+\frac{1}{2}}}{(\Sigma_t h)_{i+\frac{1}{2}}} + \hat{D}_{i+\frac{1}{2}}^{\ell+\frac{1}{2}} \right], \quad (6.7e)$$

with the other elements of the i^{th} row being 0. For row $i = J$:

$$A_{J,J-1} = \frac{1}{h_J} \left[-\frac{E_{J-1}^{\ell+\frac{1}{2}}}{(\Sigma_t h)_{J-\frac{1}{2}}} - \hat{D}_{J-\frac{1}{2}}^{\ell+\frac{1}{2}} \right], \quad (6.7f)$$

$$A_{J,J} = \frac{1}{h_J} \left[B_r^{\ell+\frac{1}{2}} + \frac{E_J^{\ell+\frac{1}{2}}}{(\Sigma_t h)_{J-\frac{1}{2}}} - \hat{D}_{J-\frac{1}{2}}^{\ell+\frac{1}{2}} \right] + \Sigma_{a,J}, \quad (6.7g)$$

with the other elements of the J^{th} row being 0.

The matrix elements $A_{i,i}$ in Eqs. (6.7) can be defined for the CMFD, QD, and GQD methods. In the case of CMFD method, we set the Eddington factors as $E_j = 1/3$. For the QD and GQD methods, we define the transport consistency term as $\hat{D}_{i+\frac{1}{2}} = 0$. The QD and GQD methods would use their specific definition of converged Eddington factors.

As previously stated, the transport correction factors may cause the matrix $\mathbf{A}$ to lose its diagonal dominance for coarser grids. The numerical results for the diagonal dominance ratio R were obtained for problem 2 (Fig. 6.34). The values were obtained by using the converged values for the transport consistency term and the respective Eddington factor used by the method.

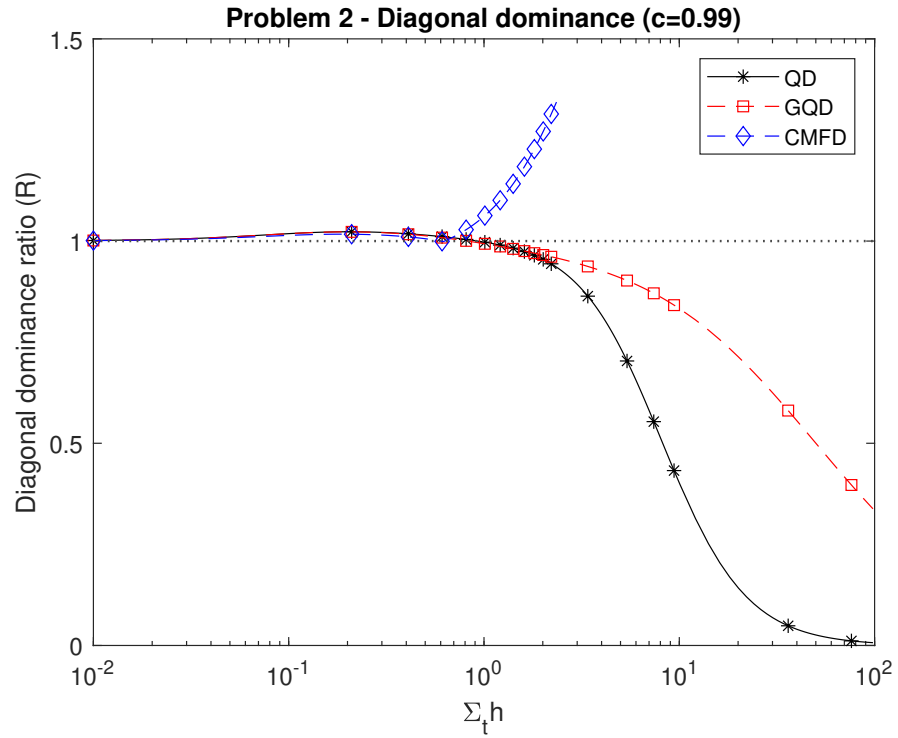


Figure 6.34: Problem 2: Diagonal dominance ratio (R) vs $\Sigma_t h$ ($c = 0.99$).

In Fig. 6.34, we observe that for optically thin cells, R is slightly above 1.0 for all tested methods, which would cause the diffusion matrices to not be diagonally dominant. Fortunately, this small deviation does not cause the method to become unstable, since we already presented that they are, in fact, stable in that region. However, as the optical thickness of the grid increases, CMFD becomes progressively less diagonally dominant. In fact, the CMFD value of R increases significantly and coincidentally in the range of $\Sigma_t h$ where the method becomes unstable. This would suggest that the CMFD's stability loss is connected to the loss of diagonal dominance of its low-order diffusion matrix. Conversely, the QD and GQD methods become progressively more diagonally dominant as $\Sigma_t h \rightarrow \infty$.

These results suggest that for transport acceleration methods having iterations consisting of a high-order transport sweep followed by a low-order diffusion calculation, there may be a theoretical link between the overall spectral radius and the diagonal dominance of the low-order diffusion matrix. If such a theoretical link can be established, it could help steer methods developers away from schemes whose low-order diffusion matrices lose their diagonal dominance, and toward schemes whose low-order diffusion matrices do not lose their diagonal dominance. In this dissertation, we do not attempt to develop such a theoretical link, but we do suggest that this link may exist. Actually developing it will be the task of future work.

Chapter 7: Conclusion

In this dissertation, we present a new acceleration technique for iteratively solving neutron transport calculations. The new method, called *Generalized Quasidiffusion* (GQD), uses the rapidly-converging high-order/low-order iterative Quasidiffusion (QD) method as a base. However, the GQD method utilizes new consistent Eddington factors, instead of the classic Eddington factors (used in the QD method) for calculating the neutron scalar flux in the low-order system. The new consistent Eddington factors eliminate the discrepancy between the high-order and low-order converged solutions observed in the QD method, making the GQD method consistent. The GQD method accomplishes this with no loss of the unconditional stability and rapid convergence of the QD method.

The new Eddington factors are calculated by solving a singular “pure diffusion” problem with no absorption. (However, in 1-D, this diffusion problem can be solved in closed form.) Again, the GQD method is consistent, unconditionally stable, and rapidly converging for spatial grids of any optical thickness. In our simulations, the GQD convergence rate is comparable to that of the QD method, which is well-known for its rapidly-converging behavior and unconditional stability. Moreover, the new “consistent” Eddington factors usually differ from the classic Eddington factors only in the second or third decimal place.

The stability of acceleration methods has been a significant challenge in the field of iteration methods for neutron transport calculations. Since the 1960’s, a major extended

effort, spanning decades, has been undertaken by many researchers to improve the efficiency and stability of iterative acceleration methods. However, a universal solution to this problem has not yet been obtained. The GQD method provides, to this field, a new technique that has displayed, so far (for physically simple tests), a consistent solution with high efficiency and stability. In principle, the development of this research could improve several already existing QD codes, providing them with a true and stable acceleration method.

However, the GQD method has two meaningful complications: it requires one to (i) solve a singular diffusion system, and (ii) choose the most appropriate solution from a pool of infinite solutions.

In the simplest case with 1-D planar geometry, the singular diffusion system can be solved in closed form. This is computationally inexpensive, making (i) straightforward. For higher spatial dimensions (2-D and 3-D), solving the singular diffusion system becomes more computationally expensive, since this must be done numerically. In this case, the GQD method would require one to solve two diffusion problems within each iteration: first, a singular diffusion problem for the consistent Eddington factors, and second, a standard diffusion problem for the new scalar flux estimate. If the new diffusion calculation, for the consistent Eddington factors, can be performed with suitable efficiency, then the cost of a GQD iteration will increase only slightly over the present cost of a QD or CMFD iteration.

The arbitrary constant (ii) requires a careful approach, since its choice can lead to a wide range of convergence performance (sometimes causing the GQD method to become unstable). In this dissertation, we provide an approach that eliminates this difficulty for all the test problems that we have run. We believe that this approach will be adequate for 2-D and 3-D problems, but this remains to be seen.

It goes without saying that logical relevant extensions of this work would include expanding its formulation for (i) coarser meshes in the low-order system and (ii) higher dimensions (2-D and 3-D). Most practical high-order/low-order algorithms use a coarser mesh in the low-order system. This can have an impact in the convergence speed of the method. At this time, it is not known how the GQD method will perform when the spatial grid on which the low-order diffusion equation is solved is coarser than the spatial grid on which the high-order S_N equations are solved. We conjecture that the GQD method will remain stable, perhaps with a somewhat slower convergence rate, but this remains to be seen. The extension to 2-D and 3-D is also one of the most natural expansion of this research.

In this dissertation, we have presented a comprehensive study for 1-D problems, which is very limited in nature. Extending this work beyond 1-D would allow a new set of validations and benchmark comparisons with realistic neutronics problems. In addition, effective algorithms to solve the singular diffusion systems to calculate the consistent Eddington factors should be explored. Also, the more mathematical question of whether there is a theoretical link between (i) the spectral radius of the QD, CMFD, and GQD schemes, and (ii) the diagonal dominance of the low-order diffusion matrices should be explored. If such a link can be established, it would motivate the examination of methods such as GQD, whose low-order diffusion matrices preserve their diagonal dominance.

Finally, one should extend the GQD method to handle more physically realistic transport physics, to account for (i) anisotropic scattering, (ii) multigroup energy-dependence, (iii) higher-order spatial discretizations schemes (e.g. Linear Discontinuous or Linear Characteristics), and (iv) multiphysics effects (e.g. temperature-dependent cross sections).

In conclusion, the Generalized Quasidiffusion (GQD) method, presented in this dissertation, provides a new, consistent, rapidly-converging, and unconditionally stable acceleration

method for neutron transport. Potentially, this technique allows us to overcome the significant challenge of acceleration methods' stability and performance for coarse mesh grids, without losing solution consistency. The findings seen in our simulation results are significant and should motivate further research and development. Although there are still complexities to be studied and addressed, especially in higher-order dimensions and more complex physical systems, the GQD method presented in this dissertation holds the promise for future improvements.

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Appendix A: Discrete Ordinates Quadratures

This Appendix presents the tables for different Gauss-Legendre quadratures used in the Discrete Ordinates (S_N) calculations.

Table A.1: Gauss-Legendre weights and angles for S_N discrete ordinates ($N = 2$).

Direction Cosine (μ_n)	Weight (w_n)
± 0.577350269189626	1.0

Table A.2: Gauss-Legendre weights and angles for S_N discrete ordinates ($N = 4$).

Direction Cosine (μ_n)	Weight (w_n)
± 0.861136311594053	0.347854845137454
± 0.339981043584856	0.652145154862546

Table A.3: Gauss-Legendre weights and angles for S_N discrete ordinates ($N = 8$).

Direction Cosine (μ_n)	Weight (w_n)
± 0.960289856497536	0.101228536290376
± 0.796666477413627	0.222381034453374
± 0.525532409916329	0.313706645877887
± 0.183434642495650	0.362683783378363

Table A.4: Gauss-Legendre weights and angles for S_N discrete ordinates ($N = 16$).

Direction Cosine (μ_n)	Weight (w_n)
± 0.095012509837637	0.189450610455067
± 0.281603550779259	0.182603415044924
± 0.458016777657227	0.169156519395003
± 0.617876244402644	0.149595988816577
± 0.755404408355003	0.124628971255534
± 0.865631202387832	0.095158511682493
± 0.944575023073233	0.062253523938648
± 0.989400934991650	0.027152459411754

Appendix B: Fredholm Alternative Theorem

In this Appendix, we present the general theory of the Fredholm Alternative Theorem and the application to the F_j system of equations. We show here that the F_j system (Eqs. (4.12)) has an infinite number of non-trivial solutions.

The Fredholm Alternative Theorem can be applied to general linear algebra problems of the form:

$$\boxed{\mathbf{M}\vec{x} = \vec{q}} \quad , \quad (\text{B.1})$$

where $\mathbf{M}$ is a known $J \times J$ matrix, $\vec{q}$ is a known $J \times 1$ “source” vector, $\vec{x}$ is an unknown to-be-determined $J \times 1$ vector, and the matrix $\mathbf{M}$ is singular – $\mathbf{M}$ has the eigenvalue 0, with eigenvector f :

$$\mathbf{M}\vec{f} = \vec{0} \quad . \quad (\text{B.2})$$

If $\mathbf{M}$ were non-singular, then $\mathbf{M}$ could be inverted. In this case, the unique solution of Eq. (B.1) exists and is given by

$$\vec{x} = \mathbf{M}^{-1}\vec{q} \quad . \quad (\text{B.3})$$

However, because M has been assumed to be singular, M^{-1} does not exist [16]. Thus, in general, a solution of Eq. (B.1) does not exist.

If a solution of Eq. (B.1) does exist, then a “necessary” condition on the source $\vec{q}$ can easily be derived. Since the matrix $\mathbf{M}$ has eigenvalue 0, the adjoint (transpose) matrix $\mathbf{M}^*$ also has eigenvalue 0, with eigenvector $\vec{f}^*$:

$$\mathbf{M}^* \vec{f}^* = 0 . \quad (\text{B.4})$$

Let us assume that a solution $\vec{x}$ of Eq. (B.1) exists. Then, taking the inner product of $\vec{f}^*$ with both sides of Eq. (B.1), we obtain:

$$(\vec{f}^*, \mathbf{M}\vec{x}) = (\vec{f}^*, \vec{q}) . \quad (\text{B.5a})$$

However, the left side of Eq. (B.5a) satisfies

$$(\vec{f}^*, \mathbf{M}\vec{x}) = (\mathbf{M}^* \vec{f}^*, \vec{x}) = (0, \vec{x}) = 0 . \quad (\text{B.5b})$$

Therefore, Eq. (B.5a) reduces to the following “solvability” condition on the source $\vec{q}$, which must hold if a solution of Eq. (B.1) exists:

$$\boxed{0 = (\vec{f}^*, \vec{q})} . \quad (\text{B.5c})$$

The Fredholm Alternative Theorem states that Eq. (B.5c) is not only *necessary*, it is also *sufficient* [75]. More precisely, the Theorem states that *a necessary and sufficient condition for a solution of Eq. (B.1) to exist is that the source q satisfy Eq. (B.5c)*. The theorem also states that if Eq. (B.5c) is satisfied, then an **infinite number of solutions exist** having the form:

$$\vec{x} = \vec{x}^{part} + c \vec{f} , \quad -\infty < c < \infty , \quad (\text{B.6})$$

where $\vec{x}^{part}$ is any particular solution, and c is any constant.

If the matrix $\mathbf{M}$ is nonsingular, then Eq. (B.1) has a unique solution. However, if the matrix $\mathbf{M}$ is singular, then either no solution exists, or there are infinitely many. The

determining factor is the solvability condition, Eq. (B.5c). If Eq. (B.5c) is not satisfied, then no solution exists. If Eq. (B.5c) is satisfied, then infinitely many solutions exist.

We can apply the Fredholm Alternative Theorem to the low-order diffusion equation derived for the constants F_j , which are the numerators of the new consistent Eddington factors Eq. (4.16). The specific set of equations in the dissertation is Eqs. (4.12) – a system of J equations in J unknowns:

$$-D_{\frac{3}{2}}^*(F_2 - F_1) = \phi_{1,\frac{3}{2}} \ , \ j = 1 \ , \quad (\text{B.7a})$$

$$\begin{aligned} -D_{j+\frac{1}{2}}^*(F_{j+1} - F_j) + D_{j-\frac{1}{2}}^*(F_j - F_{j-1}) \\ = \phi_{1,j+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}} \ , \ 2 \leq j \leq J-1 \ , \end{aligned} \quad (\text{B.7b})$$

$$D_{J-\frac{1}{2}}^*(F_J - F_{J-1}) = -\phi_{1,J-\frac{1}{2}} \ , \ j = J \ . \quad (\text{B.7c})$$

In applications of the GQD method, the right sides of these equations will consist of “known” cell edge currents, which have been estimated from the previous transport sweep and will have $\ell+\frac{1}{2}$ superscripts. Likewise, the unknowns F_j on the left sides of the equations will also have $\ell+\frac{1}{2}$ superscripts. The iterative version of Eqs. (4.12) is displayed by Eqs. (4.41):

$$-D_{\frac{3}{2}}^*(F_2^{\ell+\frac{1}{2}} - F_1^{\ell+\frac{1}{2}}) = \phi_{1,\frac{3}{2}}^{\ell+\frac{1}{2}} \ , \ j = 1 \ , \quad (\text{B.8a})$$

$$\begin{aligned} -D_{j+\frac{1}{2}}^*(F_{j+1}^{\ell+\frac{1}{2}} - F_j^{\ell+\frac{1}{2}}) + D_{j-\frac{1}{2}}^*(F_j^{\ell+\frac{1}{2}} - F_{j-1}^{\ell+\frac{1}{2}}) \\ = \phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}^{\ell+\frac{1}{2}} \ , \ 2 \leq j \leq J-1 \ , \end{aligned} \quad (\text{B.8b})$$

$$D_{J-\frac{1}{2}}^*(F_J^{\ell+\frac{1}{2}} - F_{J-1}^{\ell+\frac{1}{2}}) = -\phi_{1,J-\frac{1}{2}}^{\ell+\frac{1}{2}} \ , \ j = J \ . \quad (\text{B.8c})$$

The diffusion coefficients $D_{j+\frac{1}{2}}^*$ should be positive, but otherwise are arbitrary. We will see that the choice of these coefficients has no effect on the question of whether Eqs. (B.8) satisfies (or does not satisfy) the conditions of the Fredholm Alternative Theorem.

We can rewrite this system of equations in a matrix form similar to Eq. (B.1):

$$\mathbf{M}\vec{F}^{\ell+\frac{1}{2}} = \vec{q}^{\ell+\frac{1}{2}} , \quad (\text{B.9})$$

where $\mathbf{M}$ is the $J \times J$ matrix of the diffusion coefficients in the left side of Eq. (B.7). The matrix $\mathbf{M}$ is tridiagonal and symmetric. The vector of $\vec{F}^{\ell+\frac{1}{2}}$ is composed by $F_j^{\ell+\frac{1}{2}}$ ($1 \leq j \leq J$). The vector $\vec{q}^{\ell+\frac{1}{2}}$ is defined by the currents in the right-hand side of the Eqs. (B.8).

By setting $F_j = C$, where C is any constant, one sees that $\mathbf{M}$ annihilates the $J \times 1$ vector whose J elements are all equal to C . Therefore, the matrix $\mathbf{M}$ is *singular* – it has the eigenvalue 0, with the forward eigenvector elements $f_j = C$.

The fact that $\mathbf{M}$ is singular implies that a solution of Eq. (B.7) (and Eqs. (B.8)) may not exist. However, the Fredholm Alternative Theorem enables us to determine (i) whether a solution exists or not, and (ii) if a solution does exist, what general form it has.

Because $\mathbf{M}$ is symmetric, the adjoint matrix $\mathbf{M}^* = \mathbf{M}$ also has the eigenvalue 0, with (adjoint) eigenfunction elements $f_j^* = C^*$, where C^* is arbitrary. If we multiply the j^{th} equation in Eqs. (B.8) by $f_j^* = C^*$ and sum over $1 \leq j \leq J$, the resulting sum of the (unknown) left sides of the equations becomes:

$$\begin{aligned}
& f_1^* \left[-D_{\frac{3}{2}}^* (F_2^{\ell+\frac{1}{2}} - F_1^{\ell+\frac{1}{2}}) \right] \\
& + \sum_{j=2}^{J-1} f_j^* \left[-D_{j+\frac{1}{2}}^* (F_{j+1}^{\ell+\frac{1}{2}} - F_j^{\ell+\frac{1}{2}}) + D_{j-\frac{1}{2}}^* (F_j^{\ell+\frac{1}{2}} - F_{j-1}^{\ell+\frac{1}{2}}) \right] \\
& + f_J^* \left[D_{J-\frac{1}{2}}^* (F_J^{\ell+\frac{1}{2}} - F_{J-1}^{\ell+\frac{1}{2}}) \right] \\
& = C^* \left[-D_{\frac{3}{2}}^* (F_2^{\ell+\frac{1}{2}} - F_1^{\ell+\frac{1}{2}}) \right. \\
& \quad + \sum_{j=2}^{J-1} \left[-D_{j+\frac{1}{2}}^* (F_{j+1}^{\ell+\frac{1}{2}} - F_j^{\ell+\frac{1}{2}}) + D_{j-\frac{1}{2}}^* (F_j^{\ell+\frac{1}{2}} - F_{j-1}^{\ell+\frac{1}{2}}) \right] \\
& \quad \left. + D_{J-\frac{1}{2}}^* (F_J^{\ell+\frac{1}{2}} - F_{J-1}^{\ell+\frac{1}{2}}) \right] = 0.
\end{aligned} \tag{B.10}$$

Thus, in order for a solution of Eq. (B.1) to exist, it is necessary that the same operation, applied to the (known) quantities in the right side of Eq. (B.1), must also yield 0. Performing this operation, we obtain:

$$\begin{aligned}
& f_1^* [\phi_{1,\frac{3}{2}}] + \sum_{j=2}^{J-1} f_j^* (\phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}^{\ell+\frac{1}{2}}) + f_J^* [-\phi_{1,J-\frac{1}{2}}^{\ell+\frac{1}{2}}] \\
& = C^* \left[\phi_{1,\frac{3}{2}}^{\ell+\frac{1}{2}} + \sum_{j=2}^{J-1} (\phi_{1,j+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{1,j-\frac{1}{2}}^{\ell+\frac{1}{2}}) - \phi_{1,J-\frac{1}{2}}^{\ell+\frac{1}{2}} \right] = 0.
\end{aligned} \tag{B.11}$$

Therefore, this *solvability condition* is satisfied. This happens because of the specific definition of the known “source” terms on the right sides of Eq. (B.1).

Equation (B.11) is the “solvability condition” for Eq. (B.1) to satisfy the conditions of the Fredholm Alternative Theorem. Because Eq. (B.11) is in fact satisfied, the Fredholm Alternative Theorem guarantees that Eq. (B.1) has a solution. In fact, the Theorem states that there are an infinite number of solutions, having the following form: if F_j^{part} is any particular solution, then the general solution F_j^{gen} is given by:

$$F_j^{gen} = F_j^{part} + f_j = F_j^{part} + C, \quad 1 \leq j \leq J. \tag{B.12}$$

where C is any constant.

Appendix C: Additional results

In Table C.1 we provide the numerical values for the solution given in Fig. 6.2 with $\Sigma_t h = 0.5$.

Table C.1: Problem 1: Scalar flux results $\Sigma_r h = 0.5$.

Position (z)	SI	CMFD	QD	GQD	(z)	SI	CMFD	QD	GQD
0.25	0.5895	0.5895	0.5573	0.5895	13.25	6.5058	6.5058	6.4148	6.5058
0.75	0.9585	0.9585	0.9221	0.9585	13.75	7.3797	7.3797	7.3077	7.3797
1.25	1.3774	1.3774	1.3370	1.3774	14.25	8.7997	8.7997	8.7647	8.7997
1.75	1.8850	1.8850	1.8410	1.8850	14.75	10.9961	10.9961	11.0450	10.9961
2.25	2.5187	2.5187	2.4725	2.5187	15.25	14.2320	14.2320	14.7400	14.2320
2.75	3.3233	3.3233	3.2779	3.3233	15.75	16.6530	16.6530	17.3000	16.6530
3.25	4.3576	4.3576	4.3180	4.3576	16.25	18.3349	18.3349	19.0659	18.3349
3.75	5.7020	5.7020	5.6771	5.7020	16.75	19.3982	19.3982	20.1824	19.3982
4.25	7.4786	7.4786	7.4850	7.4786	17.25	19.8759	19.8759	20.6872	19.8759
4.75	9.9375	9.9375	10.0211	9.9375	17.75	19.7790	19.7790	20.5922	19.7790
5.25	13.3574	13.3574	13.8832	13.3574	18.25	19.1072	19.1072	19.8971	19.1072
5.75	15.9706	15.9706	16.6308	15.9706	18.75	17.8485	17.8485	18.5890	17.8485
6.25	17.8485	17.8485	18.5890	17.8485	19.25	15.9706	15.9706	16.6308	15.9706
6.75	19.1072	19.1072	19.8971	19.1072	19.75	13.3574	13.3574	13.8832	13.3574
7.25	19.7790	19.7790	20.5922	19.7790	20.25	9.9375	9.9375	10.0211	9.9375
7.75	19.8759	19.8759	20.6872	19.8759	20.75	7.4786	7.4786	7.4850	7.4786
8.25	19.3982	19.3982	20.1824	19.3982	21.25	5.7020	5.7020	5.6771	5.7020
8.75	18.3349	18.3349	19.0659	18.3349	21.75	4.3576	4.3576	4.3180	4.3576
9.25	16.6530	16.6530	17.3000	16.6530	22.25	3.3233	3.3233	3.2779	3.3233
9.75	14.2320	14.2320	14.7400	14.2320	22.75	2.5187	2.5187	2.4725	2.5187
10.25	10.9961	10.9961	11.0450	10.9961	23.25	1.8850	1.8850	1.8410	1.8850
10.75	8.7997	8.7997	8.7647	8.7997	23.75	1.3774	1.3774	1.3370	1.3774
11.25	7.3797	7.3797	7.3077	7.3797	24.25	0.9585	0.9585	0.9221	0.9585
12.25	6.0877	6.0877	5.9883	6.0877	24.75	0.5895	0.5895	0.5573	0.5895
12.75	6.0877	6.0877	5.9883	6.0877					