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*Automatic Variance Reduction for
Monte Carlo Simulations via the
Local Importance Function Transform*

Los Alamos
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Scott Allen Turner

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AUTOMATIC VARIANCE REDUCTION FOR MONTE CARLO SIMULATIONS VIA THE LOCAL IMPORTANCE FUNCTION TRANSFORM

by

Scott Allen Turner

ABSTRACT

We derive a transformed transport problem that can be solved theoretically by analog Monte Carlo with zero variance. However, the Monte Carlo simulation of this transformed problem cannot be implemented in practice, so we develop a method for approximating it. Our approximation to the zero variance method consists of replacing the continuous adjoint transport solution in the transformed transport problem by a piecewise continuous approximation containing local biasing parameters obtained from a deterministic calculation. We use the transport and collision processes of the transformed problem to bias distance-to-collision and selection of post-collision energy groups and trajectories in a traditional Monte Carlo simulation of “real” particles. We refer to the resulting variance reduction method as the Local Importance Function Transform (LIFT) method.

We demonstrate the efficiency of the LIFT method for several 3-D, linearly anisotropic scattering, one-group, and multigroup problems. In these problems the LIFT method is shown to be more efficient than the AVATAR³⁶ scheme, which is one of the best variance reduction techniques currently available in a state-of-the-art Monte Carlo code. For most of the problems we considered, the LIFT method produces higher figures of merit than AVATAR, even when the LIFT method is used as a “black box”. Like most variance reduction techniques, the LIFT method requires some fine-tuning to produce optimal results. However, it performs very well without fine tuning, and users should be able to obtain efficient solutions without any knowledge of the method, and without the need for trial and error runs.

There are some problems that cause trouble for most variance reduction techniques, and the LIFT method is no exception. For example, we demonstrate that problems with voids, or low density regions, can cause a reduction in the efficiency of the LIFT method. However, the LIFT method still performs better than survival biasing and AVATAR in these difficult cases.

CHAPTER 1

INTRODUCTION

In many radiation transport problems, one would like to determine the characteristics of radiation in some region of a system, resulting from a specified source. Unfortunately, many realistic problems are fairly complex, involving complicated geometries and a large number of mean free paths through which the radiation must pass. Currently, there are two classes of methods available for solving these problems: deterministic methods that utilize a discretization of the radiation transport equation, and the Monte Carlo method which utilizes stochastic modeling of the radiation transport process. Deterministic methods are typically much faster than Monte Carlo, but deterministic solutions contain discretization errors in space, angle, and energy that are not present in Monte Carlo solutions. On the other hand, Monte Carlo solutions contain statistical errors that are not present in deterministic solutions. In this thesis, we propose a new method which combines the best features of deterministic and Monte Carlo methodology. This method has many advantages over deterministic or Monte Carlo methods used independently of each other. In particular, it enables Monte Carlo calculations to be performed with significantly smaller variances than are currently achievable.

Traditionally, Monte Carlo methods have required users either to have a fair amount of experience or to spend a lot of time using trial and error, in order to obtain accurate, efficient answers using variance reduction techniques. The difficulties are due to the parametric nature of these techniques. Most variance reduction methods have one or more “knobs”, or biasing parameters, that the user must adjust for maximum efficiency. Unfortunately, the optimal choices are problem-dependent and often difficult to

predetermine. The Local Importance Function Transform (LIFT) method developed in this thesis does not completely escape this historical fate, but it should improve the lot of the uninitiated user, while proving to be an even more powerful tool for the Monte Carlo professional. The reason is that the LIFT method reduces the amount of “knob turning” that a user must perform by providing analytical and numerical approximations of the optimal biasing parameters. In other words, it is very nearly a fully-automatic biasing method. Optimal results for the LIFT method still require some fine tuning, but even the default settings should outperform most other variance reduction methods in many types of deep penetration shielding or source-detector problems.

There are many applications for which users may need to use variance reduction techniques in Monte Carlo simulations. This dissertation focuses on problems which involve a fixed source and a remote detector. Some examples of real-life applications include oil well-logging and radiation shielding. Well-logging tools, which are lowered down into potential oil well boreholes, involve a fixed neutron source, and one or more neutron detectors. The source neutrons begin in one section of the tool, slow down in the medium of interest, and eventually make their way to one of the detectors in another section of the tool. Usually, the neutrons must travel many mean free paths before contributing a score. Radiation shields, on the other hand, are usually designed to stop virtually all radiation from penetrating the medium of which they are made. However, shields can never be perfect, and it is important to know the characteristics of the radiation that manages to traverse the shield.

To provide a graphical example of a problem that one may want to solve with a Monte Carlo simulation, let us consider Figure 1.1, for a 2-D source-detector problem. The surfaces separating the source (lower left corner) and the detector (upper right corner), represent geometric boundaries, material boundaries, and/or conventional Splitting with Russian Roulette planes, which might be used to direct particles toward the detector. This figure is merely a cartoon representing real life problems, which are likely

to be much more complex. Directing particles is traditionally accomplished by splitting particles that cross planes into regions that are assigned a higher importance than the region from which they came, and playing Russian Roulette with particles that cross in the other direction. It is very difficult to determine the optimal placement and shape of the importance surfaces. Additional difficulties arise in determining the importance values of the cells formed by the surfaces. The LIFT method avoids these difficulties by breaking the problem up into an orthogonal grid; each cell of the grid contains functions and biasing parameters that are based on the deterministic solution of the corresponding adjoint problem. These functions and biasing parameters are automatically calculated by the code, and are used to transform the forward transport problem into a new problem which is an approximation of a zero variance problem. We will now give a brief description of the history behind the LIFT method before we go into more detail.

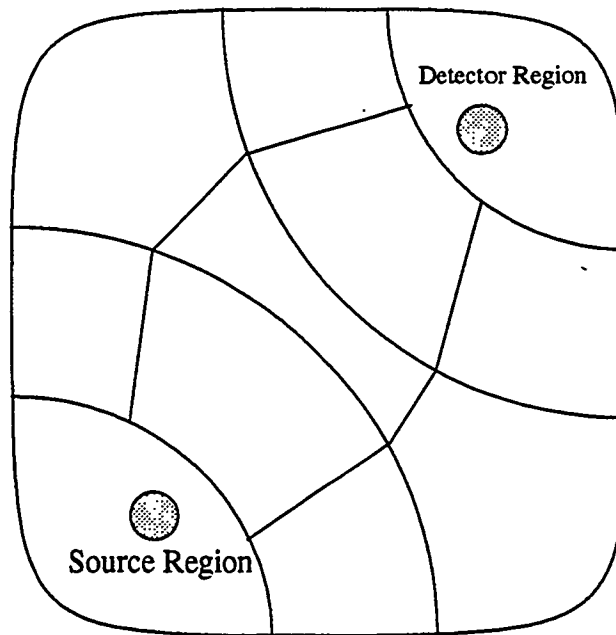


Figure 1.1: Schematic View of a Source-Detector Problem

The building blocks for the LIFT method date back to the beginning years of the development of Monte Carlo solutions to transport problems. Monte Carlo developers

have long realized that in order to transport particles through several mean free paths of material in a reasonable amount of time, one must change the rules of the game. Such rule changes are usually based on *a priori* information about the solution (e.g. knowing that a neutron population decays exponentially in space for deep penetration, fixed source problems). Kahn¹ first described the exponential transform in 1950. Briefly, the exponential transform adjusts the distance to collision so that particles travelling toward the region of interest suffer fewer collisions than particles travelling away from the region of interest. Adjustments to the particle weight keep the game fair. Later, in 1958, Goertzel and Kalos² described the potential of the zero variance problem in connection with the exponential transform. The zero variance problem is one which can theoretically be solved by a Monte Carlo simulation with zero statistical variance. We give a detailed description of this problem in Chapter 2. During the next couple of decades, methods began to include angular biasing, weight windows, and/or the use of analytic or deterministic approximations to the importance function to guide these biasing techniques³⁻¹². However, the idea of combining the biasing of the transport process with biasing of the collision process, by using a factorized analytical expression for the importance function with a common biasing parameter, seems to have originated with Dwivedi and Gupta¹³⁻¹⁵ in the early 1980's. Several proposals¹⁶⁻²⁹ involving one or more of the concepts of zero variance, angular biasing, the exponential transform, weight windows, and analytic or numerical approximations of the importance function have emerged since then. However, only the method used in the code TRIPOLI¹⁷⁻²² has combined them all into a form similar to the LIFT method (which was first proposed in a 1991 conference paper by Abotol, Larsen, and Martin³⁰, and further discussed in subsequent papers³¹⁻³⁴). Descriptions of the TRIPOLI technique provide some general information, but are lacking many details. Attempts to obtain more details have been unsuccessful. Nevertheless, it is certain that the TRIPOLI technique is not identical to the LIFT method. For example, some of the TRIPOLI biasing parameters are called from

tables for various materials and energy groups, rather than being calculated for each problem. Tables 1.1 and 1.2 summarize the key components of the references related to the exponential transform and importance function biasing. Question marks in Table 1.2 indicate areas where papers were either unclear or unspecific. [The term “local” indicates that parameters are space, energy, or angle-dependent.] Table 1.2 also list the characteristics of the LIFT method, as described in this thesis, for comparison.

	Definition
a	MC Geometry: 1-D (1), 2-D (2), 3-D (3)
b	MC Energy Treatment: One Group (), Multigroup (g), Continuous Energy (E)
c	MC Scattering: Isotropic (), Linearly Anisotropic (L), General Anisotropic (A)
d	MC Angular Treatment: Continuous (C), Discrete (D)
e	MC Biasing Parameters: Local/Deterministic (LD), Local/User (LU), Global (G)
f	MC Variable Biased: Path Length (X), Energy (E), Angle (A), All (3)
g	Weight Window Generator: None or User Defined(), Deterministic Adjoint (D), MC Adjoint (M)
h	Deterministic Geometry: 1-D (1), 2-D (2), 3-D (3)
i	Deterministic Method: None (), Diffusion (D), SP_N (SP), S_N (SN), Collision Probabilities (CP)
j	Refers Directly to Zero Variance Solution: Yes (x), No ()
k	Particle Type: Neutron Only(N), Photon Only(P)

Table 1.1: Definitions for Table 1.2 Headings

The LIFT method developed in this thesis is an approximation to the ideal, but in practice, impractical zero-variance solution. The zero-variance solution requires

	a	b	c	d	e	f	g	h	i	j	k
1	1	E	A	C	G	X					N
2	1	E	A	C	G	X				x	N
3 ^I	1	E	A	C	G	3				x	N
4	3	E	A	C	L	X					NP
5 ^{II}										x	
6	3	E?	A?	C?	L	X		1	SN		N
7	3	E?	A?	C?	L	X	D	1	SN		N
8	3	E	A	C	G	X	D	1	SN	x	N
9	3	E?	A?	C?	L	X		1	SN		N
10 ^{III}	3	g	A	D	L	X,A		2	SN		N
11 ^{IV}	3	C	A	D	L	X,A		1	SN	x	N
12 ^{IV}	3	E	L	D	L	X,A	D	1	SN		N
13-15	1 ^V			C	G	X,A				x	N
16	3	E	A	C	G	3					P
17-18	3	g ^{VI}	A	C	L	3				x	NP
19	2 1	 g	 A	C C	L L	X,A X,A	D D	2 1	CP CP	x x	N N
20-22	3	g ^{VI}	A	C	L	3	D	3	CP ^{VII}	x	N
23	3	g	A	C	L	X,E	M				N
24	3	g	A	D	L	X,A					NP
25-27	3	g	A	C	L	X,E	D	1	SN	x	NP
28	3	g	A	C	L	X,E	M			x	NP
29 ^{VIII}	3						D	3	D	x	NP
30-34	2	g	L	C	L	3	D ^{IX}	2	D	x	N
LIFT-thesis	3	g	L	C	L	3	D	3	D,SP, SN	x	N

Table 1.2: Reference Summary

^IMethod is only applicable to hydrogen.

^{II}This paper was very theoretical, and thus could not be assigned specific characteristics.

III^{Treats} Treating biasing of path length and angle independently. Path length biasing was accomplished by conventional global exponential transform. Angle biasing was done locally and was based on deterministic adjoint calculation.

IV^{Treats} Treating biasing of path length and angle independently. Both are done locally, but only the biasing of angle is based on a deterministic adjoint calculation.

V^{These} These papers reference 3-D studies for the same method.

VI^{The} The TRIPOLI method involves some apparently continuous energy functions, but also makes reference to multigroup treatments. Thus it is hard to say, without more detail, whether or not the method should be characterized as continuous energy or multigroup.

VII^{TRIPOLI} TRIPOLI also uses a method based on what the authors refer to as the “graph theoretic argument”.

VIII^{Angular} Angular biasing is also discussed, but appears to be applied globally, involves angular bins, is not derived from the zero variance solution, and is tied to the application of weight windows.

IX^{Actually,} Actually, only a weight cutoff which is based on the importance function is used, rather than a full weight window that includes splitting.

knowledge of the exact solution of a certain adjoint transport problem. Even assuming that one could obtain this, the method still may be impossible to implement. The approximation to the zero variance solution consist of replacing the exact adjoint solution with an analytical approximation containing information from a deterministic calculation (Chapter 3). The name of the method reflects the replacement of the continuous adjoint transport solution in the zero variance problem with a discretized approximation which can be used to uniquely determine biasing parameters that are local in space, energy, and angle. The conventional exponential transform formed the foundation, and gave the inspiration for the LIFT method. Within each cell of the system, the LIFT method appears to be the conventional exponential transform, but with the addition of energy and angular biasing. Angular biasing is done in a manner similar to that of Dwivedi and Gupta¹³⁻¹⁵.

The philosophy behind the LIFT method is very similar to that articulated by Lux and Koblinger³⁵. They present a generalized derivation of zero variance schemes for transport problems, including multiplying systems. They also present various ideas for approximating a zero variance simulation, including methods based on the traditional

exponential transform, and on the exponential transform with angular biasing suggested by Dwivedi and Gupta¹³⁻¹⁵. Lux and Koblinger extend the latter theory by suggesting a biasing parameter, which is local in space and energy, much like the LIFT method. However, discussions of practical applications of the theory are limited to 1-D, homogeneous, monoenergetic, isotropic scattering problems, with no numerical results. In addition, they suggest a self-learning Monte Carlo scheme for approximating the adjoint solution, rather than deterministic solutions. Overall, their work is an excellent reference for the philosophy behind the LIFT method. This thesis involves a practical implementation of this philosophy for a set of realistic problems.

For the problems considered in this dissertation, one of the most efficient variance reduction techniques currently used in a major production code, that we have full knowledge of and can implement, is a method known as AVATAR³⁶ (Chapter 4). This method utilizes deterministic approximations of the adjoint solution to generate weight windows, and is the standard by which we have chosen to measure the performance of the LIFT method. References 37 and 38 also describe methods that utilize adjoint-based weight window generators. The former utilizes a self-learning technique within the Monte Carlo simulation, while the latter utilizes a diffusion calculation to approximate the importance function. We believe that AVATAR is more efficient than either of these methods. Likewise, other variance reduction techniques exist, some of which contain techniques similar to the ones used in LIFT, but they are either proprietary, or less generalized.

LIFT and AVATAR both utilize deterministic solutions to the adjoint problem, but in different ways. AVATAR utilizes more information from the deterministic solution than LIFT, but LIFT makes a much more complete use of the limited information that it requires. AVATAR takes scalar flux and net current information, from a S_N calculation, to formulate angularly-dependent weight windows. With the exception of a variance reduction technique known as DXTRAN³⁹, which we have chosen not to implement

because it should increase the efficiency of both methods equally, and survival biasing, which is used by both methods, AVATAR does not utilize any other biasing techniques. On the other hand, LIFT only takes scalar flux information, from any suitable deterministic method, and uses this limited amount of input to bias distance-to-collision, scattering angle, and energy. LIFT also uses the scalar fluxes to formulate weight windows, which can be angularly-dependent. However, in practice, the LIFT weight windows are not angularly-dependent. In the LIFT method, angularly-dependent weight windows require the use of an analytical expression for the angular flux at every boundary and collision. The extra computing effort does not pay off, in terms of increased efficiency, as we show in Chapter 6. The algebraic cost per collision for LIFT is higher than for AVATAR. However, the extra algebra increases the efficiency of the overall transport process because LIFT particles have significantly shorter histories than AVATAR particles. This is due to the biasing utilized by the LIFT method. Particles are pushed along desired pathways, suffer fewer collisions along the preferred directions, and are more likely to scatter into preferred energy groups. In addition, LIFT particles have smaller weight fluctuations than AVATAR particles, and thus require less splitting and Russian Roulette. The overall result is that LIFT outperforms AVATAR in most problems. In some problems, where biasing is difficult, the two methods are comparable.

There are several popular methods available for obtaining the deterministic adjoint solution. Those which were utilized for this dissertation include diffusion, Simplified P_N , and three variations of S_N . The strengths and weaknesses of these methods are discussed in Chapter 5. Until recently, 3-D, multigroup, anisotropic deterministic solutions for complicated geometries were difficult if not impossible to obtain. This is no longer true, thanks to the DANTSYS⁴⁰ and NIKE/ATHENA⁴¹ code systems developed at Los Alamos National Laboratory. In addition to deterministic solutions becoming easier to obtain, the adjoint problem only needs to be solved once, before Monte Carlo histories begin. Also, the same adjoint solution can be used for several different problems in which only the

forward source changes. Therefore, several different forward source configurations can be tried, as long as the desired response function, and the remainder of the physical system (i.e. boundaries, materials, etc.) remain the same.

In Chapter 6 we demonstrate the efficiency of the LIFT method for 3-D, linearly anisotropic scattering, one-group and multigroup problems. Several comparisons are made between LIFT with various deterministic solutions, and AVATAR. This is an extension beyond previous work³⁰⁻³⁴, which was limited to 2-D problems, and only utilized diffusion approximations to the adjoint solution. Other improvements to previous work include the use of full weight windows, similar to the AVATAR method, in conjunction with LIFT biasing, as well as modifications to the treatment of linearly anisotropic angular biasing.

The following summary is a brief overview of the remainder of this thesis:

Chapter 2 describes how a transport problem is transformed in such a way that it can be solved by analog Monte Carlo with zero variance. The properties and implementation of the zero variance method are discussed.

Chapter 3 describes approximations to the zero variance solution. The implementation of the approximation in a Monte Carlo simulation is also described. Adjoint-based weight windows are formulated and discussed.

Chapter 4 provides a description of the AVATAR method. Also, two unsuccessful but instructive attempts to increase the efficiency of the LIFT method are formulated. The first is a form of generalized rejection sampling, an attempted improvement over simple rejection sampling. The second is a modification of the analytical approximation of the adjoint solution for problems where the scattering ratio is close to unity (little or no absorption).

Chapter 5 discusses the various deterministic methods utilized by the LIFT and AVATAR methods. These include diffusion, discrete ordinates (S_N), and simplified spherical harmonics (SP_N). Three variations of S_N , involving different spatial differencing

schemes, were tried. They include the diamond difference scheme, the adaptive weighted diamond difference scheme⁴⁰, and an Exponential Discontinuous differencing scheme⁴².

Chapter 6 presents the numerical results obtained from the implementation of the LIFT and AVATAR methods in a Monte Carlo simulation. The two methods are compared and discussed.

Chapter 7 summarizes the results of these experiments and our conclusions.

Chapter 8 suggests some improvements on the LIFT method, and discusses future plans for implementation and testing of the method in a major production code.

CHAPTER 2

THE ZERO VARIANCE SOLUTION

Let us consider the following 3-D, multigroup, neutron transport equation for $r \in D$, $1 \leq g \leq G$, with a fixed source in region D_s :

$$\underline{\Omega} \cdot \nabla \psi_g(r, \underline{\Omega}) + \sigma_{t,g}(r) \psi_g(r, \underline{\Omega}) \quad (2.1)$$

$$= \frac{1}{4\pi} \sum_{g'=1}^G \int_{4\pi} \sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \cdot \underline{\Omega}) \psi_{g'}(r, \underline{\Omega}') d\Omega' + \frac{1}{4\pi} Q(r) \delta_{g,1} \quad ,$$

$$\psi_g(r_b, \underline{\Omega}) = 0 \quad \text{for} \quad \underline{\Omega} \cdot \underline{n}_b < 0, \quad r_b \in \partial D, \quad 1 \leq g \leq G \quad , \quad (2.1a)$$

$$Q(r) = 1 \quad \text{for} \quad r \in D_s, \quad \text{and} \quad 0 \quad \text{otherwise.} \quad (2.1b)$$

The terms in eqn. (2.1) have the following definitions:

$r = (x, y, z) \equiv$ position,

$\underline{\Omega} = (\mu, \sqrt{1-\mu^2} \cos \phi, \sqrt{1-\mu^2} \sin \phi) \equiv$ trajectory ($\mu = \cos \theta$),

$g \equiv$ energy group (1 = highest energy, G = lowest),

$\psi_g(r, \underline{\Omega}) \equiv$ the angular neutron flux,

$\sigma_{t,g}(r) \equiv$ the macroscopic total cross section,

$\sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \cdot \underline{\Omega}) \equiv$ the macroscopic differential scattering cross section,

$Q(r) \equiv$ the fixed source,

$\underline{n}_b \equiv$ an outward normal vector on ∂D .

Figure 2.1 gives a graphical representation of the coordinate system.

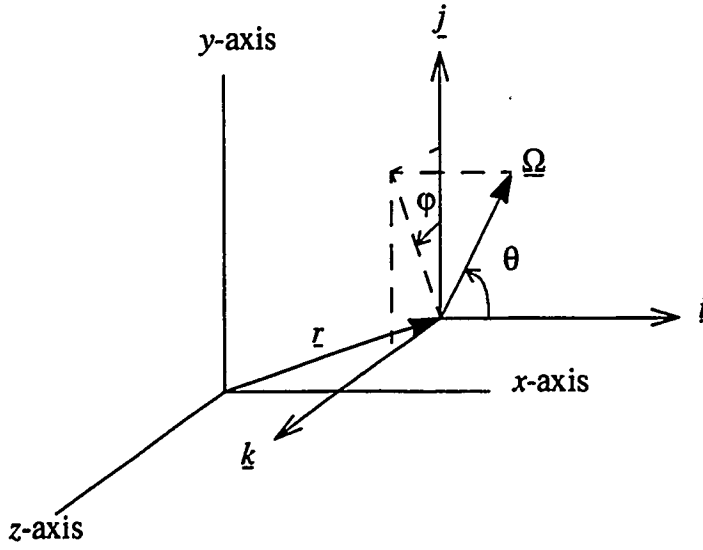


Figure 2.1: Position and Trajectory Variables

Thus, the polar angle θ is the angle between the neutron trajectory and the x -axis, while the azimuthal angle ϕ is the angle between the projection of the trajectory onto the yz -plane and the y -axis. The macroscopic total neutron cross section represents the probable number of collisions per unit path length that a neutron in group g , at position r , will undergo. The macroscopic differential scattering neutron cross section represents the probability per unit path length that a neutron in group g' , with trajectory $\underline{\Omega}'$, at position r , will scatter into group g , with trajectory $\underline{\Omega}$. (Trajectory is often referred to as direction, they are synonymous.) For linearly anisotropic scattering, we use the following form:

$$\sigma_{s, g' \rightarrow g}(r, \underline{\Omega}' \cdot \underline{\Omega}) = \sigma_{s0, g' \rightarrow g}(1 + 3\bar{\mu}_{g' \rightarrow g}\underline{\Omega}' \cdot \underline{\Omega}), \quad (2.1c)$$

$$\bar{\mu}_{g' \rightarrow g} = \frac{\sigma_{s1, g' \rightarrow g}}{\sigma_{s0, g' \rightarrow g}}. \quad (2.1d)$$

This is the highest order of scattering considered in this dissertation. (Higher orders of scattering, although possible and more realistic, add unnecessary complexity to the demonstration of the LIFT method.)

Our goal is to determine the response of a detector to neutrons in energy group G and region D_d :

$$R = \frac{1}{4\pi} \int_{D_d} \int_{4\pi} \Sigma(r) \psi_G(r, \underline{\Omega}) d\Omega dr \quad , \quad (2.2)$$

where $\Sigma(r)$, which is nonzero only in the detector region D_d , represents the type of response to be tallied (absorption, for example). We could just as easily find the response in any other energy group, or in a range of energy groups. Likewise, the source term could also involve any desired combination of energy groups. However, for the purposes of this dissertation, we have chosen to require that all particles be born in the first group and be tallied in the last group.

In problems of this nature, the source and detector regions are often separated by many mean free paths (Fig. 1.1). As a result, the difference between source strength and detector response can be many orders of magnitude. If we were to attempt a solution of this problem with analog Monte Carlo, we would find that an exceedingly large number of histories is required to achieve a low statistical uncertainty in the detector tally. As an example, if we have a source strength of 10^{14} neutrons in group 1, and only 10 of those are expected to reach the detector in group G , then more than 10^{14} histories must be run in order to achieve a statistically significant number of detector scores. This is not feasible with today's computing technology. Hence, it is necessary to develop alternative methods which more efficiently model the transport of particles from source to detector. The "ultimate" such method would be to follow a single particle from the source to the detector, and to have its score determine the correct answer. This would eliminate the need to run more than one history. Theoretically, such a method exists; it involves using

the solution of an adjoint transport problem to transform the forward problem into one that can be solved by analog Monte Carlo with zero variance. We will now describe how such a method might be developed.

First, we must define the adjoint problem. The adjoint solution is also known as the *importance function*, because it represents the expected contribution of a particle, at any point in phase space (energy group, position, trajectory), to the response of a detector. Hence, every point in phase space has a value, $\psi_g^*(\underline{r}, \underline{\Omega})$, which indicates how important particles, at spatial point $\underline{r}$, in group g , with trajectory $\underline{\Omega}$, are to the desired answer. Eqs. (2.1) are known as the *forward problem* because particles are run “forward” from the phase space of the source. In adjoint problems, particles are run “backward” from the phase space of the response function. Thus, the response function serves as the source for the adjoint problem. Let us now consider the *adjoint problem* for eqs. (2.1):

$$\begin{aligned} & -\underline{\Omega} \cdot \nabla \psi_g^*(\underline{r}, \underline{\Omega}) + \sigma_{t,g}(\underline{r}) \psi_g^*(\underline{r}, \underline{\Omega}) \\ & = \frac{1}{4\pi} \sum_{g'=1}^G \int_{4\pi} \sigma_{s,g \rightarrow g'}(\underline{r}, \underline{\Omega}' \cdot \underline{\Omega}) \psi_{g'}^*(\underline{r}, \underline{\Omega}') d\Omega' + \frac{1}{4\pi} \Sigma(\underline{r}) \delta_{g,G} \quad , \end{aligned} \quad (2.3)$$

$$\psi_g^*(\underline{r}_b, \underline{\Omega}) = 0 \quad \text{for} \quad \underline{\Omega} \cdot \underline{n}_b > 0, \quad \underline{r}_b \in \partial D, \quad 1 \leq g \leq G \quad , \quad (2.3a)$$

$$\Sigma(\underline{r}) = 1 \quad \text{for} \quad \underline{r} \in D_d, \quad \text{and} \quad 0 \quad \text{for} \quad \underline{r} \notin D_d \quad . \quad (2.3b)$$

To provide the mathematical connection between the forward and adjoint problems, we operate on eqn. (2.1) by $\sum_{g=1}^G \psi_g^*(\underline{r}, \underline{\Omega})$, and on eqn. (2.3) by $\sum_{g=1}^G \psi_g(\underline{r}, \underline{\Omega})$. Then, we operate on each of the resulting equations by $\int_{4\pi} d\Omega$, and subtract to obtain:

$$\begin{aligned}
& \int_{4\pi} \sum_{g=1}^G \psi_g^*(r, \underline{\Omega}) \underline{\Omega} \cdot \underline{\nabla} \psi_g(r, \underline{\Omega}) d\Omega + \int_{4\pi} \sum_{g=1}^G \psi_g(r, \underline{\Omega}) \underline{\Omega} \cdot \underline{\nabla} \psi_g^*(r, \underline{\Omega}) d\Omega \\
& = \int_{4\pi} \psi_1^*(r, \underline{\Omega}) \frac{Q(r)}{4\pi} d\Omega - \int_{4\pi} \psi_G(r, \underline{\Omega}) \frac{\Sigma(r)}{4\pi} d\Omega .
\end{aligned} \tag{2.4}$$

Applying the chain rule and operating by $\int_D dr$, we get:

$$\sum_{g=1}^G \int_D \int_{4\pi} \underline{\Omega} \cdot \underline{\nabla} \psi_g(r, \underline{\Omega}) \psi_g^*(r, \underline{\Omega}) d\Omega dr = \int_D \int_{4\pi} \psi_1^*(r, \underline{\Omega}) \frac{Q(r)}{4\pi} d\Omega dr - R , \tag{2.5}$$

where R is defined by eqn. (2.2). Using Gauss's Divergence Theorem to convert the LHS of this equation to a surface integral, and applying boundary conditions (2.1a) and (2.3a), we arrive at the following result:

$$R = \frac{1}{4\pi} \int_D \int_{4\pi} \psi_1^*(r, \underline{\Omega}) Q(r) d\Omega dr . \tag{2.6}$$

This supports our assertion that the adjoint solution represents the expected response of a detector to a particle at a given point in phase space. For example, if the source term Q in eqn. (2.6) were a mono-directional point source:

$$Q = Q(r, \underline{\Omega}) = \delta(r - r_0) \delta(\underline{\Omega} - \underline{\Omega}_0) , \tag{2.7}$$

then

$$R = \frac{1}{4\pi} \psi_1^*(r_0, \underline{\Omega}_0) . \tag{2.8}$$

Thus, $\psi_1^*(r, \underline{\Omega})$ is (proportional to) the response R due to a unit delta-function source of particles at position r , with trajectory $\underline{\Omega}$. Also, if we obtain $\psi_g^*(r, \underline{\Omega})$, the solution to eqs. (2.3), then by eqn. (2.6), we automatically have the solution to eqs. (2.1) and (2.2).

Considering the connection between the forward and adjoint problems, it makes sense to combine the adjoint solution with the forward solution. Then, the particles in the new problem, created by this transformation, will carry along information about their importance to the response of the detector. Thus we create a new function, defined by:

$$\xi_g(r, \underline{\Omega}) \equiv \psi_g(r, \underline{\Omega}) \psi_g^*(r, \underline{\Omega}) . \quad (2.9)$$

Substituting eqn. (2.9) into eqn. (2.1), we get:

$$\begin{aligned} & \frac{1}{\psi_g^*(r, \underline{\Omega})} \underline{\Omega} \cdot \nabla \xi_g(r, \underline{\Omega}) - \frac{\xi_g(r, \underline{\Omega})}{(\psi_g^*(r, \underline{\Omega}))^2} \underline{\Omega} \cdot \nabla \psi_g^*(r, \underline{\Omega}) + \sigma_{t,g}(r) \frac{\xi_g(r, \underline{\Omega})}{\psi_g^*(r, \underline{\Omega})} \\ & = \frac{1}{4\pi} \sum_{g'=1}^G \int_{4\pi} \sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \cdot \underline{\Omega}) \frac{\xi_{g'}(r, \underline{\Omega}')}{\psi_{g'}^*(r, \underline{\Omega}')} d\Omega' + \frac{1}{4\pi} Q(r) \delta_{g,1} . \end{aligned} \quad (2.10)$$

Multiplying by $\psi_g^*(r, \underline{\Omega})$, we obtain:

$$\begin{aligned} & \underline{\Omega} \cdot \nabla \xi_g(r, \underline{\Omega}) + \left[\sigma_{t,g}(r) - \frac{1}{\psi_g^*(r, \underline{\Omega})} \underline{\Omega} \cdot \nabla \psi_g^*(r, \underline{\Omega}) \right] \xi_g(r, \underline{\Omega}) \\ & = \frac{1}{4\pi} \sum_{g'=1}^G \int_{4\pi} \sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \cdot \underline{\Omega}) \frac{\psi_g^*(r, \underline{\Omega})}{\psi_{g'}^*(r, \underline{\Omega}')} \xi_{g'}(r, \underline{\Omega}') d\Omega' + \frac{\psi_g^*(r, \underline{\Omega})}{4\pi} Q(r) \delta_{g,1} . \end{aligned} \quad (2.11)$$

This is a transport equation for $\xi_g(r, \underline{\Omega})$, containing the “effective” cross sections:

$$\Sigma_{t,g}(r, \underline{\Omega}) = \sigma_{t,g}(r) - \frac{1}{\psi_g^*(r, \underline{\Omega})} \underline{\Omega} \cdot \nabla \psi_g^*(r, \underline{\Omega}) , \quad (2.12)$$

$$\Sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega}) = \sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \cdot \underline{\Omega}) \frac{\psi_g^*(r, \underline{\Omega})}{\psi_{g'}^*(r, \underline{\Omega}')} . \quad (2.13)$$

(At first, the “effective” total cross section appears capable of being negative. However, after we present the new transformed transport problem, we will show that this is not the

case.) We can now rewrite eqn. (2.11), along with the corresponding boundary conditions derived from eqs. (2.1), for $r \in D$, $1 \leq g \leq G$:

$$\begin{aligned} \underline{\Omega} \cdot \underline{\nabla} \xi_g(r, \underline{\Omega}) + \Sigma_{t,g}(r, \underline{\Omega}) \xi_g(r, \underline{\Omega}) \\ = \frac{1}{4\pi} \sum_{g'=1}^G \int_{4\pi} \Sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega}) \xi_{g'}(r, \underline{\Omega}') d\Omega' + \frac{\psi_g^*(r, \underline{\Omega})}{4\pi} Q(r) \delta_{g,1} , \end{aligned} \quad (2.14)$$

$$\xi_g(r_b, \underline{\Omega}) = 0 \text{ for } \underline{\Omega} \cdot \underline{n}_b < 0, \quad r_b \in \partial D, \quad 1 \leq g \leq G , \quad (2.14a)$$

$$Q(r) = 1 \text{ for } r \in D_s, \text{ and } 0 \text{ otherwise.} \quad (2.14b)$$

Eqs. (2.14) describe a transport process, for $\xi_g(r, \underline{\Omega})$, that is different from either the original problem (2.1), or the adjoint problem (2.3). Let us examine the properties of the transformed problem (2.14). First, as with the original forward problem, all particles are born in the original source region, D_s , and in the first energy group. Now, let us consider the “effective” cross sections defined by eqs. (2.12) and (2.13). If we divide eqn. (2.3) by $\psi_g^*(r, \underline{\Omega})$, switch primes throughout, and move the source term over to the LHS:

$$\begin{aligned} \frac{-\underline{\Omega}' \cdot \underline{\nabla} \psi_{g'}^*(r, \underline{\Omega}')}{\psi_{g'}^*(r, \underline{\Omega}')} + \sigma_{t,g'}(r) - \frac{\frac{1}{4\pi} \Sigma(r) \delta_{g',G}}{\psi_{g'}^*(r, \underline{\Omega}')} \\ = \frac{1}{4\pi} \sum_{g=1}^G \int_{4\pi} \frac{\Sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega}) \psi_g^*(r, \underline{\Omega})}{\psi_{g'}^*(r, \underline{\Omega}')} d\Omega , \end{aligned} \quad (2.15)$$

then we see that with eqs. (2.12) and (2.13);

$$\Sigma_{t,g'}(r, \underline{\Omega}') - \frac{\frac{1}{4\pi} \Sigma(r) \delta_{g',G}}{\psi_{g'}^*(r, \underline{\Omega}')} = \frac{1}{4\pi} \sum_{g=1}^G \int_{4\pi} \Sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega}) d\Omega . \quad (2.16)$$

This indicates that particles at position r , in group g' , with trajectory $\underline{\Omega}'$, enter collisions at the same rate per unit path length as they leave collisions, everywhere except group G in the detector region. Thus, the collision process in eqn. (2.14) is *conservative* (no particles are created or lost), in all phase space, except in the detector region and in group G . Collisions in the detector region, in group G , are not conservative, because eqn. (2.16) contains the response function $\Sigma(r)$, which plays the role of a capture cross section.

We can also show that for the transformed problem, defined by eqs. (2.14), leakage from the system is impossible. To do this, we only need to examine eqn. (2.12), rewritten in the following form:

$$\Sigma_{t,g}(r, \underline{\Omega}) = \frac{-\underline{\Omega} \cdot \nabla \psi_g^*(r, \underline{\Omega}) + \sigma_{t,g}(r) \psi_g^*(r, \underline{\Omega})}{\psi_g^*(r, \underline{\Omega})} . \quad (2.17)$$

The numerator of eqn. (2.17) can be replaced, using eqn. (2.3):

$$\Sigma_{t,g}(r, \underline{\Omega}) = \frac{\frac{1}{4\pi} \sum_{g'=1}^G \int_{4\pi} \sigma_{s,g \rightarrow g'}(r, \underline{\Omega} \cdot \underline{\Omega}') \psi_{g'}^*(r, \underline{\Omega}') d\Omega' + \frac{1}{4\pi} \Sigma(r) \delta_{g,G}}{\psi_g^*(r, \underline{\Omega})} . \quad (2.18)$$

Along with boundary condition (2.3a), this implies that the total cross section approaches infinity as a particle approaches any system boundary. Thus leakage is impossible. [Also, we see why the “effective” total cross section cannot be negative. Eqn. (2.18) explicitly shows that $\Sigma_{t,g}(r, \underline{\Omega})$ must always be positive.]

Now let us examine the results of applying analog Monte Carlo to the transformed problem, defined by eqs. (2.14). The transformed source is defined by:

$$\bar{Q}(r, \underline{\Omega}) = \frac{\psi_g^*(r, \underline{\Omega})}{4\pi} Q(r) \delta_{g,1} , \quad (2.19)$$

which can be rewritten, using eqn. (2.6), as:

$$\bar{Q}(r, \underline{\Omega}) = \delta_{g,1} \left[\frac{\psi^*_{1}(r, \underline{\Omega}) Q(r)}{\int_{D, 4\pi} \psi^*_{1}(r, \underline{\Omega}) Q(r) d\Omega dr} \right] R. \quad (2.20)$$

The term in brackets is a probability distribution function for selecting a source particle, and R is the weight of each source particle. Thus every particle is born with an identical weight.

Having defined the source particles, we now examine distance-to-collision. Referring to eqn. (2.12), we see that the mean distance to collision (which is proportional to $\Sigma_{t,g}^{-1}$) depends on the slope of the adjoint solution. If a particle is headed in a direction of increasing slope (increasing importance), then $\Sigma_{t,g}$ is small, so the distance to collision increases, allowing the particle to suffer fewer collisions as it travels towards the region of interest. On the other hand, if a particle is headed in a direction of decreasing slope (decreasing importance), then $\Sigma_{t,g}$ is large, so the distance to collision decreases, causing the particle to suffer more frequent collisions when it attempts to travel away from the region of interest. This effect alone would cause particles to concentrate in the area of interest, where the peak of the importance function exist. But eqn. (2.14) also biases selection of trajectory and energy group after a collision.

In the event of a collision, we need to determine probability distribution functions for the new energy group and the new trajectory, and an expression for the probability of survival. All of these can be found by examining the scattering integral in eqn. (2.14), which can be written as:

$$\sum_{g'=1}^G \int_{4\pi} \Sigma_{t,g'}(r, \underline{\Omega}') \xi_{g'}(r, \underline{\Omega}') \left[\frac{\frac{1}{4\pi} \Sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega})}{\Sigma_{t,g'}(r, \underline{\Omega}')} \right] d\Omega'. \quad (2.21)$$

Using eqn. (2.16), the bracket term can be rewritten again as:

$$\begin{aligned}
& \frac{\Sigma_{s, g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega})}{\int_{4\pi} \Sigma_{s, g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega}'') d\Omega''} \cdot \frac{\int_{4\pi} \Sigma_{s, g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega}'') d\Omega''}{\sum_{g''=1}^G \int_{4\pi} \Sigma_{s, g' \rightarrow g''}(r, \underline{\Omega}' \rightarrow \underline{\Omega}'') d\Omega''} \\
& \cdot \frac{\frac{1}{4\pi} \sum_{g''=1}^G \int_{4\pi} \Sigma_{s, g' \rightarrow g''}(r, \underline{\Omega}' \rightarrow \underline{\Omega}'') d\Omega''}{\frac{1}{4\pi} \sum_{g=1}^G \int_{4\pi} \Sigma_{s, g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega}) d\Omega + \frac{\frac{1}{4\pi} \Sigma(r) \delta_{g', G}}{\psi_{g'}^*(r, \underline{\Omega}')}} \cdot
\end{aligned} \tag{2.22}$$

The second term, which is equal to unity when summed over g , is the probability distribution function for the new energy group ($p_{g' \rightarrow g}$). The first term, which is equal to unity when integrated over $\underline{\Omega}$, is the probability distribution function for the new trajectory ($p_{\underline{\Omega}' \rightarrow \underline{\Omega}}$) given knowledge of the new energy group g . The third term is the probability of survival (non-absorption). This is equal to unity, except in the detector region and in group G , where it is less than unity. Referring to eqn. (2.13), we see that both the probability distribution functions for new trajectory and new energy group are biased toward angles and energies that give the highest value of $\psi_g^*(r, \underline{\Omega})$. In other words, the maximum values of the probability distribution functions occur for new trajectories that point toward the region of interest, and for new energy groups that are equal to the energy groups of the detector response. Finally, referring to eqn. (2.16), we see that the probability of survival for collisions outside of the detector region, or outside of group G , is equal to unity, and that the probability of survival for collisions inside the detector region, in group G , is less than unity (we already know this from our earlier discussion).

Let us now consider how particles are terminated. We have already shown that a particle can die only via absorption in the detector region, in group G , since the collision process outside of the detector region, or outside of group G , is conservative, and particles are not allowed to leak out. Inside the detector region, in group G , every collision can

have two results. Either the particle is absorbed, in which case it contributes its entire weight to the detector tally, or it survives the collision and scatters. Eventually, this process results in every particle being absorbed in the detector and contributing its entire weight to the detector tally in group G .

In summary, we have shown that the use of the adjoint solution in the definition of $\xi_g(\underline{r}, \underline{\Omega})$ in the transformed problem results in an analog Monte Carlo simulation with the following properties: Particles are born only in the first group, in the source region of the forward problem, and every particle is born with exactly the same weight. This weight is equal to the final weight deposited in the detector region, in group G , that will result in the correct detector response. A particle's weight never changes during transport from the source to the detector. In addition, no particles are gained or lost in collisions outside of the detector region, or outside of group G , and none can leak out of the system. A particle can be lost only by absorption in the detector region, in group G . When this happens, its entire weight is contributed to the detector tally. Thus, every particle is guaranteed to score, and will contribute exactly the same score. As a result, only one particle history needs to be run. Thus, eqs. (2.14) describe a transport process which can be solved by a Monte Carlo simulation with zero variance in the desired response function tally.

Before we get too excited about the possibility of solving deep penetration source-detector problems with only one Monte Carlo particle, we need to determine whether or not it is possible, or desirable, to implement the zero variance method. In fact, it is not clear that even with the exact continuous solution of the adjoint problem, one could implement the zero variance method in a Monte Carlo code. The effective cross sections, which are now functions of the adjoint solution, would be prohibitively complex, making distance-to-collision, trajectory selection, and other Monte Carlo calculations very expensive, if not impossible, to carry out. This is in addition to the fact that obtaining the adjoint solution throughout the system is far more difficult than our original goal of obtaining a response function in a small region of the system! These arguments clearly

indicate that the zero variance method is impractical to implement. However, this does not mean that it is only useful for philosophical discussions. If one can obtain a good approximation to the adjoint solution, then this ought to yield a good approximation to the zero variance method. Approximating the zero variance method in this way should result in low variances in the desired tally. In other words, the zero variance method is (in principle) the best variance reduction technique possible, and an approximation of it should be the next best thing.

It is worth noting that at least one other variance reduction technique can be related to the zero variance method. It has long been known that the adjoint solution can be used as a guide for determining the proper weight of a particle at each point of phase space, throughout a system. Thus, upper and lower weight limits can be based on the adjoint solution and used to control a particle's weight. This is one way of attempting to approximate the zero variance method's ability to maintain constant and identical particle weights. The LIFT and AVATAR methods utilize this strategy in their implementation of weight windows. Since AVATAR is not derived from the zero variance method, and can only be related to one of its characteristics (that of keeping a particle's weight constant, or at least close to its theoretical value), there is a limit to the amount of variance reduction that can be achieved, even with a very accurate approximation of the adjoint solution. LIFT, on the other hand, is derived directly from the zero variance method, and with an accurate enough approximation of the adjoint solution, weight windows would not even be needed to achieve lower variance. However, due to the limits of our ability to approximate the adjoint solution, we have found that LIFT and weight windows usually work more efficiently together than either method alone.

The following chapters describe in detail how we plan to implement our approximation to the zero variance method. In brief, our strategy involves the following steps:

1. We derive an analytical function, piecewise continuous in space and angle, which approximates the adjoint solution within each energy group and spatial cell of the Monte Carlo system. This function utilizes information from a deterministic approximation of the adjoint solution on a spatial grid, which can be obtained in several ways. For this dissertation, the deterministic approximations include diffusion, SP_N , and three variations of S_N .
2. We use our approximate representation of the adjoint solution to transform the original forward problem into a new problem which can be solved by a Monte Carlo simulation with reduced variance. Greater accuracy in the approximation of the adjoint solution should result in greater reduction of the variance, but at a greater cost of obtaining (and using) the more accurate adjoint solution. The limit, which is unachievable, is an exact representation resulting in zero variance. There is, however, a balance to be achieved between increased accuracy and increased computing time. This will also be addressed.

CHAPTER 3

APPROXIMATIONS TO THE ZERO VARIANCE SOLUTION

As we discussed in the previous chapter, determining the adjoint solution everywhere is more difficult than the original task of finding the response function in a single region of the system. Therefore, we approximate the zero variance method by obtaining a reasonably accurate, easily-calculated approximation to the adjoint solution.

The Exponential Transform

The simplest approximation, and one that has been in use since the about the beginning of Monte Carlo transport, leads to a variance reduction technique known as the exponential transform. This method approximates the adjoint solution with a function independent of Ω , and exponentially varying in space:

$$\psi^*(r) \approx e^{\sigma_0 \lambda \cdot r} . \quad (3.1)$$

Here λ is a user-defined parameter that controls the amount and direction of biasing; it is chosen through either experience or trial and error. The method was sometimes localized by making λ a vector that always pointed toward the region of interest⁴. However, the magnitude of λ was constant, independent of space and energy. One of the greatest problems with this method, or any method that alters the transport or collision process, is that adjustments to the weight of the particle are necessary in order to maintain a fair game. These adjustments often result in undesirable weight fluctuations that increase the variance of the tally. A significant improvement over the plain exponential transform is

achieved by using the discrete Case mode or asymptotic solution to the adjoint problem with isotropic scattering⁴³:

$$\psi^*(r, \underline{\Omega}) \approx \frac{\sigma_{s0} e^{\sigma_t \underline{\lambda} \cdot r}}{4\pi\sigma_t(1 - \underline{\lambda} \cdot \underline{\Omega})} , \quad (3.2)$$

where $\underline{\lambda}$ satisfies the following dispersion law:

$$1 = \int_{4\pi} \frac{\sigma_{s0}}{4\pi\sigma_t(1 - \underline{\lambda} \cdot \underline{\Omega})} d\Omega . \quad (3.3)$$

This method, minus the dispersion law requirement for $\underline{\lambda}$, was first proposed by Dwivedi¹³. He found that by combining the biasing of the transport and collision processes, the weight fluctuations caused by each one nearly cancelled out. However, the magnitude of the biasing parameter is still a constant, and thus neither of these methods works well in heterogeneous or multigroup problems. These more complex and realistic types of problems are the target of the LIFT method.

The Local Importance Function Transform (LIFT) Method

For heterogeneous or multigroup problems, one needs an approximation of the adjoint solution that is space, angle, and energy-dependent. In addition, the expression should contain information derived from a deterministic approximation of the adjoint solution. The approximation used by the Local Importance Function Transform satisfies these criteria. The physical system is split into a number of regions (V_n) centered around position r_n , and the expression given below, for linearly anisotropic scattering, holds for all $|\underline{\Omega}| = 1$ and $r \in V_n$:

$$\psi_{g,n}^*(r, \underline{\Omega}) \approx \phi_{g,n}^* V_n \left[\beta_{g,n} \frac{\sigma_{s0,g \rightarrow g,n} b_{g,n}(\underline{\Omega})}{\sigma_{t,g,n} - \underline{\rho}_{g,n} \cdot \underline{\Omega}} e^{\underline{\rho}_{g,n} \cdot (r - r_n)} \right], \quad (3.4)$$

with the normalization factor:

$$\beta_{g,n} = \left[\left(\int_{V_n} e^{\underline{\rho}_{g,n} \cdot (r - r_n)} dr \right) \left(\int_{4\pi} \frac{\sigma_{s0,g \rightarrow g,n} b_{g,n}(\underline{\Omega})}{\sigma_{t,g,n} - \underline{\rho}_{g,n} \cdot \underline{\Omega}} d\Omega \right) \right]^{-1}, \quad (3.4a)$$

and the linearly anisotropic factor:

$$b_{g,n}(\underline{\Omega}) = 1 + 3\bar{\mu}_{g \rightarrow g,n} \frac{\sigma_{t,g,n} - \sigma_{s0,g \rightarrow g,n}}{|\underline{\rho}_{g,n}|^2} \underline{\rho}_{g,n} \cdot \underline{\Omega}, \quad (3.4b)$$

and the biasing parameter:

$$\underline{\rho}_{g,n} = \sigma_{t,g,n} \underline{\lambda}_{g,n}. \quad (3.4c)$$

We see that eqn. (3.4) is very similar to eqn. (3.2), except that the biasing parameter is now dependent on energy group g and spatial cell n . In this case, $\underline{\lambda}_{g,n}$ is determined by a deterministic adjoint calculation, rather than a dispersion law. However, its maximum value is guided by a dispersion law, as we will explain. For now, we only point out that $|\underline{\lambda}_{g,n}|$ is required to be between zero and unity, to insure that $\psi_{g,n}^*(r, \underline{\Omega})$ is always positive. This in turn insures that the “effective” cross sections given by eqs. (2.12) and (2.13) are positive. Eqn. (3.4a) is used to make the bracketed term in eqn. (3.4) a *shape function* (its integral over $\underline{\Omega}$ and $r \in V_n$ is unity), insuring that information from $\phi_{g,n}^*$, the deterministically calculated scalar flux, is preserved.

Evaluating the integrals in eqn. (3.4a) is simplified by choosing a coordinate system such that:

$$\underline{\rho}_g = |\underline{\rho}_g| \hat{i} \Rightarrow \underline{\Omega} \cdot \underline{\rho}_g = \mu |\underline{\rho}_g| \quad (3.5)$$

Then,

$$\frac{1}{\beta_{g,n}} = \frac{8 \sinh(\rho_{x,g,n} \Delta x_n / 2) \sinh(\rho_{y,g,n} \Delta y_n / 2) \sinh(\rho_{z,g,n} \Delta z_n / 2) \sigma_{s0,g \rightarrow g,n} 2\pi}{\rho_{x,g,n} \rho_{y,g,n} \rho_{z,g,n} |\underline{\rho}_{g,n}|} \left[\frac{-6\bar{\mu}_{g \rightarrow g,n}(\sigma_{t,g,n} - \sigma_{s0,g \rightarrow g,n})}{|\underline{\rho}_{g,n}|} - \left(1 + \frac{3\bar{\mu}_{g \rightarrow g,n}(\sigma_{t,g,n} - \sigma_{s0,g \rightarrow g,n})\sigma_{t,g,n}}{|\underline{\rho}_{g,n}|^2} \right) \gamma_{g,n} \right], \quad (3.6)$$

with

$$\gamma_{g,n} = \ln \left(\frac{\sigma_{t,g,n} - |\underline{\rho}_{g,n}|}{\sigma_{t,g,n} + |\underline{\rho}_{g,n}|} \right). \quad (3.7)$$

Later, [see eqn. (3.42)] we will describe a method known as simplified linearly anisotropic scattering, which involves setting $b_{g,n}(\underline{\Omega}) = 1$.

We will now discuss the derivation of eqn. (3.4). Unless we attempt to write a discrete ordinates Monte Carlo code, we need only obtain a deterministic approximation to the scalar flux $\phi_{g,n}^*$. Having the scalar flux, we can approximate the angular flux for each group independently. Thus, we treat each group as a separate one-group problem, when deriving eqn. (3.4). So, for linearly anisotropic scattering, we have:

$$\begin{aligned} & -\underline{\Omega} \cdot \underline{\nabla} \psi_g^*(r, \underline{\Omega}) + \sigma_{t,g}(r) \psi_g^*(r, \underline{\Omega}) \\ & = \frac{1}{4\pi} \int_{4\pi} \sigma_{s0,g \rightarrow g} (1 + 3\bar{\mu}_{g \rightarrow g} \underline{\Omega} \cdot \underline{\Omega}') \psi_g^*(r, \underline{\Omega}') d\Omega' \quad . \end{aligned} \quad (3.8)$$

Since $\Sigma(r) = 0$, except in the detector region, the adjoint source has been eliminated. However, this approximation is used everywhere, including the detector region, when the method is implemented. Future work could attempt a more accurate approximation that

includes the adjoint source.

We will now apply separation of variables to solve eqn. (3.8). We assume the spatial component of the solution to be an exponential, and leave the angular component unspecified:

$$\psi_g^*(r, \underline{\Omega}) = f_g(\underline{\Omega}) e^{\underline{\rho}_g \cdot (\underline{r} - \underline{r}_n)} = F_g(\underline{\Omega} \cdot \underline{\rho}_g) e^{\underline{\rho}_g \cdot (\underline{r} - \underline{r}_n)} . \quad (3.9)$$

We require that $f_g(\underline{\Omega})$ satisfy a normalization condition (also called a dispersion law), which if we choose a coordinate system such that $\underline{\rho}_g = |\underline{\rho}_g| \hat{i}$ and $\underline{\Omega} \cdot \underline{\rho}_g = \mu |\underline{\rho}_g|$, can be written as:

$$\int_{4\pi} F_g(\underline{\Omega} \cdot \underline{\rho}_g) d\Omega = 2\pi \int_{-1}^1 F_g(\mu |\underline{\rho}_g|) d\mu = 1 . \quad (3.10)$$

Substituting eqn. (3.9) into eqn. (3.8), carrying out the derivative, and cancelling the exponential terms, we obtain:

$$(\sigma_{t,g} - \underline{\Omega} \cdot \underline{\rho}_g) F_g(\underline{\Omega} \cdot \underline{\rho}_g) = \frac{\sigma_{s0,g \rightarrow g}}{4\pi} \int_{4\pi} (1 + 3\bar{\mu}_{g \rightarrow g} \underline{\Omega} \cdot \underline{\Omega}') F_g(\underline{\Omega}' \cdot \underline{\rho}_g) d\Omega' , \quad (3.11)$$

or

$$(\sigma_{t,g} - \mu |\underline{\rho}_g|) F_g(\mu |\underline{\rho}_g|) = \frac{\sigma_{s0,g \rightarrow g}}{2} \int_{-1}^1 (1 + 3\bar{\mu}_{g \rightarrow g} \mu \mu') F_g(\mu' |\underline{\rho}_g|) d\mu' . \quad (3.12)$$

Eqn. (3.12) can be rewritten, using eqn. (3.10), in the following form:

$$(\sigma_{t,g} - \mu |\underline{\rho}_g|) F_g(\mu |\underline{\rho}_g|) = \frac{\sigma_{s0,g \rightarrow g}}{4\pi} + \frac{3\bar{\mu}_{g \rightarrow g} \mu \sigma_{s0,g \rightarrow g}}{2} \int_{-1}^1 \mu' F_g(\mu' |\underline{\rho}_g|) d\mu' . \quad (3.13)$$

If we operate on eqn. (3.13) by $\int_{-1}^1 () d\mu$, then, again using eqn. (3.10), we obtain:

$$\frac{\sigma_{t,g} - |\underline{\rho}_g|}{2\pi} \int_{-1}^1 \mu F_g(\mu |\underline{\rho}_g|) d\mu = \frac{\sigma_{s0,g \rightarrow g}}{2\pi} . \quad (3.14)$$

If we replace μ by μ' in eqn. (3.14), and substitute the result into eqn. (3.13), we obtain:

$$(\sigma_{t,g} - \mu |\underline{\rho}_g|) F_g(\mu |\underline{\rho}_g|) = \frac{\sigma_{s0,g \rightarrow g}}{4\pi} + \frac{3\bar{\mu}_{g \rightarrow g} \mu \sigma_{s0,g \rightarrow g}}{2} \left(\frac{\sigma_{t,g} - \sigma_{s0,g \rightarrow g}}{2\pi |\underline{\rho}_g|} \right) . \quad (3.15)$$

We can then solve for $f_g(\underline{\Omega})$, if we recall that $\underline{\Omega} \cdot \underline{\rho}_g = \mu |\underline{\rho}_g|$:

$$f_g(\underline{\Omega}) = \frac{\frac{1}{4\pi} \sigma_{s0,g \rightarrow g} \left[1 + 3\bar{\mu}_{g \rightarrow g} \left(\frac{\sigma_{t,g} - \sigma_{s0,g \rightarrow g}}{|\underline{\rho}_g|^2} \right) \underline{\rho}_g \cdot \underline{\Omega} \right]}{\sigma_{t,g} - \underline{\Omega} \cdot \underline{\rho}_g} = \frac{\frac{1}{4\pi} \sigma_{s0,g \rightarrow g} b_g(\underline{\Omega})}{\sigma_{t,g} - \underline{\Omega} \cdot \underline{\rho}_g} . \quad (3.16)$$

Now that we have obtained an approximation for the adjoint solution, in terms of the scalar flux and a biasing parameter, let us determine how $\underline{\rho}_g$ is obtained. Ideally, $\underline{\rho}_g$ is chosen to satisfy eqn. (3.10), leading to the following equation:

$$\frac{\sigma_{s0,g \rightarrow g,n}}{2|\underline{\rho}_{g,n}|} * \left[\frac{-6\bar{\mu}_{g \rightarrow g,n}(\sigma_{t,g,n} - \sigma_{s0,g \rightarrow g,n})}{|\underline{\rho}_{g,n}|} - \left(1 + \frac{3\bar{\mu}_{g \rightarrow g,n}(\sigma_{t,g,n} - \sigma_{s0,g \rightarrow g,n})\sigma_{t,g,n}}{|\underline{\rho}_{g,n}|^2} \right) \gamma_{g,n} \right] = 1 . \quad (3.17)$$

This can be solved, numerically, for $|\underline{\rho}_{g,n}|$. However, this is for the deep penetration part of an infinite slab. Thus we use eqn. (3.17) as a guide only. In practice, we define the biasing parameter in terms of the adjoint scalar flux, as we will see next, and eqn. (3.17) is used to set a maximum value of $|\underline{\rho}_{g,n}|$. Recalling eqn. (3.4c), this maximum value can be overridden by the user choosing the weighting factor ($f4$) in the following expression:

$$|\underline{\lambda}_{g,n}|_{max} = f4 + (1 - f4) |\underline{\lambda}_{0,g}| , \quad (3.18)$$

where $\lambda_{0,g}$ is the eigenvalue of eqn. (3.10), and f_4 is between 0 and 1. Thus, choosing f_4 to be zero sets the maximum biasing parameter magnitude equal to the magnitude of the eigenvalue for deep penetration, while choosing f_4 to be unity sets the maximum biasing parameter magnitude equal to $\sigma_{t,g,n}$ (the highest value allowed, to insure that the effective total cross section remains positive). To see how $\rho_{g,n}$ is obtained from the deterministic approximation of the adjoint scalar flux, let us consider the following 1-D representation of the angular flux given by eqn. (3.4):

$$\psi_{g,n}^*(x, \mu) \approx A_{g,n} f_{g,n}(\mu) e^{\rho_{x,g,n}(x-x_n)}, \quad (3.19)$$

where $A_{g,n}$ is a constant. Integrating over μ , we get the scalar flux and a new constant:

$$\phi_{g,n}^*(x) = B_{g,n} e^{\rho_{x,g,n}x}. \quad (3.20)$$

Taking the natural log and derivative gives us an expression for the biasing parameter:

$$\frac{d}{dx} \ln[\phi_{g,n}^*(x)] = \rho_{x,g,n}. \quad (3.21)$$

Thus, we define the biasing parameters in eqs. (3.4) in terms of the deterministic scalar fluxes by the following formulas [$n \Leftrightarrow (i, j, k)$]:

$$\rho_{x,g,n} = \frac{1}{\Delta x_n} \ln \left(\frac{\phi_{g,i+1/2}^*}{\phi_{g,i-1/2}^*} \right), \quad (3.22a)$$

$$\rho_{y,g,n} = \frac{1}{\Delta y_n} \ln \left(\frac{\phi_{g,j+1/2}^*}{\phi_{g,j-1/2}^*} \right), \quad (3.22b)$$

$$\rho_{z, g, n} = \frac{1}{\Delta z_n} \ln \left(\frac{\phi_{g, k+1/2}^*}{\phi_{g, k-1/2}^*} \right). \quad (3.22c)$$

To summarize, we use the approximate expression for $\psi_{g, n}^*(z, \underline{\Omega})$ in region V_n given by eqn. (3.4), with the biasing parameter defined by eqs. (3.22).

We are now ready to examine a Monte Carlo transport process guided by the zero variance problem. There are two strategies for approximating the zero variance solution. Unfortunately, the author of this thesis may have chosen the less efficient strategy for the numerical calculations presented in Chapter 6. This strategy is based in traditional Monte Carlo biasing techniques. We start with “real” particles, that obey the laws of eqs. (2.1). Every time that some aspect of the “real” particle’s transport is biased, thus transforming it into a “biased” particle, we convert it back to a “real” particle by altering its weight. Hence, we use eqs. (2.1) as our base, from which we start particles, and to which we always return after some aspect of the equation has been biased (e.g. distance-to-collision, scattering angle or energy). This particular strategy is probably less efficient than the second strategy (discussed in the next paragraph), and it caused the author to overlook the possibility of source biasing. Eqs. (2.1) have a uniformly distributed, isotropically-emitted source. The transformed problem defined by eqs. (2.14), does not. We recognized the ability to bias path length in eqn. (2.1) by using the “effective” total cross section from eqn. (2.14) each time that we calculated distance-to-collision. We also recognized the ability to bias scattering angles and energies in eqn. (2.1) by using the “effective” scattering cross section from eqn. (2.14) each time that particles underwent collisions. However, we did not recognize the ability to use the source from eqn. (2.14) in eqn. (2.1), along with a weight correction. Had this additional aspect of the zero variance problem been employed, source particles would have been biased in position and trajectory, resulting in a more efficient calculation because their histories would be shorter. Thus, the results presented in Chapter 6, for the LIFT method, would have been better to some

degree.

The second strategy, which is probably more efficient, is to apply a Monte Carlo simulation directly to eqs. (2.14). We have already shown in Chapter 2 that eqs. (2.14) can be solved by analog Monte Carlo with zero variance. After completing the numerical testing of the strategy used in this thesis, described in the previous paragraph, it was discovered that approximating an analog Monte Carlo simulation of eqs. (2.14) would probably be more efficient. Instead of beginning with “real” particles, and converting back to “real” particles after every biased event, one would simply carry out the entire simulation with “biased” particles. The “real” response would then be defined by substituting eqn. (2.9) into eqn. (2.2). This would eliminate the time-consuming conversions back to real particles at every boundary and every collision. The author regrets having discovered these strategies after very lengthy numerical studies had been conducted. It is unfortunate that time constraints for completing this thesis prevent the use of a biased source in the first strategy, or the implementation of the even more efficient second strategy that involves direct application of a Monte Carlo simulation to eqs. (2.14). (Chapter 6 is the result of approximately 2000 calculations, involving 11 problems, up to 11 methods, and several trial and error optimization runs for each method on each problem.) However, even with this presumably less efficient strategy, the LIFT method is shown in this thesis to be very advantageous. The implementation of the second, presumably more efficient strategy, will be considered in future work, as we discuss in Chapter 8.

We will now describe the Monte Carlo simulation employed in this thesis. We begin each Monte Carlo “history” by creating a source particle with weight equal to unity. As discussed above, Eqn. (2.20), along with a weight modification, can be used to bias the source’s spatial distribution and emission of particles in desired energy groups and directions. However, all of the source particles for this thesis are born isotropically in group 1, and are uniformly distributed in the source region. Our simulation is based on

eqs. (2.1), utilizing biased transport and collision processes derived from eqs. (2.14) with conversions back to “real” particles. Let us write down the probability distribution function for the uniformly distributed position of a source particle along the x -axis, within the user-defined source cell(s):

$$p(x) = \begin{cases} \frac{1}{x_1 - x_2} & (x_1 < x < x_2) \\ 0 & \text{otherwise} \end{cases} . \quad (3.23)$$

If we integrate the probability distribution function to obtain a cumulative distribution function, and set that equal to a random number (ζ) between 0 and 1, then we have an explicit expression for x :

$$\zeta = P(x) = \int_0^x p(x') dx' = \frac{x - x_1}{x_2 - x_1} \quad \text{for } (x_1 < x < x_2) , \quad (3.24)$$

which can be rewritten as:

$$x = x_1 + \zeta(x_2 - x_1) . \quad (3.25a)$$

Likewise:

$$y = y_1 + \zeta(y_2 - y_1) , \quad (3.25b)$$

$$z = z_1 + \zeta(z_2 - z_1) , \quad (3.25c)$$

Next, we determine the trajectory of the isotropic source particle. The probability distribution functions for average cosine, and azimuthal angle are, respectively:

$$p(\mu) = \frac{1}{2} , \quad (3.26)$$

$$p(\varphi) = \frac{1}{2\pi} . \quad (3.27)$$

Repeating the procedure used for position, we obtain expressions for μ and φ :

$$\zeta = \int_{-1}^{\mu} p(\mu') d\mu' = \frac{\mu+1}{2} \Rightarrow \mu = 2\zeta - 1 , \quad (3.28)$$

$$\zeta = \int_0^{\varphi} p(\varphi') d\varphi' = \frac{\varphi}{2\pi} \Rightarrow \varphi = 2\pi\zeta . \quad (3.29)$$

(Every reference to ζ indicates a new random number, unless otherwise noted.)

Having defined the source particles, we need to determine the distance to collision. From here on, we are referring to any particle anywhere in the system, rather than just source particles. For analog, or survival biasing Monte Carlo, we solve the following 1-D streaming problem in the n^{th} cell:

$$\frac{d}{ds} \psi_{g,n}(s) + \sigma_{t,g,n} \psi_{g,n}(s) = 0 , \quad (3.30)$$

where s is the distance to collision. So, the probability distribution function for the distance to collision is:

$$p(s) = \sigma_{t,g,n} e^{-\sigma_{t,g,n}s} , \quad (3.31)$$

leading to an expression for s :

$$\zeta = \int_0^s p(s') ds' = 1 - e^{-\sigma_{t,g,n}s} \Rightarrow s = \frac{-1}{\sigma_{t,g,n}} \ln(1 - \zeta) . \quad (3.32)$$

However, since the random number ζ is between 0 and 1, this is equivalent to:

$$s = \frac{-1}{\sigma_{t,g,n}} \ln(\zeta) . \quad (3.33)$$

Similarly, for LIFT Monte Carlo, we have the local probability distribution function:

$$p(s) = \Sigma_{t,g,n} e^{-\Sigma_{t,g,n}s} , \quad (3.34)$$

where $\Sigma_{t,g,n}$ is given by eqn. (2.12), which when combined with eqn. (3.4) simplifies to:

$$\Sigma_{t,g,n} = \sigma_{t,g,n} - \underline{\Omega} \cdot \underline{\rho}_{g,n} . \quad (3.35)$$

Therefore,

$$s = \frac{-1}{\sigma_{t,g,n} - \underline{\Omega} \cdot \underline{\rho}_{g,n}} \ln(\zeta) . \quad (3.36)$$

We can see that if $\underline{\rho}_{g,n} = 0$ (unbiased game), then eqn. (3.36) is equal to eqn. (3.33). In both cases, the change in coordinates, if the particle does not escape the cell, is given by:

$$\Delta x = \mu s , \quad (3.37a)$$

$$\Delta y = \sqrt{1 - \mu^2} \cos(\varphi) s , \quad (3.37b)$$

$$\Delta z = \sqrt{1 - \mu^2} \sin(\varphi) s . \quad (3.37c)$$

Having the distance to collision, we test to see if the particle collides in the cell, or escapes the cell. If the particle escapes the cell, the particle is stopped at the cell boundary and the point of escape becomes the new position, rather than the position given by eqs. (3.37). A new distance-to-collision is then sampled. Before proceeding, we need to adjust the particle's weight to account for the biased game. In this case, escape from a cell, the particle's weight is multiplied by the following factor:

$$w_{esc} = \frac{\psi_{g,n}^*(r_i, \underline{\Omega}_i)}{\psi_{g,n}^*(r_f, \underline{\Omega}_f)} = e^{\rho_{g,n} \cdot (r_i - r_f)}, \quad (3.38)$$

where i indicates initial parameters, and f indicates final parameters. Since the particle has not suffered a collision, the initial and final energy groups and trajectories are equal. Clearly, if $\rho_{g,n} = 0$ (unbiased game), then $w_{esc} = 1$.

In the event of a collision within the cell, we need to determine probability distribution functions for new energy group and new trajectory, and an expression for weight change due to the probability of survival. All of these can be found by examining the scattering integral in eqn. (2.14), which can be written as:

$$\sum_{g'=1}^G \int_{4\pi} \Sigma_{t,g'}(r, \underline{\Omega}') \xi_{g'}(r, \underline{\Omega}') \left[\frac{\frac{1}{4\pi} \Sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega})}{\Sigma_{t,g'}(r, \underline{\Omega}')} \right] d\Omega' . \quad (3.39)$$

The bracket term can be rewritten again:

$$\begin{aligned} & \frac{\Sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega})}{\int_{4\pi} \Sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega}'') d\Omega''} \cdot \frac{\int_{4\pi} \Sigma_{s,g' \rightarrow g}(r, \underline{\Omega}' \rightarrow \underline{\Omega}'') d\Omega''}{\sum_{g''=1}^G \int_{4\pi} \Sigma_{s,g' \rightarrow g''}(r, \underline{\Omega}' \rightarrow \underline{\Omega}'') d\Omega''} \\ & \cdot \frac{\frac{1}{4\pi} \sum_{g''=1}^G \int_{4\pi} \Sigma_{s,g' \rightarrow g''}(r, \underline{\Omega}' \rightarrow \underline{\Omega}'') d\Omega''}{\Sigma_{t,g'}(r, \underline{\Omega}')} . \end{aligned} \quad (3.40)$$

The second term, which is equal to unity when summed over g , is the probability distribution function for the new energy group ($p_{g' \rightarrow g}$). The first term, which is equal to unity when integrated over $\underline{\Omega}$, is the probability distribution function for the new trajectory ($p_{\underline{\Omega}' \rightarrow \underline{\Omega}}$) given knowledge of the new energy group g . The third term is the weight change factor (w_c) accounting for the survival of the particle (non-absorption).

Since the probability distribution function for new trajectory involves old and new energy groups, we must determine the new energy group first. Using eqs. (2.13) and (3.4) in the second term of eqn. (3.40), we have, for linearly anisotropic scattering:

$$P_{g' \rightarrow g} = \frac{\sigma_{s0, g' \rightarrow g, n} \phi_{g, n}^* \beta_{g, n} \sigma_{s0, g \rightarrow g, n} e^{\rho_{g, n} \cdot (\underline{\tau} - \underline{\tau}_n)} \int \frac{(1+3\bar{\mu}_{g' \rightarrow g, n} \underline{\Omega}'' \cdot \underline{\Omega}') b_{g, n}(\underline{\Omega}'')}{\sigma_{t, g, n} - \underline{\Omega}'' \cdot \underline{\rho}_{g, n}} d\Omega''}{\sum_{g''=1}^G \sigma_{s0, g' \rightarrow g'', n} \phi_{g'', n}^* \beta_{g'', n} \sigma_{s0, g'' \rightarrow g'', n} e^{\rho_{g'', n} \cdot (\underline{\tau} - \underline{\tau}_n)} \int \frac{(1+3\bar{\mu}_{g' \rightarrow g'', n} \underline{\Omega}'' \cdot \underline{\Omega}') b_{g'', n}(\underline{\Omega}'')}{\sigma_{t, g'', n} - \underline{\Omega}'' \cdot \underline{\rho}_{g'', n}} d\Omega''} \quad (3.41)$$

Here we recognize that with $b_{g, n}(\underline{\Omega})$ defined by eqn. (3.4b), the above integrals become very complicated, resulting in expressions for $p_{g' \rightarrow g}$, $p_{\underline{\Omega}' \rightarrow \underline{\Omega}}$, and w_c , which involve an inordinate amount of algebra. All of this number crunching at every collision consumes a great deal of cpu time. Since $b_{g, n}(\underline{\Omega})$ is just the linearly anisotropic part of the angular biasing, we should get roughly the same amount of acceleration, with fewer computations, by using angular biasing based on isotropic scattering ($b_{g, n}(\underline{\Omega}) = 1$). In addition, we can adjust the biasing parameter in the angular term of eqn. (3.9) to simulate biasing based on linearly anisotropic scattering:

$$\frac{\frac{1}{4\pi} \sigma_{s0, g \rightarrow g} \left[1 + 3\bar{\mu}_{g \rightarrow g} \left(\frac{\sigma_{t, g} - \sigma_{s0, g \rightarrow g}}{|\underline{\rho}_g|^2} \right) \underline{\rho}_g \cdot \underline{\Omega} \right]}{\sigma_{t, g} - \underline{\Omega} \cdot \underline{\rho}_g} \approx \frac{\frac{1}{4\pi} \sigma_{s0, g \rightarrow g}}{\sigma_{t, g} - \underline{\Omega} \cdot \underline{L}_g \underline{\rho}_g}, \quad (3.42)$$

where L_g is the adjustment to the biasing parameter. Note that L_g is not used in the spatial biasing term of eqn. (3.9). We call this method simplified linearly anisotropic biasing. This strategy can also be used for higher-order anisotropic scattering.

In determining L_g , we have to choose the way in which the RHS function of $\underline{\Omega}$ in eqn. (3.42) is going to fit the LHS function of $\underline{\Omega}$. The simplest way to do this, is to choose a coordinate system in which $\underline{\rho}/|\underline{\rho}| = i$, and require the two functions to be equivalent at $\mu = 1$. Thus, particles are treated most accurately when scattering forward. This is probably desirable, since we will be biasing scattering toward forward directions any time a particle is headed toward the detector. Other fits were tried, such as a least squares fit, where:

$$A(L_g) = \int_{4\pi} \left[\sigma_{t,g} - \underline{\Omega} \cdot L_g \underline{\rho}_g - \frac{\sigma_{t,g} - \underline{\Omega} \cdot \underline{\rho}_g}{1 + 3\bar{\mu}_{g \rightarrow g} \left(\frac{\sigma_{t,g} - \sigma_{s0,g \rightarrow g}}{|\underline{\rho}_g|^2} \right) \underline{\rho}_g \cdot \underline{\Omega}} \right]^2 d\Omega \quad (3.43)$$

$A(L_g)$ is then minimized. However, simply choosing $\mu = 1$ proved to be more efficient, when comparing the two fits in a 1-D, 4-group simulation. Getting back to our method of choice, after some cancellation, and choosing $\underline{\rho}/|\underline{\rho}| = i$, and $\mu = 1$, eqn. (3.42) becomes:

$$\frac{1 + 3\bar{\mu}_{g \rightarrow g} \left(\frac{\sigma_{t,g} - \sigma_{s0,g \rightarrow g}}{|\underline{\rho}_g|} \right)}{\sigma_{t,g} - |\underline{\rho}_g|} = \frac{1}{\sigma_{t,g} - L_g |\underline{\rho}_g|} \quad (3.44)$$

After some simplification, this gives:

$$L_g = \frac{|\underline{\rho}_g| + 3\bar{\mu}_{g \rightarrow g} \left(\frac{\sigma_{t,g} - \sigma_{s0,g \rightarrow g}}{|\underline{\rho}_g|} \right) \sigma_{t,g}}{|\underline{\rho}_g| + 3\bar{\mu}_{g \rightarrow g} (\sigma_{t,g} - \sigma_{s0,g \rightarrow g})} \quad (3.45)$$

If $|\underline{\rho}_g| = \sigma_{t,g}|\underline{\lambda}_g| = \sigma_{t,g}|\underline{\lambda}_{0,g}|$, where $\underline{\lambda}_{0,g}$ is the eigenvalue of eqn. (3.10), then we have:

$$L_g = \frac{|\underline{\rho}_g| + 3\bar{\mu}_{g \rightarrow g}(\sigma_{t,g} - \sigma_{s0,g \rightarrow g})(1/|\underline{\lambda}_{0,g}|)}{|\underline{\rho}_g| + 3\bar{\mu}_{g \rightarrow g}(\sigma_{t,g} - \sigma_{s0,g \rightarrow g})} . \quad (3.46)$$

Since $|\underline{\lambda}_{0,g}| \leq 1$, then we see that $L_g \geq 1$, which means that L_g never reduces the amount of biasing. However, as described earlier, in practice, $|\underline{\rho}_g| = \sigma_{t,g}|\underline{\lambda}_g|_{max} \neq \sigma_{t,g}|\underline{\lambda}_{0,g}|$ because the code calculates $\underline{\rho}_g$ based on ϕ_g^* , and $\underline{\rho}_g$ is limited in size by the user choosing $0 \leq f4 \leq 1$ in:

$$|\underline{\lambda}_g|_{max} = f4 + (1 - f4)\sigma_{t,g}|\underline{\lambda}_{0,g}| . \quad (3.47)$$

So, in fact we have $|\underline{\rho}_g| > \sigma_{t,g}|\underline{\lambda}_{0,g}|$, which is why we have chosen eqn. (3.46) for L_g , to insure that $L_g \geq 1$. A test on the new biasing parameter insures that the effective total cross section is always positive by printing out an error message telling the user to reduce $f4$ when the effective total cross section becomes negative. Testing of the simplified linearly anisotropic biasing method demonstrated the usefulness of L_g . When $L_g = 1$ is used in the right hand side of eqn. (3.42) (equivalent to angular biasing based on isotropic scattering), the figure of merit (defined by eqn. 3.83) was lower than that obtained by using the left hand side of eqn. (3.42) for angular biasing. The latter figure of merit was, in turn, lower than that obtained by using L_g defined by eqn. (3.46) in the right hand side of eqn. (3.42). Thus, we see that the right hand side of eqn. (3.42) with $L_g = 1$ is algebraically simple, but introduces too much "error" into the biasing of trajectory, while the left hand side of eqn. (3.42) is accurate, but too algebraically complex. Eqn. (3.46) allows us to maintain the algebraic simplicity of angular biasing based on isotropic scattering, while retaining part of the accuracy of true linearly anisotropic angular biasing.

We now return to eqn. (3.41) with $b_{g,n}(\underline{\Omega}) = 1$. We still need to evaluate the

integral terms, which after some work become:

$$\int \frac{1 + 3\bar{\mu}_{g' \rightarrow g, n} \underline{\Omega}'' \cdot \underline{\Omega}'}{\sigma_{t, g, n} - \underline{\Omega}'' \cdot \underline{L}_{g, n} \rho_{g, n}} d\Omega'' = 4\pi \Gamma_{g, n}(\underline{\Omega}') , \quad (3.48)$$

where,

$$\Gamma_{g, n}(\underline{\Omega}') = \frac{1}{2L_{g, n} |\rho_{g, n}|} * \quad (3.49)$$

$$\left[\frac{-6\bar{\mu}_{g' \rightarrow g, n} \underline{\Omega}' \cdot \underline{L}_{g, n} \rho_{g, n}}{L_{g, n} |\rho_{g, n}|} - \left(1 + \frac{3\bar{\mu}_{g' \rightarrow g, n} \sigma_{t, g, n} \underline{\Omega}' \cdot \underline{L}_{g, n} \rho_{g, n}}{L_{g, n}^2 |\rho_{g, n}|^2} \right) \ln \left(\frac{\sigma_{t, g, n} - L_{g, n} |\rho_{g, n}|}{\sigma_{t, g, n} + L_{g, n} |\rho_{g, n}|} \right) \right].$$

Eqn. (3.41) can now be rewritten as:

$$p_{g' \rightarrow g} = \frac{\sigma_{s0, g' \rightarrow g, n} \phi_{g, n}^* \beta_{g, n} \sigma_{s0, g \rightarrow g, n} e^{\rho_{g, n} \cdot (\tau - \tau_n)} \Gamma_{g, n}(\underline{\Omega}')}{\sum_{g''=1}^{g_c} \sigma_{s0, g' \rightarrow g'', n} \phi_{g'', n}^* \beta_{g'', n} \sigma_{s0, g'' \rightarrow g'', n} e^{\rho_{g'', n} \cdot (\tau - \tau_n)} \Gamma_{g'', n}(\underline{\Omega}')} . \quad (3.50)$$

We can see how energy selection is biased toward groups where the adjoint scalar flux is largest, causing particles to be “directed” toward the energy group of the response function. As before, we obtain the cumulative distribution function:

$$\zeta = \int_0^{g_c} p_{g' \rightarrow g} dE \Rightarrow \sum_{g=1}^{g_c-1} p_{g' \rightarrow g} < \zeta \leq \sum_{g=1}^{g_c} p_{g' \rightarrow g} . \quad (3.51)$$

We pick the random number ζ , then sum $p_{g' \rightarrow g}$ until it is greater than or equal to ζ . At that point, we set $g = g_c$.

Now we can determine the new trajectory after collision. Using eqs. (2.13) and (3.4) in the first term of eqn. (3.40), we have, for linearly anisotropic scattering:

$$p_{\underline{\Omega}' \rightarrow \underline{\Omega}} = \frac{1 + 3\bar{\mu}_{g' \rightarrow g, n} \underline{\Omega}' \cdot \underline{\Omega}}{4\pi\Gamma_{g, n}(\underline{\Omega}')(\sigma_{t, g, n} - \underline{\Omega} \cdot L_{g, n} \underline{\rho}_{g, n})} . \quad (3.52)$$

We can see how trajectory is biased toward directions where $\underline{\Omega} = \underline{\rho}_{g, n}$, since $p_{\underline{\Omega}' \rightarrow \underline{\Omega}}$ is maximized when the new trajectory points toward the direction of fastest gain in importance. It turns out that if we try to solve the cumulative distribution function:

$$\zeta = \int_0^{\varphi_c \mu_c} \int_{-1}^1 p_{\underline{\Omega}' \rightarrow \underline{\Omega}} d\mu d\varphi , \quad (3.53)$$

analytically, we end up with a complicated equation, which must be solved numerically for μ_c (φ_c is taken care of by rotation of the coordinate system, and can be sampled uniformly). As a result, we have chosen to use simple rejection to sample $p_{\underline{\Omega}' \rightarrow \underline{\Omega}}$. Another form of rejection, referred to as generalized rejection, was tried and is discussed later. For these problems, and for our random number generator, simple rejection resulted in higher figures of merit.

Simple rejection requires us to determine the minimum and maximum values of the probability distribution function:

$$p_{\underline{\Omega}' \rightarrow \underline{\Omega}, min} = 0 , \quad (3.54)$$

and

$$p_{\underline{\Omega}' \rightarrow \underline{\Omega}, max} = \frac{1 + 3\bar{\mu}_{g' \rightarrow g, n}}{4\pi\Gamma_{g, n}(\underline{\Omega}' = \underline{\rho}_{g, n})(\sigma_{t, g, n} - L_{g, n} |\underline{\rho}_{g, n}|)} . \quad (3.55)$$

Next, we pick new values of μ and φ uniformly, using eqs. (3.28) and (3.29). Then we sample uniformly between the minimum and maximum values of the probability distribution function:

$$p_{sel} = \zeta p_{\underline{\Omega}' \rightarrow \underline{\Omega}, max} . \quad (3.56)$$

If $p_{\underline{\Omega}' \rightarrow \underline{\Omega}}$ with the new values of μ and ϕ is greater than or equal to p_{sel} then we keep μ and ϕ . Otherwise, we reject them and start over.

In analog or survival biasing Monte Carlo, the probability distribution function for the new energy group is:

$$p_{g' \rightarrow g} = \frac{\sigma_{s0, g' \rightarrow g, n}}{\sum_{g''=1}^G \sigma_{s0, g' \rightarrow g'', n}} . \quad (3.57)$$

The probability distribution function for new trajectory is:

$$p_{\underline{\Omega}' \rightarrow \underline{\Omega}} = \frac{1}{4\pi} (1 + 3\bar{\mu}_{g \rightarrow g, n} \underline{\Omega}' \cdot \underline{\Omega}) . \quad (3.58)$$

Simple rejection is fairly efficient for sampling from eqn. (3.58).

Having determined the results of a collision, we need to adjust the particle's weight to account for the biased game, and to account for its survival. So, the adjustment consists of two factors:

$$w_{adj} = w_c w_{tr} , \quad (3.59)$$

where

$$w_{tr} = \frac{\psi_{g', n}^*(r, \underline{\Omega}')}{\psi_{g, n}^*(r, \underline{\Omega})} , \quad (3.60)$$

and w_c is given by the third part of eqn. (3.40), which with eqs. (2.12), (2.13) and (3.4) for

simplified linearly anisotropic scattering gives:

$$w_c = \frac{\sum_{g''=1}^G \sigma_{s0, g' \rightarrow g'', n} \phi_{g'', n}^* \beta_{g'', n} \sigma_{s0, g'' \rightarrow g'', n} e^{\rho_{g'', n} \cdot (t - t_n)} \Gamma_{g'', n}(\Omega')}{\phi_{g', n}^* \beta_{g', n} \sigma_{s0, g' \rightarrow g', n} e^{\rho_{g', n} \cdot (t - t_n)}} , \quad (3.61)$$

and

$$w_{tr} = \frac{\phi_{g', n}^* \beta_{g', n} \sigma_{s0, g' \rightarrow g', n} e^{\rho_{g', n} \cdot (t_i - t_n)} (\sigma_{t, g, n} - \Omega \cdot L_{g, n} \rho_{g, n})}{\phi_{g, n}^* \beta_{g, n} \sigma_{s0, g \rightarrow g, n} e^{\rho_{g, n} \cdot (t - t_n)} (\sigma_{t, g', n} - \Omega' \cdot L_{g', n} \rho_{g', n})} . \quad (3.62)$$

For survival biasing Monte Carlo, the weight adjustment is the scattering ratio:

$$w_{adj} = \frac{\sum_{g''=1}^G \sigma_{s0, g' \rightarrow g'', n}}{\sigma_{t, g', n}} . \quad (3.63)$$

This concludes the basic description of the LIFT method. However, we have found that the method works best when used with weight windows. Fortunately, the adjoint solution can also be used to generate the weight windows. Reference 37 gives an argument supporting the theory that a particle's weight should be proportional to the inverse of the importance function:

$$ww_{cen, g, n} = \frac{\psi_{g, src}^*}{\psi_{g, n}^*} . \quad (3.64)$$

This gives the center value of the weight window in cell n , normalized by the initial importance value of each source particle. Unfortunately, using the full approximation of the adjoint solution given by eqn. (3.4), is very cpu intensive. The weight of a particle is checked at every boundary and collision. Hence, we have chosen to use:

$$ww_{cen, g, n} = \frac{\phi_{g, src}^*}{\phi_{g, n}^*} . \quad (3.65)$$

This allows all weight window values to be calculated before histories are even started, thus saving calculation time, while retaining much of the accuracy of eqn. (3.64). Overall, this strategy results in higher figures of merit, as we demonstrate later.

Having determined the center of the weight window in each cell, we need to set limits on the width of the window, and the survival parameter:

$$ww_{cut, g, n} = (ww_{cen, g, n})(cf) , \quad (3.66)$$

$$ww_{split, g, n} = (ww_{cen, g, n})(spf) , \quad (3.67)$$

$$ww_{surv, g, n} = (ww_{cen, g, n})(survf) . \quad (3.68)$$

Typically, $cf < 1$ and $spf > 1$, although in some cases, this may not be true for optimal weight windows. In any case, $cf < survf < spf$. Thus, if a particle's weight (w) falls below $ww_{cut, g, n}$, then Russian Roulette is played, with $w/ww_{surv, g, n}$ probability of surviving. So, if $w < ww_{cut, g, n}$, then we pick ζ . If $\zeta < w/ww_{surv, g, n}$, then the particle survives, and its weight is $w = ww_{surv, g, n}$. Otherwise the particle is terminated. The maximum probability of survival is $cf/surf$. If a particle's weight exceeds $ww_{split, g, n}$, then $npas$ new particles are created:

$$npas = Int[w/(ww_{split, g, n})] , \quad (3.69a)$$

$$\text{if } (npas > n5) \text{ then } npas = n5 , \quad (3.69b)$$

where n_5 is a parameter chosen by the user. Each particle's weight is then $w/(npas + 1)$. The new particles are stored, and run after the parent particle is terminated. Note that a particle should never be allowed to travel more than about one mean free path before its weight is checked. Otherwise, the ratio of actual weight to expected weight can become too large or too small. If the ratio becomes too large, then excessive splitting occurs when the weight is checked. If the ratio becomes too small, then time is wasted following unimportant particles. Our Monte Carlo cells are about one mean free path thick, as measured by the energy group with the shortest mean free path. Thus, in some groups, weight is checked several times per mean free path.

Now that we have described how to transport particles throughout the system, let us look at keeping score (tally accumulation). Tallying absorption in the internal detector is fairly simple. The scalar flux in a group is defined by:

$$\phi_g(r) = v_g n_g(r) , \quad (3.70)$$

where $n_g(r)$ is the number of particles in a unit volume, and v_g is the speed of the particles. Now, since $v_g n_g(r) dt dr$ is equal to the total track length traversed in dt by all particles, then $\phi_g(r)$ is the track length density per unit time. So, let $l_{g,n}^i$ be the total track length traversed by a particle in group g , in history n and region i . Then $l_{g,n}^i/V_i$ is the track length density, and:

$$\phi_{i,g} = \frac{1}{N} \sum_{n=1}^N \frac{l_{g,n}^i}{V_i} . \quad (3.71)$$

We note that time has been eliminated because the problems are time-independent.

To implement this in our method, we tally the track length inside the detector for each history, along with its average weight over each part of the track length:

$$ttl_{g,n} = \sum_{k=1}^{kt} \frac{w_{avg,g}}{V_d} s_d . \quad (3.72)$$

Where kt is the number of times a particle passes through the detector region during a history, including any daughters; $w_{g,avg}$ is the average weight of a particle over each track in group g ; V_d is the volume of the detector; and s_d is the distance travelled by the particle inside the detector. A particle's weight at any point, before a collision, is determined by:

$$w_g = w_{g,i} w_{tr,g} , \quad (3.73)$$

where $w_{g,i}$ is its initial weight before travelling to a point of collision or a cell boundary and $w_{tr,g}$ is given by eqn. (3.62). Since no collision has taken place yet, eqn. (3.62) simplifies to:

$$w_{tr,g} = e^{\rho_{g,n} \cdot (z_i - z)} . \quad (3.74)$$

Thus, the average weight over the track is:

$$w_{avg,g} = \frac{w_{g,i}}{\Delta x \Delta y \Delta z} \int_{z_i}^z \int_{y_i}^y \int_{x_i}^x e^{\rho_{x,g,n}(x_i - x')} e^{\rho_{y,g,n}(y_i - y')} e^{\rho_{z,g,n}(z_i - z')} dx' dy' dz' , \quad (3.75)$$

giving:

$$\begin{aligned} w_{avg,g} & \quad (3.76) \\ &= \frac{1}{\rho_{x,g,n} \rho_{y,g,n} \rho_{z,g,n}} \frac{w_{g,i}}{\Delta x \Delta y \Delta z} \left(1 - e^{-\rho_{x,g,n} \Delta x}\right) \left(1 - e^{-\rho_{y,g,n} \Delta y}\right) \left(1 - e^{-\rho_{z,g,n} \Delta z}\right) . \end{aligned}$$

This simplifies to $w_{avg,g} = w_{g,i}$ for analog or survival biasing Monte Carlo. The total

track length over all histories is:

$$tl_g = \sum_{n=1}^N tt l_{g,n} . \quad (3.77)$$

Finally, the flux is defined by:

$$\phi_g = \frac{tl_g}{N} , \quad (3.78)$$

which is used in the calculation of absorption:

$$R_{abs,g} = \phi_g \sigma_{a,g} V_d . \quad (3.79)$$

In order to determine the variance of the tally, we also keep track of the sum of the squares of the track lengths of each history:

$$tlsq_g = \sum_{n=1}^N (tt l_{g,n})^2 . \quad (3.80)$$

Then the variance in the flux or absorption rate is:

$$var_g = \frac{tlsq_g - \frac{tl_g^2}{N}}{N(N-1)} . \quad (3.81)$$

The estimated relative error is:

$$\epsilon_g = \frac{\sqrt{var_g}}{\phi_g} . \quad (3.82)$$

Variance and error are only one measure of the method's performance. The other important measure is the amount of cpu time that the calculation uses. Error and cpu time

can be combined into a measure of efficiency known as the “relative” Figure of Merit (*FOM*):

$$FOM = \frac{1}{\epsilon^2 T} , \quad (3.83)$$

where T is the cpu time (we have used seconds in the results section). Since the relative error is proportional to $1/\sqrt{N}$, and cpu time is proportional to N , a reliable tally should have a roughly constant *FOM*. A method that reduces error only at the expense of cpu time is not much of an improvement. The same is true for a method that runs faster, but at the expense of statistical error. An efficient variance reduction technique must reduce error and running time, or at least reduce one without significantly increasing the other. As we will see in Chapter 6, LIFT accomplishes this feat. We note that the figure of merit defined by eqn. (3.83) is not the traditional figure of merit used by many other codes. The traditional figure of merit uses the variance defined by eqn. (3.81) in place of the relative error defined by eqn. (3.82), in the denominator of eqn. (3.83). This is fine for comparing Monte Carlo methods used on the same problem, but it does not allow comparisons of the same methods used on different problems. Using the relative error takes the size of the answer, which is problem-dependent, out of the figure of merit. Thus, our definition of the figure of merit is somewhat less problem-dependent than the usual definition.

So far, we have described the techniques used in the LIFT method. The next chapter briefly describes a method called AVATAR³⁶, which is currently one of the most efficient variance reduction techniques available for shielding type problems in the production code MCNP³⁹. This is the method against which we have chosen to gauge the performance of LIFT. Also included in the next chapter, is a discussion of two techniques that we tried as attempts to improve the LIFT method.

CHAPTER 4

AVATAR AND OTHER TECHNIQUES

AVATAR³⁶ can be considered to be an earlier, simpler version of the LIFT method, involving only weight windows. The weight windows used in LIFT, which are based on adjoint scalar fluxes, are very similar to the original version of AVATAR. However, the current version of AVATAR, used in MCNP³⁹, utilizes angular information for adjoint angular fluxes, and is used in conjunction with a method called DXTRAN³⁹. We have chosen not to include DXTRAN in LIFT or in our approximation to AVATAR, because it is simply another variance reduction technique which should aid both methods equally, and would only cloud the comparison of the two techniques. Note that AVATAR without DXTRAN only involves weight windows; no other biasing is utilized.

AVATAR multiplies adjoint scalar fluxes by an angular term in order to approximate the adjoint angular flux:

$$\begin{aligned} \psi_{g,n}^*(\underline{\Omega}) &\approx \phi_{g,n}^* \frac{\lambda(\bar{\mu}_{g,n}) e^{\lambda(\bar{\mu}_{g,n})(\underline{\Omega} \cdot \underline{u}_{g,n})}}{2 \sinh \lambda(\bar{\mu}_{g,n})} \\ &= \phi_{g,n}^* \frac{\lambda(\bar{\mu}_{g,n})}{e^{\lambda(\bar{\mu}_{g,n})(1 - \underline{\Omega} \cdot \underline{u}_{g,n})} - e^{-\lambda(\bar{\mu}_{g,n})(1 + \underline{\Omega} \cdot \underline{u}_{g,n})}} \end{aligned} \quad (4.1)$$

where

$$\bar{\mu}_{g,n} = \frac{|J_{g,n}^*|}{\phi_{g,n}^*} \quad (4.2)$$

is the average cosine of the adjoint flux, and:

$$\underline{n}_{g,n} = \frac{\underline{J}_{g,n}^*}{|\underline{J}_{g,n}^*|} \quad (4.3)$$

is a unit vector in the direction of the cell-average net current. For $\bar{\mu}_{g,n} < 0.8001$ we have:

$$\lambda(\bar{\mu}_{g,n}) = \frac{2.99821\bar{\mu}_{g,n} - 2.2669248\bar{\mu}_{g,n}^2}{1 - 0.769332\bar{\mu}_{g,n} - 0.519928\bar{\mu}_{g,n}^2 + 0.2691594\bar{\mu}_{g,n}^3}, \quad (4.4)$$

and for $\bar{\mu}_{g,n} \geq 0.8001$ we have:

$$\lambda(\bar{\mu}_{g,n}) = \frac{1}{1 - \bar{\mu}_{g,n}}. \quad (4.5)$$

This method, proposed by J. E. Morel at Los Alamos National Laboratory, is based on the maximum entropy distribution, preserving the first two moments of the angular flux³⁶.

The resulting expression for $\psi_{g,n}^*$ is then used in eqn. (3.64), and the same procedures for LIFT weight windows are then followed. For computational stability, the restriction:

$$\lambda(\bar{\mu}_{g,n})(1 - \underline{\Omega} \cdot \underline{n}_{g,n}) \leq 11, \quad (4.6)$$

is applied. Each time this is required, eqn. (4.6) is solved for $\lambda(\bar{\mu}_{g,n})$, which is then used in eqn. (4.1).

Generalized Rejection Sampling

One of the most inefficient aspects of the LIFT method is the selection of a new trajectory after collision, using the rejection technique (see Chapter 3). One attempt to address this problem involved testing a generalized rejection scheme⁴⁴ as an alternative to

simple rejection. To demonstrate, let us consider the 1-D, mono-energetic version of eqn. (3.52):

$$p_{\mu' \rightarrow \mu} = \frac{1 + 3\bar{\mu}\mu'\mu}{2\Gamma(\mu')[\sigma_t - L\rho\mu]} , \quad (4.7)$$

where

$$\Gamma(\mu') = \left[\frac{1}{2L\rho} + \frac{3\bar{\mu}\mu'}{2L\rho\lambda} \right] \ln\left(\frac{1+\lambda}{1-\lambda}\right) - \frac{3\bar{\mu}\mu'}{L\rho} . \quad (4.8)$$

We recall that $\rho = \sigma_t\lambda$. Now eqn. (4.7) can be rewritten as:

$$p_{\mu' \rightarrow \mu} = g(\mu)f(\mu, \mu') , \quad (4.9)$$

with

$$g(\mu) = \frac{N}{\sigma_t - L\rho\mu} , \quad (4.10)$$

and

$$f(\mu, \mu') = \frac{1 + 3\bar{\mu}\mu'\mu}{2\Gamma(\mu')N} , \quad (4.11)$$

where N is a normalization factor that makes $g(\mu)$ a probability distribution function. We sample μ explicitly from $g(\mu)$. At this value of μ , we sample uniformly from 0 to $Ag(\mu)$, where A is chosen to insure that $g(\mu) \geq p_{\mu' \rightarrow \mu}$. In other words $A \geq f(\mu, \mu')_{\max}$. If the sampled value is less than $p_{\mu' \rightarrow \mu}$, then μ is accepted. If not, then μ is rejected, and resampled from $g(\mu)$. As a proof of the method, we see that the above technique gives the probability of picking μ to be:

$$g(\mu) \left[\frac{p_{\mu' \rightarrow \mu}}{g(u)} \right] = p_{\mu' \rightarrow \mu} . \quad (4.12)$$

This method significantly reduced the number of random numbers required, compared to simple rejection. However, our code utilizes an efficient two line random number generator, so the added computational time exceeded the reduced random number generator time, resulting in lower overall efficiency. If a more sophisticated, and usually more cpu intensive, random number generator is used, then the generalized rejection method may result in an overall increase in efficiency.

Linear Adjoint Solution Approximation For $c=1$

So far, we have analyzed problems in which the forward and adjoint solutions are exponential. This is fine for scattering ratios (c) less than unity. But what happens when the scattering ratio is approximately equal to unity? Experiments show that as $c \rightarrow 1$, the LIFT method, as described up to this point, begins to lose its advantage over survival biasing. Figures of merit increase as $c \rightarrow 1$, but the acceleration of the method compared to survival biasing becomes negligible. We believe that this is due to the fact that as $c \rightarrow 1$, $\rho \rightarrow 0$. So, as the scattering ratio approaches unity, the amount of biasing in LIFT decreases to zero. However, another contributing factor to LIFT's reduced advantage may be due to the fact that the forward and adjoint angular fluxes vary linearly in space rather than exponentially at $c \approx 1$. To demonstrate this, consider the 1-D, monoenergetic, isotropic equivalent of eqn. (3.4), without normalization, or information from ϕ^* :

$$\psi^*(x, \mu) = \frac{\sigma_{s0} e^{\rho x}}{2(\sigma_t - \rho \mu)} . \quad (4.13)$$

This was the result of the specific problems that we chose to solve. However, in general,

the following form should be used:

$$\psi_{\pm}^*(x, \mu) = \frac{\sigma_{s0} e^{\pm \rho x}}{2(\sigma_r \mp \rho \mu)} . \quad (4.14)$$

As $c \rightarrow 1$, the dispersion law

$$\int_{-1}^1 \frac{\sigma_{s0}}{2(\sigma_r - \rho \mu)} d\mu = 1 \quad (4.15)$$

becomes,

$$\int_{-1}^1 \frac{1}{1 - \lambda \mu} d\mu = 2 . \quad (4.16)$$

Thus we see that λ must approach zero as $c \rightarrow 1$. So let us set λ equal to some small number (ϵ) in eqn. (4.14) for $c \rightarrow 1$. We obtain:

$$\begin{aligned} \psi_{\pm}^*(x, \mu) &\rightarrow \frac{e^{\pm \epsilon \sigma_r x}}{2(1 \mp \epsilon \mu)} \approx \frac{1}{2}(1 \pm \epsilon \sigma_r x)(1 \pm \epsilon \mu) \approx \frac{1}{2}(1 \pm \epsilon \sigma_r x \pm \epsilon \mu) \\ &= \frac{1}{2}[1 \pm \epsilon(\sigma_r x + \mu)] , \end{aligned} \quad (4.17)$$

giving two independent solutions:

$$\psi_{+}^* + \psi_{-}^* = 1 , \quad (4.18)$$

and

$$\psi_{+}^* - \psi_{-}^* = \epsilon(\sigma_r x + \mu) . \quad (4.19)$$

Thus, we have a linear combination:

$$\psi^*(x, \mu) = a^* + b^*(\sigma_t x + \mu) . \quad (4.20)$$

One might expect that using eqn. (4.20) would help in problems where $c \approx 1$. However, algebraic difficulties arise when eqn. (4.20) is used in the LIFT method. To see why, consider the 1-D, monoenergetic version of the effective total cross section in eqn. (2.12):

$$\Sigma_t(x, \mu) = \sigma_t - \frac{\mu}{\psi^*(x, \mu)} \frac{d}{dx} \psi^*(x, \mu) . \quad (4.21)$$

When ψ^* was approximated as an exponential, Σ_t was not a function of x :

$$\Sigma_t(\mu) = \sigma_t - \rho \mu . \quad (4.22)$$

Now, with ψ^* approximated as a linear function, Σ_t is a function of x :

$$\Sigma_t(x, \mu) = \sigma_t - \frac{\mu(b^* \sigma_t)}{a^* + b^*(\sigma_t x + \mu)} . \quad (4.23)$$

Thus, the distance to collision varies continuously with position. This causes a significant increase in algebra. This difficulty, in addition to others, resulted in a large decrease in efficiency. In the end, using the more accurate representation of the angular flux for $c \approx 1$ did not result in increased figures of merit. The reason was that the extra algebra caused by the space-dependent total cross section in eqn. (4.23) more than cancelled out the slight gain in accuracy of the representation of the adjoint angular flux. The lesson to be drawn from this is that *for the LIFT method to be efficient, it is not enough that the representation for the adjoint angular flux be accurate. The representation of the adjoint angular flux must also lead to an algebraically simple scheme for sampling the distance to collision.*

CHAPTER 5

DETERMINISTIC METHODS

Solving transport problems, such as those defined by eqs. (2.1) or (2.3), is generally difficult. Writing all of the 3-D deterministic algorithms used to obtain the numerical input for the LIFT method would make completion of this thesis nearly impossible. Fortunately, the LIFT method is able to use off-the-shelf software for performing the adjoint calculations. Until recently, even production-quality deterministic transport codes did not offer complete and reliable treatments of problems in 3-D. Many of the authors in the references of Chapter 1 were forced to either work in 1-D, or use 1-D adjoint solvers to patch together 3-D approximations. However, all of the deterministic calculations for this thesis were done with modified versions of the existing THREEDANT⁴⁰ and NIKE/ATHENA⁴¹ codes. Except for the Exponential Discontinuous⁴² method, all modifications were minor. In the Exponential Discontinuous differencing scheme, the released version of THREEDANT does not yet contain an option for selecting that method. Nonetheless, an experimental version did exist which was used in this thesis. The other modifications mostly involved output formats required by the new LIFT Monte Carlo code.

The methods described here involve two primary types of approximations; discretizations of variables, and representations of functions by truncated expansions. All of the methods use discretization of space and energy. Their handling of angular dependence is what really sets them apart. The discrete ordinates (S_N) methods discretize the angular variable and require particles to follow a limited set of trajectory paths. The spherical harmonics (P_N) methods approximate angular functions by expanding them into a linear combination of spherical harmonic functions. Diffusion methods approximate the

angular flux by a linear combination of the zeroth and first order spherical harmonics, thus setting all higher order terms of the expansion to zero. SP_N methods are an approximation to P_N methods. The rest of this chapter will briefly describe these methods in a little more detail, and discuss the advantages and disadvantages of each. An important feature of the LIFT method is that it works regardless of the method chosen for calculating the adjoint solution, as long as the calculations are done with reasonable accuracy.

Diffusion

We begin with the simplest, and least accurate, method. Diffusion methods represent the angular flux by a two-term spherical harmonics expansion:

$$\psi_g(r, \underline{\Omega}) \approx \frac{1}{4\pi} [\phi_g(r) + 3 \underline{\Omega} \cdot \underline{J}_g(r)] . \quad (5.1)$$

This simple representation allows one to solve transport problems on a discretized spatial grid very quickly. Unfortunately, except for large homogeneous systems with high scattering ratios, this method is fairly inaccurate. Diffusion is especially inaccurate near boundaries and sources. Speed is the primary advantage of diffusion. All of the transport problems in this thesis were solved by diffusion in less than 10 seconds on a Cray-YMP. The other methods required on the order of 100 or a 1000 seconds, depending on the problem.

All diffusion calculations for the LIFT method involved adjustments to the diffusion constant to increase their accuracy for deep penetration. We have shown, in Chapter 3, that the spatial component of the adjoint angular flux can have the following form in 1-D:

$$\psi_g^*(x) \approx e^{\lambda_{0,g} \sigma_{t,g} x} , \quad (5.2)$$

where $\lambda_{0,g}$ is the eigenvalue of eqn. (3.10). To retain some of this information, we set the analytical representation of the diffusion scalar flux equal to eqn. (5.2):

$$\phi_g^*(x) \approx e^{x\sqrt{\sigma_{a,g}/D_g}} = e^{\lambda_{0,g}\sigma_{t,g}x}, \quad (5.3)$$

resulting the modified diffusion coefficient:

$$D_g = \frac{\sigma_{a,g}}{(\lambda_{0,g}\sigma_{t,g})^2}. \quad (5.4)$$

Other than the above modification, the only other alteration of the off-the-shelf version of THREEEANT was a change in the output of the scalar fluxes. LIFT requires either cell-edge, or cell-vertex fluxes, in addition to the cell-average fluxes output by the unmodified version. Cell-edge fluxes are required for calculating the biasing parameters in eqs. (3.22), while cell-average fluxes are required in the approximation of the adjoint angular flux, given by eqn. (3.4). Cell-edge fluxes are obtained simply by averaging the two vertex fluxes defining each edge of a cell.

Spherical Harmonics

We now consider methods that can be very accurate, but that can also be very costly. P_N methods involve the following expansion of the angular flux into a linear combination of spherical harmonic functions:

$$\psi_g(r, \underline{\Omega}) \approx \sum_{l=0}^N \sum_{m=-l}^l f_{lmg}(r) Y_{lm}(\underline{\Omega}). \quad (5.2)$$

The user must decide, for each problem, where to truncate the expansion (the N in P_N). Spherical harmonics methods, due to their rotational symmetry, do not suffer from the “ray effects” associated with discrete ordinates methods, which is discussed in the next

section. The primary disadvantage of the P_N method is the expense of the calculation, which is due to the large number of unknowns and the complicated structure of the equations. The Simplified P_N method reduces the expense of the calculation while remaining significantly more accurate than diffusion⁴¹. The simplification consists of the creation of 3-D SP_N equations from 1-D P_N equations by replacing the partial derivatives in the 1-D equations by divergence and gradient operators. The following equations, which demonstrate the simplification, are from reference 41, and thus are not specifically related to eqs. (2.1) or (2.3). One writes down the planar-geometry P_N equations:

$$\frac{n+1}{2n+1} \cdot \frac{\partial \phi_{n+1}}{\partial z} + \frac{n}{2n+1} \cdot \frac{\partial \phi_{n-1}}{\partial z} + (\sigma_t - \sigma_n) \phi_n = q_n \quad (n = 0, N) . \quad (5.5)$$

For n odd, one replaces ϕ_n by $\underline{\phi}_n$, and $\partial \phi_n / \partial z$ by $\underline{\nabla} \cdot \underline{\phi}_n$; for n even, one replaces $\partial \phi_n / \partial z$ by $\underline{\nabla} \phi_n$. The result is the SP_N equations:

$$\frac{n+1}{2n+1} \underline{\nabla} \cdot \underline{\phi}_{n+1} + \frac{n}{2n+1} \underline{\nabla} \cdot \underline{\phi}_{n-1} + (\sigma_t - \sigma_n) \phi_n = q_n \quad (n = 0, 2, N-1) , \quad (5.6)$$

$$\frac{n+1}{2n+1} \underline{\nabla} \phi_{n+1} + \frac{n}{2n+1} \underline{\nabla} \phi_{n-1} + (\sigma_t - \sigma_n) \underline{\phi}_n = \underline{q}_n \quad (n = 1, 3, N) . \quad (5.7)$$

This derivation, credited to Gelbard⁴⁵, is mathematically dubious. However, it has been shown that the SP_N equations are an asymptotic approximation of the transport equation in the classical diffusion limit, and can be restated in such a way as to allow solution by standard diffusion methods⁴⁶⁻⁴⁸.

In one respect, the SP_N calculations were obtained from an off-the-shelf code (NIKE/ATHENA⁴¹). However, NIKE/ATHENA is not exactly on the shelf yet. It is still being developed, with certain features, such as downscatter, being added as needed for this thesis. However, no modifications by the code developers were made specifically for use with LIFT. The released version of NIKE/ATHENA will probably be capable of

providing input for LIFT without modification.

Discrete Ordinates

Discrete ordinates (S_N) methods require neutrons to travel along a discrete set of trajectories $\underline{\Omega}_m$, ($m = 1, N$). Each trajectory is weighted by w_m , a section of the unit sphere. Thus, integration of angular variables is handled as follows:

$$\phi_g(r) = \int_{4\pi} \psi_g(r, \underline{\Omega}) d\Omega \approx \sum_{m=1}^N \psi_g(r, \underline{\Omega}_m) w_m . \quad (5.8)$$

The sum of the weights cover the unit sphere:

$$\sum_{m=1}^N w_m = 4\pi . \quad (5.9)$$

Together, $\underline{\Omega}_m$ and w_m are known as a quadrature set. The S_N solutions should converge to the true transport solution as the order of the quadrature set goes to infinity. Thus, the S_N equations are capable of great accuracy, given enough time. However, due to the peculiarities of the angular discretization, S_N methods suffer from two phenomenon known as “ray effects” and “non-streaming effects”.

Ray effects are unphysical oscillations in the scalar flux distribution, and are most prevalent in problems with low scattering ratios (high absorption), and deep penetration. They are caused by the inability of a finite quadrature set to accurately propagate particles far away from a source. As N increases, the oscillations increase in frequency and decrease in amplitude. In addition, the oscillations usually occur around the true solution; thus integrated quantities are often (but not always) fairly accurate. In fact, this quality makes spatially-integrated S_N calculations more accurate than P_{N-1} calculations for some problems. However, in other problems, the oscillations may not occur around the true solution. Users must learn through experience when to trust answers produced by S_N

methods (and most other methods as well). The ray effects can sometimes be offset somewhat by the truncation errors in the spatial differencing scheme.

Non-streaming effects cause a smooth solution to be produced instead of a physically-correct peaked solution, due to the method's inability to model streaming through narrow voids. (The S_N method does not accurately model strong angular dependence.) Thus, real angular peaks in a solution, caused by uncollided particles, are often grossly underestimated. It is helpful for one to know whether or not a solution will have oscillations, before running a S_N calculation. Otherwise, the lack of (or presence of) oscillations in the solution may be unduly comforting. Unfortunately, complicated geometries and complicated sources make such foreknowledge difficult.

Three different types of spatial discretizations are utilized in the S_N calculations performed in this thesis. Discretization of the transport equation results in more unknowns than equations. The standard "closure" technique to account for this utilizes diamond differencing, which represents cell-centered fluxes as an average of the cell-edge fluxes, to complete the system of equations:

$$\psi_{g,m,i,j,k} = \frac{1}{2}(\psi_{g,m,i+1/2,j,k} + \psi_{g,m,i-1/2,j,k}) , \quad (5.10a)$$

$$\psi_{g,m,i,j,k} = \frac{1}{2}(\psi_{g,m,i,j+1/2,k} + \psi_{g,m,i,j-1/2,k}) , \quad (5.10b)$$

$$\psi_{g,m,i,j,k} = \frac{1}{2}(\psi_{g,m,i,j,k+1/2} + \psi_{g,m,i,j,k-1/2}) , \quad (5.10c)$$

$$\psi_{g,m,i,j,k} = \frac{1}{2}(\psi_{g,m+1/2,i,j,k} + \psi_{g,m-1/2,i,j,k}) . \quad (5.10d)$$

The problem with this method is that the resulting edge fluxes can extrapolate to negative values, requiring a fixup. The fixup sets the negative values to zero, and recalculates with this forced condition.

An alternative technique, selected as an option in THREEEDANT for use in this thesis, involves a weighting scheme with a predictor corrector method determining the weights that produce positive edge fluxes. This technique is known as Adaptive Weighted Diamond Differencing (AWDD)⁴⁰. As an example, eqn. (5.10a) would become:

(5.11a)

$$(1 + P_{x,g,m,i,j,k})\psi_{g,m,i,j,k} = \frac{1}{2}(\psi_{g,m,i+1/2,j,k} + P_{x,g,m,i,j,k}\psi_{g,m,i-1/2,j,k}) ,$$

for $\mu_m > 0$, and

(5.11b)

$$(1 + P_{x,g,m,i,j,k})\psi_{g,m,i,j,k} = \frac{1}{2}(P_{x,g,m,i,j,k}\psi_{g,m,i+1/2,j,k} + \psi_{g,m,i-1/2,j,k}) ,$$

for $\mu_m < 0$. The absolute value of the weighting parameter P , is always less than or equal to unity, and always begins equal to unity, corresponding to regular diamond differencing. After the cell-edge fluxes are obtained, they are tested for positivity. If any are negative, the weights are recalculated based on the information just obtained, and the calculations are repeated. Monotonicity can be imposed to spatially smooth the solution. The amount of smoothness and the corresponding reduction of accuracy are controlled by a group-dependent input parameter called WDAMP. If WDAMP is zero, then standard diamond differencing is used. If WDAMP is set to its maximum value of 4, then oscillations are heavily damped. For this thesis, the optimal value of WDAMP appeared to be 2, but the effect was not very significant (meaning that the figures of merit in the Monte Carlo calculations that used input from THREEEDANT⁴⁰ did not vary much as a function of WDAMP).

The third technique used in this thesis, for obtaining the additional spatial discretization equations, was the Exponential Discontinuous method⁴². This was chosen for its use of an approximation to the angular flux that is very similar to the approximation used by the LIFT method. Thus parameters used in both analytical forms of the

approximation, calculated by the Exponential Discontinuous algorithm, could be used almost directly in the LIFT algorithm. The spatial form of the one group adjoint angular flux in the n^{th} cell, for the Exponential Discontinuous method is:

$$\psi_{m,n}^*(r) \approx A_{m,n} e^{2\lambda_{x,m,n}(x-x_i)/\Delta x_n + 2\lambda_{y,m,n}(y-y_j)/\Delta y_n + 2\lambda_{z,m,n}(z-z_k)/\Delta z_n}, \quad (5.12)$$

with

$$A_{m,n} = \frac{\phi_{m,n}^* \lambda_{x,m,n} \lambda_{y,m,n} \lambda_{z,m,n}}{\sinh(\lambda_{x,m,n}) \sinh(\lambda_{y,m,n}) \sinh(\lambda_{z,m,n})}. \quad (5.12a)$$

The spatial part of the adjoint angular flux in the LIFT method is:

$$\psi_n^*(r) \approx \beta_n e^{\lambda_{x,n}(x-x_i) + \lambda_{y,n}(y-y_j) + \lambda_{z,n}(z-z_k)}, \quad (5.13)$$

with

$$\beta_n = \frac{\phi_n^* \lambda_{x,n} \lambda_{y,n} \lambda_{z,n}}{\sinh(\lambda_{x,n}) \sinh(\lambda_{y,n}) \sinh(\lambda_{z,n})}. \quad (5.13a)$$

The simplest way to utilize the scalar flux and decay constants from the Exponential Discontinuous method is to have the algorithm integrate them over angle. They can then be used almost directly in the LIFT method. Alternatively, the LIFT method could be altered to work in a discrete ordinates Monte Carlo simulation, thus utilizing more of the information from the Exponential Discontinuous calculation. The former technique is used in this thesis, the latter is suggested for future work. This method is very promising, because it has been shown that the Exponential Discontinuous method is far more accurate than the diamond differencing methods for many deep penetration problems⁴².

As mentioned at the beginning of this chapter, the Exponential Discontinuous

method is not yet a part of the released version of THREEDANT. Other than that, the only modifications made to THREEDANT for use with LIFT, was a change in the output of scalar fluxes; the cell-vertex scalar fluxes had to be saved rather than discarded, so that they could be output to a file.

CHAPTER 6

RESULTS AND COMPARISONS

We present here the results of applying the LIFT method to a set of problems. The results are compared to those obtained from applying survival biasing and AVATAR³⁶ weight windows to the same set of problems. All results were obtained from a code that was written specifically for this thesis, rather than from a modified production code. For each problem, up to 11 variations of the Monte Carlo variance reduction techniques discussed in this thesis were tried.

Eight of the methods tested are variations of the LIFT method that utilize the approximation of the angular flux given by eqn. (3.4) to approximate the zero variance solution. The variations of the LIFT method are due to the type of deterministic method used to obtain the scalar fluxes used in eqn. (3.4), and to the type of weight window used. There are four deterministic methods, and three weight window methods. The deterministic methods include diffusion, S_N with Adaptive Weighted Diamond Differencing⁴⁰, S_N with Exponential Discontinuous⁴² spatial differencing, and SP_N . The weight window methods include those described by eqs. (3.64) and (3.65), which utilize angular and scalar fluxes respectively, and the AVATAR style of weight windows discussed in Chapter 4.

The other three methods tested were analog Monte Carlo with survival biasing, and two variations of the AVATAR method of weight windows. The first variation is simply the same weight window used in LIFT, defined by eqn. (3.65). The second variation utilizes currents from the deterministic calculation to make the weight windows angularly-dependent, and is similar to the LIFT weight windows defined by eqn. (3.64), but with a different analytical expression for the approximation of the angular flux.

The following acronyms denote the methods used in the results sections:

SB:	Analog Monte Carlo with Survival Biasing
LIFT/D/PHI:	The Local Importance Function Transform and scalar flux-based weight windows, both using scalar flux input from a diffusion calculation.
LIFT/SN/PHI:	The Local Importance Function Transform and scalar flux-based weight windows, both using scalar flux input from a S_N calculation with Adaptive Weighted Diamond Differencing ⁴⁰ .
LIFT/SNED/PHI:	The Local Importance Function Transform and scalar flux-based weight windows, both using scalar flux input from a S_N calculation with Exponential Discontinuous ⁴² spatial differencing.
LIFT/SPN/PHI:	The Local Importance Function Transform and scalar flux-based weight windows, both using scalar flux input from a SP_N calculation.
AV/D/PHI:	The AVATAR method of weight windows using scalar flux input from a diffusion calculation.
AV/SN/PSI:	The AVATAR method of weight windows using scalar flux and currents from a S_N calculation with Adaptive Weighted Diamond Differencing.
LIFT/AV/SN/PSI:	The Local Importance Function Transform with the AVATAR method of weight windows, using scalar flux and currents from a S_N calculation with Adaptive Weighted Diamond Differencing.
LIFT/SN/PSI:	The Local Importance Function Transform and angular flux-based weight windows, both using scalar flux input from a S_N calculation with Adaptive Weighted Diamond Differencing.
LIFT/SPN/PSI:	The Local Importance Function Transform and angular flux-based weight windows, both using scalar flux input from a SP_N calculation.
LIFT/SN/PSI-E:	The Local Importance Function Transform and angular flux-based weight windows minus exponential terms, both using scalar flux input from a S_N calculation with Adaptive Weighted Diamond Differencing.

We note that all of the results presented in this thesis represent the best that can be obtained from the methods tested. By that, we mean that each parameter of each method was optimized by trial and error. As mentioned in the introduction, no variance reduction technique devised so far escapes the fate of requiring user experience or trial and error for optimal results. The goal that we believe we have reached, is the development of a method (LIFT) that can either outperform other methods even when it is unoptimized, or at least match their best performance when it is used as a “black box”. The results demonstrate the advantages of “black box”-LIFT over AVATAR weight windows, and the gains that can be achieved by a little optimization. Optimization of the LIFT method involves trial and error adjustment of f_4 in eqn. (3.18), and the weight window parameters (cf , spf , $survf$, $n5$) in eqs. (3.66), through (3.69). Optimization of the AVATAR method involves trial and error adjustment of the weight window parameters. The deterministic methods were also optimized by refining the differencing (space and angle, where applicable), or increasing the order of the expansions, until the scalar flux point furthest from the source and the peak scalar flux no longer changed significantly. Refining beyond this point should only increase the calculation time.

One Group Homogeneous Problems

The system for this group of problems is a 15 x 15 x 15 cm cube. The cube is uniformly divided into 15 x 15 x 15 Monte Carlo cells (so each cell has dimensions equal to one cm = one mean free path). The number of cells used for the deterministic calculations varies with the method. Scattering is always linearly anisotropic, with $\bar{\mu} = 0.2$. The total cross section is always 1 cm^{-1} , and the absorption and scattering cross sections vary in order to create four problems with different scattering ratios. The scattering ratios used were 0.9, 0.7, 0.5, and 0.3. All sources are uniform, isotropic, and located between $x = y = z = 2.0 \text{ cm}$ and $x = y = z = 3.0 \text{ cm}$. The flux is tallied for each problem by a track length flux detector located between $x = y = z = 12.0 \text{ cm}$ and

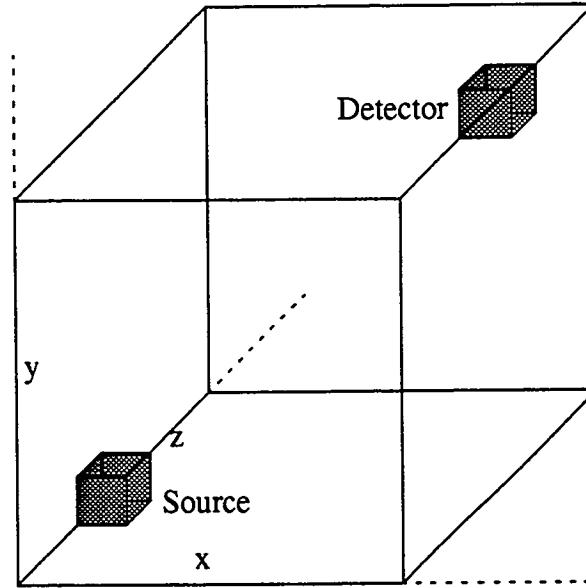


Figure 6.1: Source-Detector Arrangement

$x = y = z = 13.0$ cm. The flux obtained from the tally is used to determine the absorption rate in that cell. Figure 6.1 depicts the arrangement of the source (near the lower left corner) and detector (near the upper right corner). (Neither the source nor the detector touch any sides of the system, although this 2-D drawing may make it appear that way.)

The diffusion calculation was carried out by setting the number of iterations to unity in the S_N code THREEDANT⁴⁰. Each Monte Carlo cell was divided into $3 \times 3 \times 3$ cells, resulting in a $45 \times 45 \times 45$ cell calculation. Thus, each cell had dimensions equal to one third of a mean free path. Throughout this thesis, fine-grid data from deterministic calculations were run through a filter to select the coarse-grid values used on the Monte Carlo grid. The only place where fine grid data are used directly, is in the determination of weight windows. When particle weight is checked, the comparison between its weight and the weight window limits determined by eqs. (3.64) through (3.68), is done using fine grid data.

The S_N calculation was carried out by THREEDANT. Each Monte Carlo cell was divided into $2 \times 2 \times 2$ cells, resulting in a $30 \times 30 \times 30$ cell calculation. Thus, each cell had dimensions equal to one half of a mean free path. We used the rectangular Chebychev-Legendre quadrature set of order $N=8$. The rectangular Chebychev-Legendre set was chosen because it produced slightly better results than the default set. WDAMP, the damping factor for the Adaptive Weighted Diamond Differencing⁴⁰ method, was set to 2.0 for problems with scattering ratios of 0.7, 0.5, and 0.3. WDAMP was not used in the problem with a scattering ratio of 0.9.

The Exponential Discontinuous calculation was carried out by a modified version of THREEDANT. One advantage of this method, is that it allows the use of coarser discretization compared to standard S_N . Thus, we were allowed to use the same cells as the Monte Carlo calculation, which had dimensions equal to one mean free path. We were also able to use a lower quadrature-set order, $N=6$. This helped mitigate the extra time required by the Exponential Discontinuous method. The rectangular Chebychev-Legendre quadrature set was also used here.

The SP_N calculation was carried out by the NIKE/ATHENA⁴¹ code. The only reasonable choices for dividing the Monte Carlo cells up into tetrahedrons (tets), required by the code, were to use 6 tets per cell or 24 tets per cell. The 6 tets per cell option left out 2 cell vertices due to the way tets were defined for this option. Thus, we were forced to use 24 tets per cell, resulting in 81000 total tets. Fortunately, the code is very efficient, with run times between standard THREEDANT and the Exponential Discontinuous method. In several cases, after correcting for the difference in hardware, the SP_N calculation took less time than the more coarsely differenced S_N calculation. The order of the calculation was $N=7$ (specified by $N=8$ in the code input).

Each Monte Carlo run, except survival biasing, was carried out for 100,000 histories. The survival biasing runs required more histories. All but one took up to the limit of the random number generator to even approach statistically meaningful tallies.

The survival biasing problem with a scattering ratio of 0.9 was carried out for 1,000,000 histories, while each of the other problems were carried out for 8,000,000 histories. The random number generator used in this thesis was taken from EGS4⁴⁹, another Monte Carlo code. It was chosen for its simplicity and efficiency, while being known as a “reliable” random number generator. Use of this generator only requires two program lines, and thus can be inserted where needed, rather than called from a subroutine:

$$iseed = iseed \times 663608941 \quad (6.1a)$$

$$\zeta = 0.5 + iseed \times 0.23283064^{-9} . \quad (6.1b)$$

The period for this generator is 10^9 . A more sophisticated, and thus more expensive, random number generator with a longer period could have been used. However, obtaining trustworthy answers from survival biasing would have required an inordinate amount of computing time.

In all methods with weight windows (every method except survival biasing), the parameter $n5$, which controls the number of splits allowed per encounter with a weight window, was set to 4. This limited the number of particles that could be created in a single split to 5 (4 daughters and one parent). Table 6.1 provides the parameters used to control weight windows and the LIFT biasing, along with the effects of each parameter, for the problem with a scattering ratio of 0.9. Table 6.2 provides the cpu times, statistical errors, and “relative” figures of merit [see eqn. (3.83)] for the calculations. Tables 6.3 and 6.4 are for the problem with a scattering ratio of 0.7. Likewise, Tables 6.5 and 6.6 apply to $c = 0.5$, and Tables 6.7 and 6.8 apply to $c = 0.3$. Blanks in the tables indicate that either the variable is not applicable to the method, or the method was not used for that problem (in particular, the last three methods of each table were not tried on every problem). The following list provides meanings for each of the variables used in the tables.

<i>f4:</i>	The weighting factor in eqn. (3.18), that affects the maximum magnitude of the LIFT biasing parameter $P_{g,n}$. When set to zero, the maximum is controlled by the eigenvalue in eqn. (3.17), and when set to unity, the maximum is controlled by the total cross section, which the biasing parameter can never exceed.
<i>nadjust:</i>	The number of adjustments to the LIFT biasing parameter as a result of restricting the deterministically calculated values to the maximum allowed by parameter <i>f4</i> . The maximum number is the number of cells times the number of groups (3375 for 1-group, 16875 for 5-group).
<i>cf:</i>	The factor applied to the center value of the weight window, determining the weight at which particles will undergo Russian Roulette. See eqn. (3.66).
<i>spf:</i>	The factor applied to the center value of the weight window, determining the weight at which particles will be split. See eqn. (3.67).
<i>sur:</i>	The factor applied to the center value of the weight window, affecting the probability of survival in the Russian Roulette game. See eqn. (3.68).
<i>spl:</i>	The total number of daughters created by splitting particles. This number plus the original number of histories, is the total number of particles followed.
<i>cut:</i>	The total number of particles that did not survive Russian Roulette.
<i>D-time:</i>	The cpu time in seconds required by the deterministic method used for a given problem. All deterministic methods except SP_N were calculated on a Cray-YMP. The SP_N calculations were done on a Sun SPARCstation 20. As a rough guess, based on some experience with a wide variety of hardware, the SP_N time are cut in half to make up for the platform difference. The NIKE/ATHENA code has been designed for a parallel machine, allowing for the possibility of even less expensive SP_N calculations.
<i>MC-time:</i>	The cpu time in seconds required by the Monte Carlo code for running histories. All Monte Carlo runs for one group problems were done on a Sun SPARCstation 20. Multigroup problems utilized an IBM RISC6000/590 (about 4 times faster than a Sun SPARCstation 20). This is

the time used in the “relative” figure of merit, since it is the only time that provides a constant and meaningful figure of merit. Including *D-time* or Monte Carlo overhead time, would make the figure of merit a function of the number of histories.

Err %: The relative statistical error, given by eqn. (3.82), converted to a percentage.

FOM-W: The worst “relative” figure of merit encountered during the optimization trials. See the next definition for a description of figure of merit. This is not the worst figure of merit possible, since really bad choices of weight window parameters could make it even smaller. The optimization procedure consisted of starting with reasonable choices for all parameters, such as those which one might choose for default values, and adjusting them from there. Also, the trials were done with a factor of 10 less histories, so these figures of merit are not as reliable as the optimal ones.

FOM-O: The optimal “relative” figure of merit achieved through trial and error adjustments of parameters. The standard by which the methods are compared. The “relative” figure of merit is a measure of efficiency, as described in eqn. (3.83). The higher this number is, the better the method. For example, increasing the *FOM* by a factor of two means that the same statistical accuracy was achieved in half the cpu time, or the statistical error was reduced by the square root of two in the same amount of cpu time. This is not the traditional figure of merit, which is based on the variance. As discussed in Chapter 3, eqn. (3.83) is based on the relative error, and thus can be used to compare a method across a variety of problems.

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0.6	1860	0.05	5.5	0.15	102658	152467
LIFT/SN/PHI	0.5	1350	0.01	1.5	0.03	196931	187491
LIFT/SNED/PHI	0.5	1581	0.01	1.5	0.03	254917	236646
LIFT/SPN/PHI	0.5	1650	0.01	2.0	0.03	165898	173762
AV/D/PHI	-	-	0.1	0.5	0.2	3198863	2804040
AV/SN/PSI	-	-	0.1	0.5	0.15	1506087	1546080
LIFT/AV/SN/PSI	0.6	965	0.05	1.0	0.1	103381	167283
LIFT/SN/PSI	0.5	1350	0.1	1.5	0.3	92712	141661
LIFT/SPN/PSI	0.5	1650	0.1	1.5	0.3	98321	150254
LIFT/SN/PSI-E	0.5	1350	0.1	1.5	0.3	115063	160492

Table 6.1: Monte Carlo Parameters and Effects for $c = 0.9$

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	2101	21.2	-	0.01
LIFT/D/PHI	7	1565	0.641	12.3	15.6
LIFT/SN/PHI	49	2518	0.477	16.7	17.5
LIFT/SNED/PHI	110	2782	0.449	16.1	17.8
LIFT/SPN/PHI	47	2185	0.576	15.7	17.4
AV/D/PHI	6	3765	0.850	3.24	3.68
AV/SN/PSI	49	1539	1.32	2.25	3.72
LIFT/AV/SN/PSI	49	1512	0.571	13.7	20.3
LIFT/SN/PSI	49	1490	0.624	14.1	17.3
LIFT/SPN/PSI	47	1544	0.632	no trials	16.2
LIFT/SN/PSI-E	49	1591	0.594	no trials	17.8

Table 6.2: Performance for $c = 0.9$

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0.4	3374	0.2	8.0	0.3	249822	309118
LIFT/SN/PHI	0.4	2658	0.01	2.0	0.03	121618	177886
LIFT/SNED/PHI	0.3	3374	0.01	2.5	0.03	116371	175642
LIFT/SPN/PHI	0.4	3374	0.05	3.0	0.1	99905	172299
AV/D/PHI	-	-	0.5	1.0	0.75	5218051	5162668
AV/SN/PSI	-	-	0.1	0.25	0.15	3487481	3565689
LIFT/AV/SN/PSI	0.6	1356	0.05	1.0	0.1	104355	187852
LIFT/SN/PSI	0.4	2658	0.1	1.5	0.15	68706	144006
LIFT/SPN/PSI	-	-	-	-	-	-	-
LIFT/SN/PSI-E	0.4	2658	0.1	1.5	0.15	95572	168157

Table 6.3: Monte Carlo Parameters and Effects for $c = 0.7$

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	17008	47.9	-	2.6e-4
LIFT/D/PHI	5	1540	0.666	6.77	14.7
LIFT/SN/PHI	36	1559	0.678	8.43	14.0
LIFT/SNED/PHI	116	1411	0.741	11.5	12.9
LIFT/SPN/PHI	50	1214	0.759	14.6	16.5
AV/D/PHI	6	1903	1.51	0.98	2.30
AV/SN/PSI	36	1352	1.53	2.85	3.15
LIFT/AV/SN/PSI	36	1299	0.670	12.4	17.1
LIFT/SN/PSI	36	1037	0.871	9.61	12.7
LIFT/SPN/PSI	-	-	-	-	-
LIFT/SN/PSI-E	36	1167	0.836	no trials	12.3

Table 6.4: Performance for $c = 0.7$

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0.2	3374	0.1	60.0	0.3	122461	203003
LIFT/SN/PHI	0.2	2917	0.01	2.0	0.03	86982	163041
LIFT/SNED/PHI	0.2	3374	0.01	2.0	0.03	168239	251746
LIFT/SPN/PHI	0.0	3374	0.05	3.0	0.1	144864	224507
AV/D/PHI	-	-	0.5	1.5	1.25	11340962	11180093
AV/SN/PSI	-	-	0.1	0.5	0.15	1463388	1557449
LIFT/AV/SN/PSI	0.2	2917	0.1	1.0	0.2	108341	202975
LIFT/SN/PSI	0.0	2987	0.5	1.5	0.75	55569	147510
LIFT/SPN/PSI	-	-	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-	-	-

Table 6.5: Monte Carlo Parameters and Effects for $c = 0.5$

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	17270	75.1	-	1.0e-4
LIFT/D/PHI	5	1107	1.38	0.54	4.77
LIFT/SN/PHI	34	1213	1.32	3.17	4.75
LIFT/SNED/PHI	120	1014	1.55	2.77	4.10
LIFT/SPN/PHI	46	1009	1.28	3.57	6.40
AV/D/PHI	6	3329	2.93	0.21	0.35
AV/SN/PSI	34	518	3.32	1.02	1.75
LIFT/AV/SN/PSI	34	787	1.22	4.08	8.57
LIFT/SN/PSI	34	537	2.05	2.77	4.43
LIFT/SPN/PSI	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-

Table 6.6: Performance for $c = 0.5$

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0	3374	0.1	60.0	0.3	798011	858799
LIFT/SN/PHI	0	2952	0.01	2.0	0.03	68571	157158
LIFT/SNED/PHI	0	3374	0.05	3.0	0.15	101052	194986
LIFT/SPN/PHI	0	3374	0.1	4.0	0.2	480499	557753
AV/D/PHI	-	-	0.5	2.0	1.25	34136959	33530389
AV/SN/PSI	-	-	0.1	0.5	0.15	1442048	1540714
LIFT/AV/SN/PSI	0	3374	0.05	1.0	0.1	137554	235062
LIFT/SN/PSI	0	3374	0.5	1.5	0.75	171466	266246
LIFT/SPN/PSI	-	-	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-	-	-

Table 6.7: Monte Carlo Parameters and Effects for $c = 0.3$

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	16711	87.9	-	7.7e-5
LIFT/D/PHI	5	7265	4.12	0.01	0.08
LIFT/SN/PHI	28	1499	3.70	0.20	0.49
LIFT/SNED/PHI	48	1027	6.11	0.12	0.26
LIFT/SPN/PHI	8	3365	3.67	no trials	0.22
AV/D/PHI	6	8174	7.72	0.006	0.02
AV/SN/PSI	28	372	7.46	no trials	0.48
LIFT/AV/SN/PSI	28	1259	3.08	no trials	0.84
LIFT/SN/PSI	28	775	4.87	no trials	0.55
LIFT/SPN/PSI	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-

Table 6.8: Performance for $c = 0.3$

From the results presented in Tables 6.1-6.8, we see that the “relative” figures of merit for survival biasing drop off rapidly as the scattering ratio (c) drops below 0.9, and the “relative” figures of merit for the LIFT and AVATAR methods drop off rapidly as the scattering ratio drops below 0.7. In both cases, some particles reach the detector region after only a few collisions, while others suffer many collisions. When the scattering ratio is high, the difference in their weights is not that significant, since each collision only reduces weight by a factor only slightly smaller than unity. However, when the scattering ratio is low (high absorption), the difference in the weights of particles can be great. For example, in survival biasing, if a particle with an initial weight equal to unity suffers 30 collisions in a problem with $c=0.9$, then its weight would be 0.0424. If $c=0.5$, then its weight would be $9.31 \cdot 10^{-10}$. Thus, the potential variance in the weight of particles arriving at the detector in problems with $c=0.9$ is much less than the potential variance in the weight of particles in problems with $c=0.5$. The Monte Carlo time per particle, for each problem should be about the same, as verified in the tables (recall that for $c=0.9$, survival biasing was only run for $1/8^{\text{th}}$ as many histories as the other problems). Higher variances, in equal calculation times, result in lower figures of merit. An additional source of error for the LIFT and AVATAR methods is the fact that deterministic methods are less accurate in highly absorbing problems. Thus, the adjoint solution required by these methods is not as accurate when the scattering ratio is low.

We note here that the traditional figure of merit, based on the variance rather than the relative error, would increase as the scattering ratio decreased. This is because the answer to the problem becomes much smaller, and only the relative error takes this into account. Thus smaller answers have smaller variances relative to larger answers, even though both may have comparable relative errors. Use of the traditional figure of merit is misleading when comparing a given method used on different problems. The traditional figure of merit could mislead one into thinking that a method was becoming more efficient as the scattering ratio decreased. This would be supported by knowledge that the amount

of biasing increases as the scattering ratio decreases. However stronger biasing has never been a reliable indication of higher efficiency.

Fortunately, a figure of merit by itself does not determine the worth of a method. The value of the LIFT method is seen in the *ratios* of the figures of merits. If we define a benefit factor as being the ratio of one method's figure of merit to that of another method's figure of merit, then we can compare methods on the basis of how efficient they are relative to each other. In Table 6.2, the best method is the combination of LIFT with AVATAR. This method has a benefit factor of about 5.5 when compared to AVATAR with angularly-dependent weight windows, and a benefit factor of about 2030 when compared to survival biasing. As the scattering ratio becomes smaller, we see in Tables 6.4, 6.6, and 6.8, that the benefit factors for the LIFT/AVATAR combination increases by up to an order of magnitude when compared to survival biasing (the benefit factor is 85700 in Table 6.6), but decreases slightly when compared to AVATAR with angularly-dependent weight windows. The decrease in benefit factors for LIFT compared to AVATAR is probably due to the lack of source biasing, an oversight explained in Chapter 3. Some of the decreased efficiency of the LIFT method for low scattering ratios might be mitigated by strong source biasing. *From the comparison of benefit factors as the scattering ratio decreases, we can see that the LIFT method is most valuable in problems with high absorption.* Problems that cannot be solved in a reasonable amount of time with survival biasing are handled relatively efficiently by the LIFT method.

The variable f_4 decreases as the scattering ratio decreases. This is due to the behavior of the eigenvalue ($|\lambda_{0,g}|$) in eqn. (3.18). As the scattering ratio goes to zero, the eigenvalue approaches unity. Thus, the user cannot increase the maximum limit of the biasing by much. When $c=0.9$, $|\lambda_{0,g}|$ is only about 0.5, leaving plenty of room for adjustment. The number of adjustments caused by setting the maximum limit of the biasing parameter increases as the scattering ratio decreases. This is due to the decrease in accuracy of the deterministic methods. They do not do as good a job of estimating the

optimal biasing parameters as the scattering ratio decreases, thus more adjustments are necessary. The number of adjustments is comparable for each method, with diffusion requiring slightly more than the others, and S_N requiring slightly less.

We can see from the tables that the AVATAR methods rely much more heavily on Russian Roulette and splitting for optimal results than do the LIFT methods. This supports the statement made in earlier chapters that the LIFT method does a good job of controlling variations in weight. Another indication of weight control is given in the figures for relative statistical error. The LIFT methods have lower errors than the AVATAR methods, even though they rely less heavily on weight windows. The type of weight window is also important. In the AVATAR methods, angular dependence of the weight windows was an important feature, resulting in higher figures of merit. In the LIFT-only methods, weight windows based on angular fluxes sometime resulted in higher figures of merit compared to weight windows based on scalar fluxes. But, they never outperformed the LIFT method with AVATAR weight windows.

None of the deterministic methods required a significant amount of computing time, compared to the Monte Carlo calculations. We see that not only did the LIFT/ SP_N combination produce some of the highest figures of merit, but the SP_N calculations took less time, corrected for hardware, than did some of the S_N calculations. The methods based on diffusion suffered the most as the scattering ratio decreased, emphasizing the inability of diffusion to produce good approximations of the adjoint solution for low scattering ratios. The lack of ray effects in SP_N methods is probably responsible for the larger figures of merit compared to the S_N methods for some problems.

The final observations to be made here are that even the worst figures of merit for the LIFT methods usually exceed the best of the AVATAR methods, and the figures of merit for angularly-dependent AVATAR usually exceed those for AVATAR without angular dependence. Thus, even as a black box, the LIFT method is an improvement over AVATAR. Except when the scattering ratio is very low ($c=0.3$), where the results are very

unreliable, all of the figures of merit for all of the LIFT methods exceed all of the figures of merit for both of the AVATAR methods. However, the combination of LIFT and AVATAR resulted in the highest figures of merit for each problem.

One Group Heterogeneous Problems

The system for this group of problems is defined by a 15 x 15 x 15 cm cube. In the first two problems, a low-density crooked duct runs between the source and detector regions. In the third problem, a highly absorbing region is inserted midway between the source and detector. The cube is uniformly divided into 15 x 15 x 15 Monte Carlo cells (each cell has dimensions equal to one cm = one mean free path, except in the low density ducts where one cm is equivalent to a fraction of a mean free path). The number of cells used for the deterministic calculations varies with the method. Scattering is always linearly anisotropic with $\bar{\mu} = 0.2$. All sources are uniform, isotropic, and located between $x = y = z = 2.0$ cm and $x = y = z = 3.0$ cm. The flux is tallied for each problem by a track length flux detector located between $x = y = z = 12.0$ cm and $x = y = z = 13.0$ cm. The flux obtained from the tally is used to determine the absorption rate in that cell.

In the first two problems, the total cross section is 1 cm^{-1} for the bulk of the material through which a lower density duct runs. The duct material has the same scattering ratio as the bulk material in both problems ($c = 0.9$), and has a total cross section of 0.1 cm^{-1} in the first problem, and 0.01 cm^{-1} in the second problem. Figure 6.2 provides a rough idea of how the duct appears to the particle in the first two problems, as it travels between the source and detector. The duct runs between the source and detector, but it has 3 bends in it that are very difficult to depict on a flat piece of paper. Thus, Figure 6.2 is a slice diagonally through the cube, representing the plane containing the source and detector. The darkest squares are where the duct exists in cells intersected by the plane of the paper, *and* by planes above or below the paper. The next shade represents cells where

the duct is intersected by the plane of the paper. The lightest shade represents cells where the duct is in cells above *or* below the paper. White cells do not contain duct material on the plane of the paper, *or* above *or* below it. So, in words, the duct heads from the upper right corner of the source cell straight towards the detector cell, turns so that it travels in the x - y plane, turns again so that it travels along the z -axis, turns a final time to once again lie along the path between the source and detector. The cross sectional area of the duct varies, depending on whether it is running diagonally or along an axis, but it is fairly narrow compared to the overall dimensions of the system, never exceeding 3 cm^2 in area.

The third problem contains a strong absorber region (a $5 \times 5 \times 5 \text{ cm}$ cube) midway between the source and detector. Figure 6.3 shows its position relative to the source and detector. Both the bulk and the absorber regions have a total cross section equal to 1 cm^{-1} . The scattering ratio for the bulk material is 0.9, while the scattering ratio for the absorber material is 0.3.

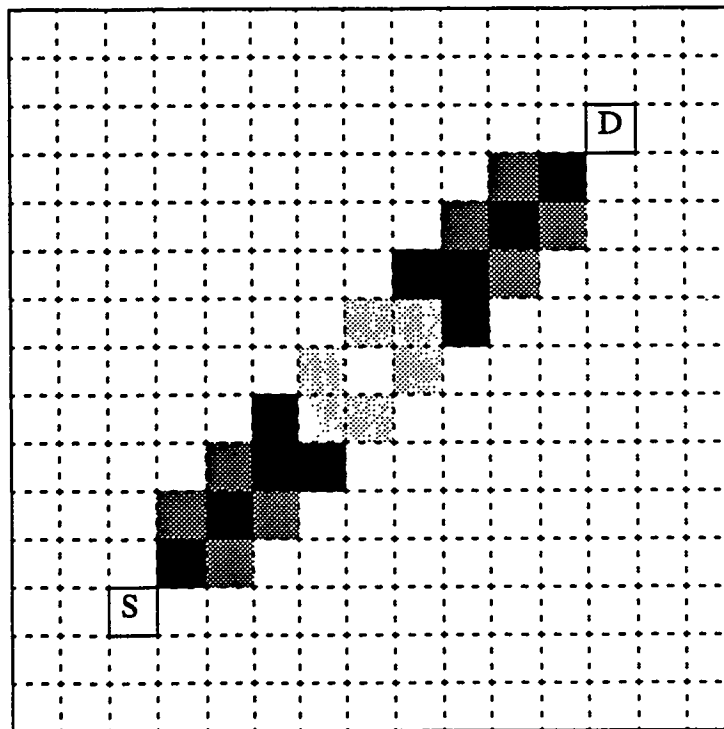


Figure 6.2: Planar Representation of 3-D Duct

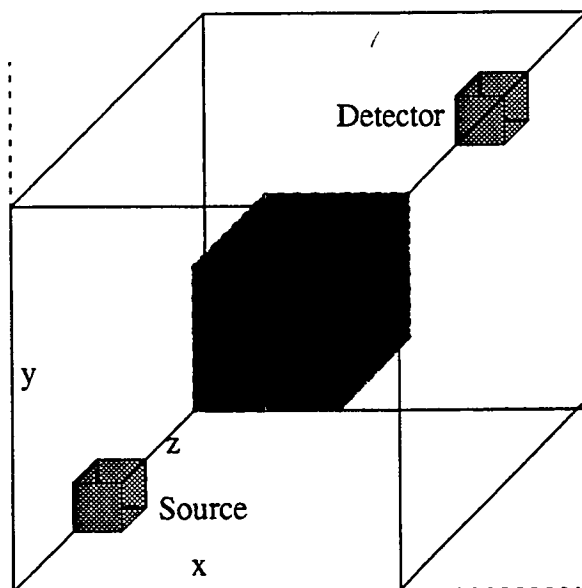


Figure 6.3: Representation of the Absorber Region

All deterministic calculations were carried out in the same way as the previous section, with a couple of exceptions. For these problems, the order of the regular S_N calculation was increased from $N=8$ to $N=16$, and the order of the Exponential Discontinuous calculation was increased from $N=6$ to $N=8$. All Monte Carlo runs were done in the same way as the previous section, except that all survival biasing runs were for 8,000,000 histories. Tables 6.9 and 6.10 present the results for the first problem (Duct 1) with a duct density equal to 0.1 times the density of the bulk material. Tables 6.11 and 6.12 present the results for the second problem (Duct 2) with a duct density equal to 0.01 times the density of the bulk material. Tables 6.13 and 6.14 present the results for the third problem containing an absorber region.

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0.5	2246	0.5	7.0	1.5	277620	1189248
LIFT/SN/PHI	0.5	1201	0.5	2.5	1.0	2425622	3174706
LIFT/SNED/PHI	0.5	1620	0.5	7.5	1.0	466953	1339603
LIFT/SPN/PHI	0.5	1622	0.5	3.5	1.0	511265	1422026
AV/D/PHI	-	-	0.5	2.0	1.0	2118313	1838157
AV/SN/PSI	-	-	1.0	3.0	2.0	2657532	3620829
LIFT/AV/SN/PSI	0.4	1722	0.5	2.5	1.0	845743	1788579
LIFT/SN/PSI	0.5	1201	0.5	2.5	1.0	15362212	16158149
LIFT/SPN/PSI	-	-	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-	-	-

Table 6.9: Monte Carlo Parameters and Effects for Duct 1

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	17053	6.19	-	0.015
LIFT/D/PHI	5	3137	1.87	0.43	0.91
LIFT/SN/PHI	126	6468	1.44	0.27	0.74
LIFT/SNED/PHI	211	3853	1.61	0.31	1.00
LIFT/SPN/PHI	66	3045	1.75	0.65	1.08
AV/D/PHI	6	3036	2.44	0.23	0.56
AV/SN/PSI	126	1741	2.36	0.46	1.03
LIFT/AV/SN/PSI	126	4267	1.41	0.52	1.18
LIFT/SN/PSI	126	10550	1.68	0.30	0.34
LIFT/SPN/PSI	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-

Table 6.10: Performance for Duct 1

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0.7	1539	2.0	4.5	3.0	438098	1417484
LIFT/SN/PHI	0.4	1774	0.5	8.0	1.0	367620	1200923
LIFT/SNED/PHI	0.5	1637	0.5	9.5	1.0	361131	1252390
LIFT/SPN/PHI	0.0	3327	0.5	1.5	1.0	866667	1787479
AV/D/PHI	-	-	0.5	1.0	0.75	1790940	2648260
AV/SN/PSI	-	-	1.0	5.0	2.0	1421949	2389786
LIFT/AV/SN/PSI	0.4	1774	0.5	5.5	1.0	376148	1327513
LIFT/SN/PSI	0.4	1774	0.5	8.5	1.0	353117	1187050
LIFT/SPN/PSI	-	-	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-	-	-

Table 6.11: Monte Carlo Parameters and Effects for Duct 2

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	17133	5.31	-	0.021
LIFT/D/PHI	6	1032	6.25	0.12	0.25
LIFT/SN/PHI	157	3913	2.41	0.19	0.44
LIFT/SNED/PHI	356	3261	2.32	0.35	0.57
LIFT/SPN/PHI	88	1715	4.14	0.17	0.34
AV/D/PHI	6	1630	3.86	0.18	0.41
AV/SN/PSI	162	1311	3.88	0.21	0.51
LIFT/AV/SN/PSI	160	3281	2.32	0.23	0.57
LIFT/SN/PSI	157	3818	2.43	0.22	0.45
LIFT/SPN/PSI	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-

Table 6.12: Performance for Duct 2

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0.4	3151	0.2	4.0	0.3	236786	238112
LIFT/SN/PHI	0.5	1409	0.1	6.0	0.2	265465	792618
LIFT/SNED/PHI	0.5	1824	0.5	11.0	0.75	182420	952548
LIFT/SPN/PHI	0.5	1934	0.1	2.5	0.2	1322136	1696277
AV/D/PHI	-	-	0.5	1.0	0.75	2853756	2726401
AV/SN/PSI	-	-	0.5	2.5	0.75	2926166	3738405
LIFT/AV/SN/PSI	0.6	844	0.5	2.5	0.75	517581	1365059
LIFT/SN/PSI	-	-	-	-	-	-	-
LIFT/SPN/PSI	-	-	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-	-	-

Table 6.13: Monte Carlo Parameters and Effects for Absorber

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	16787	12.0	-	0.004
LIFT/D/PHI	5	1939	0.666	9.58	11.6
LIFT/SN/PHI	127	8959	0.318	6.72	11.0
LIFT/SNED/PHI	372	5310	0.434	7.97	10.0
LIFT/SPN/PHI	54	14530	0.236	10.5	12.4
AV/D/PHI	5	1835	1.24	2.96	3.55
AV/SN/PSI	126	3142	0.963	2.68	3.43
LIFT/AV/SN/PSI	127	5811	0.384	7.37	11.7
LIFT/SN/PSI	-	-	-	-	-
LIFT/SPN/PSI	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-

Table 6.14: Performance for Absorber

We see immediately that the figures of merit for the LIFT and AVATAR methods applied to the duct problems (Tables 6.10 and 6.12), are much lower than those observed for the homogeneous problem (Table 6.2) with the same scattering ratio ($c=0.9$). But the figures of merit for survival biasing actually increased slightly when the duct problems are compared to the homogeneous problem with the same scattering ratio. The reason for this is that particles streaming through the duct save time without driving up the variance much in survival biasing runs. Particles streaming through the duct suffer fewer collisions (saving time), but the resulting higher variance in the number of collisions is not very important in problems with high scattering ratios. However, the deterministic methods do not handle ducts very well, causing the efficiency of the LIFT and AVATAR methods to suffer. The approximations of the adjoint solution are not good enough to cause accurate biasing of trajectories through narrow ducts. In addition, since $c=0.9$, the biasing is not very strong. Another effect of inaccurate deterministic solutions is that statistical errors for the LIFT and AVATAR methods have increased, compared to homogeneous problems, despite increased reliance on Russian Roulette and splitting.

The computing time required by the deterministic methods for the duct problems increased compared to the homogeneous problems. This is to be expected, given the difficulty deterministic methods have with voids or low density regions. Monte Carlo times also increased, due to the decreased efficiency, and increased reliance on Russian Roulette and splitting. Once again, the best method was LIFT combined with AVATAR angularly-dependent weight windows. Of the LIFT-only methods, those utilizing SP_N and Exponential Discontinuous S_N calculations performed the best. Superior accuracy is probably responsible for the performance of the Exponential Discontinuous method, while lack of ray-effects is probably responsible for the performance of the SP_N method. Angularly-dependent AVATAR once again performed better than diffusion-based AVATAR. Since the worst figures of merit for the LIFT methods did not always exceed the best for AVATAR, LIFT may not be the best “black box” method for problems with

voids or low density ducts.

Comparing Table 6.14 to Table 6.2, we see that adding the strong absorber in between the source and detector caused some problems for all of the methods. The same arguments that were used for low scattering ratios apply here, except that the LIFT and AVATAR methods were able to steer particles around the troublesome absorber region, to some degree. Thus, they did not suffer decreases in efficiency as strongly as did survival biasing. The absorber also seems to have caused more trouble for S_N methods than the SP_N method. In fact, the LIFT/ SP_N combination outperformed the LIFT/AVATAR combination. The LIFT/AVATAR combination was not the best this time, because angularly-dependent AVATAR did not do as well as diffusion-based AVATAR. Thus, using angularly-dependent AVATAR with LIFT hurt more than it helped. Overall, ray-effects seem to be responsible for the lower performance of the S_N -based methods, compared to the diffusion and SP_N -based methods.

Multigroup Homogeneous Problems

The system for this group of problems is defined by a 15 x 15 x 15 cm cube. The cube is uniformly divided into 15 x 15 x 15 Monte Carlo cells (so each cell has dimensions equal to about one cm = one mean free path in the energy group with the shortest mean free path). The number of cells used for the deterministic calculations varies with the method. Scattering is always linearly anisotropic with $\bar{\mu}$ dependent on the material, energy group, and whether scattering is within-group, or out-of-group.

The cross sections for each of the three materials (water, carbon, concrete) were obtained from the libraries used by MCNP³⁹. The cross sections for all but one element (iron), were taken from the ENDF/B version V evaluation. Iron cross sections were taken from the Group T-2 evaluation done at Los Alamos National Laboratory (LANL). The data was then collapsed down to 5 energy groups by codes at LANL, and cross section data for each element were combined into materials by THREEDANT.

	Concrete Weight Fractions	Water Atom Fractions	Carbon Atom Fractions
Hydrogen	4.532e-3	2/3	-
Oxygen	5.12597e-1	1/3	-
Sodium	1.1553e-2	-	-
Magnesium	3.866e-3	-	-
Aluminum	3.5548e-2	-	-
Silicon	3.60364e-1	-	-
Potassium	1.4219e-2	-	-
Calcium	4.3546e-2	-	-
Iron	1.3775e-2	-	-
Carbon	-	-	1

Table 6.15: Material Data

Energy Group	1	2	3	4	5
Lower E (MeV)	2.87	2.48e-2	1.67e-4	4.14e-7	1.39e-10
$\sigma_{t,g}$	3.1846e-1	6.2625e-1	7.6180e-1	7.5340e-1	8.9120e-1
$\sigma_{a,g}$	1.2750e-2	1.5000e-4	2.5000e-4	1.4500e-3	1.5600e-2
$\sigma_{s0,g \rightarrow g}$	2.2849e-1	5.8655e-1	6.9675e-1	6.9665e-1	8.7560e-1
$\sigma_{s0,g \rightarrow g+1}$	7.7220e-2	3.9450e-2	6.4800e-2	5.5300e-2	0
within-group c	0.7175	0.9368	0.9146	0.9247	0.9825
$\sigma_{s1,g \rightarrow g}$	6.8547e-2	1.0415e-1	1.7542e-1	1.8511e-1	2.6268e-1
$\sigma_{s1,g \rightarrow g+1}$	-2.2505e-3	1.1835e-2	1.9440e-2	1.6590e-2	0
$\bar{\mu}_{g \rightarrow g}$ used	3.0000e-1	1.7756e-1	2.5177e-1	2.6571e-1	3.0000e-1
$\bar{\mu}_{g \rightarrow g}$ real	4.859e-1	same	same	same	3.177e-1
$\bar{\mu}_{g \rightarrow g+1}$ used	-2.9144e-2	3.0000e-1	3.0000e-1	3.0000e-1	-
$\bar{\mu}_{g \rightarrow g+1}$ real	same	3.184e-1	3.311e-1	3.315e-1	-
$ \lambda_{0,g} $	0.7546	0.3826	0.4419	0.4161	0.2039

Table 6.16: Cross Section Data for Concrete

Energy Group	1	2	3	4	5
Lower E (MeV)	2.87	2.48e-2	1.67e-4	4.14e-7	1.39e-10
$\sigma_{t,g}$	3.5266e-1	1.3198e-0	2.9064e-0	3.0034e-0	4.1444e-0
$\sigma_{a,g}$	4.2000e-3	2.0000e-5	2.0000e-4	3.4000e-3	3.8200e-2
$\sigma_{s0,g \rightarrow g}$	1.6406e-1	1.0033e-0	2.3596e-0	2.5332e-0	4.1062e-0
$\sigma_{s0,g \rightarrow g+1}$	1.8440e-1	3.1648e-1	5.4660e-1	4.6680e-1	0
within-group c	0.4652	0.7602	0.8119	0.8434	0.9908
$\sigma_{s1,g \rightarrow g}$	5.0400e-2	2.9097e-1	7.7040e-1	8.1975e-1	1.2893e-0
$\sigma_{s1,g \rightarrow g+1}$	4.3236e-2	7.3795e-2	1.2053e-1	1.0271e-1	0
$\bar{\mu}_{g \rightarrow g}$ used	3.0720e-1	2.9001e-1	3.2650e-1	3.2360e-1	3.1399e-1
$\bar{\mu}_{g \rightarrow g}$ real	6.1441e-1	5.8002e-1	6.5300e-1	6.4719e-1	6.2798e-1
$\bar{\mu}_{g \rightarrow g+1}$ used	2.3447e-1	2.3317e-1	2.2051e-1	2.2003e-1	-
$\bar{\mu}_{g \rightarrow g+1}$ real	4.6893e-1	4.6636e-1	4.4102e-1	4.4006e-1	-
$ \lambda_{0,g} $	0.9391	0.7055	0.6354	0.5856	0.1482

Table 6.17: Cross Section Data for Water

Table 6.15 provides information on the components of each material. Tables 6.16-6.18 provide cross section data (in cm^2) used for all multigroup calculations performed for this thesis, values for the within-group scattering ratio (c), $\bar{\mu}$, and the eigenvalue for eqn. (3.10). We note here, that in some cases, $\bar{\mu}$ has been artificially reduced to insure that the macroscopic differential scattering cross section remains positive ($\bar{\mu}$ has to be less than one third, or eqn. (2.1c) can become negative). The real and artificial values are noted in the tables. This is only necessary when using linearly anisotropic scattering. There is no upscatter, and downscatter is directly coupled. These modifications were made to keep the calculations simple and to accommodate some of the deterministic codes that did not allow upscatter. Overall, the cross sections are fairly realistic. Finally, the cross sections were multiplied by a constant greater than unity, to simulate more mean free paths without changing the dimensions of the system. The cross sections were multiplied by 5.0 for concrete, by 2.0 for water, and by 3.5 for carbon.

Energy Group	1	2	3	4	5
Lower E (MeV)	2.87	2.48e-2	1.67e-4	4.14e-7	1.39e-10
$\sigma_{t,g}$	3.1318e-1	5.8818e-1	8.2898e-1	8.3279e-1	8.6671e-1
$\sigma_{a,g}$	3.8100e-3	1.5100e-4	7.0000e-6	4.7000e-5	5.3000e-4
$\sigma_{s0,g \rightarrow g}$	2.0448e-1	5.6721e-1	8.0252e-1	8.1060e-1	8.6618e-1
$\sigma_{s0,g \rightarrow g+1}$	1.0489e-1	2.0819e-2	2.6453e-2	2.2143e-2	0
within-group c	0.6529	0.9644	0.9681	0.9734	0.9994
$\sigma_{s1,g \rightarrow g}$	9.7639e-2	5.6154e-2	5.4812e-2	5.3175e-2	4.8506e-2
$\sigma_{s1,g \rightarrow g+1}$	-4.4956e-2	-6.1166e-3	-7.7983e-3	-6.5255e-3	0
$\bar{\mu}_{g \rightarrow g}$ used	3.0000e-1	9.9000e-1	6.8300e-1	6.5600e-1	5.6000e-1
$\bar{\mu}_{g \rightarrow g}$ real	4.775e-1	same	same	same	same
$\bar{\mu}_{g \rightarrow g+1}$ used	-3.0000e-1	-2.9380e-1	-2.9480e-1	-2.9470e-1	-
$\bar{\mu}_{g \rightarrow g+1}$ real	-4.286e-1	same	same	same	-
$ \lambda_{0,g} $	0.8172	0.2894	0.2743	0.2508	0.0379

Table 6.18: Cross Section Data for Carbon

All sources are uniform, isotropic, in group 1 and located between $x = y = z = 2.0$ cm and $x = y = z = 3.0$ cm. The flux is tallied for each problem by a track length flux detector in group 5, located between $x = y = z = 12.0$ cm and $x = y = z = 13.0$ cm. The flux obtained from the tally is used to determine the absorption rate in that cell. Figure 6.1 depicts the arrangement of the source and detector.

All deterministic calculations are carried out in the same way as the first section, with a couple of exceptions. For these problems, the default quadrature set ("traditional built-in constants") was used in the S_N calculations, and the order of the SP_N calculation was decreased from $N=7$ to $N=3$. All Monte Carlo runs were done in the same way as the previous section, except that survival biasing runs were for 17,000,000 histories, 1,700,000 histories, and 18,000,000 histories respectively. Tables 6.19 and 6.20 are the results for the first problem (concrete). Tables 6.21 and 6.22 are the results for the second problem (water). Tables 6.23 and 6.24 are the results for the third problem (carbon).

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0.6	8066	0.2	4.0	0.4	854456	890814
LIFT/SN/PHI	0.5	6856	0.1	3.0	0.3	1226595	736270
LIFT/SNED/PHI	0.7	1660	0.5	7.0	0.75	451618	619819
LIFT/SPN/PHI	0.4	10837	0.3	3.0	0.6	996831	1025565
AV/D/PHI	-	-	1.0	2.0	1.5	5181376	4987592
AV/SN/PSI	-	-	0.5	5.0	1.0	1091963	1806638
LIFT/AV/SN/PSI	0.6	5097	0.1	1.5	0.2	1159324	1415279
LIFT/SN/PSI	0.5	6856	0.2	2.0	0.6	538145	674577
LIFT/SPN/PSI	-	-	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-	-	-

Table 6.19: Monte Carlo Parameters and Effects for Concrete

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	4550	3.67	-	0.16
LIFT/D/PHI	8	3298	0.374	16.8	21.7
LIFT/SN/PHI	92	4247	0.317	19.1	23.5
LIFT/SNED/PHI	618	1717	0.448	21.0	29.0
LIFT/SPN/PHI	360	2103	0.483	16.7	20.4
AV/D/PHI	5	1635	0.732	9.04	11.4
AV/SN/PSI	92	779	1.18	5.45	9.23
LIFT/AV/SN/PSI	92	4000	0.323	14.4	24.0
LIFT/SN/PSI	92	2945	0.487	11.8	14.3
LIFT/SPN/PSI	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-

Table 6.20: Performance for Concrete

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0.3	6075	0.2	45.0	0.4	99648	702574
LIFT/SN/PHI	0.1	5249	0.3	15.0	0.45	127131	708613
LIFT/SNED/PHI	0.1	12450	1.0	14.0	1.5	523739	1243987
LIFT/SPN/PHI	-	-	-	-	-	-	-
AV/D/PHI	-	-	1.0	4.0	2.0	5409085	5861265
AV/SN/PSI	-	-	0.6	2.0	1.2	5416524	6324625
LIFT/AV/SN/PSI	0.2	3767	0.4	12.0	0.8	64983	1003012
LIFT/SN/PSI	-	-	-	-	-	-	-
LIFT/SPN/PSI	-	-	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-	-	-

Table 6.21: Monte Carlo Parameters and Effects for Water

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	3325	16.5	-	0.01
LIFT/D/PHI	8	2473	0.706	3.37	8.10
LIFT/SN/PHI	119	2827	0.615	4.48	9.35
LIFT/SNED/PHI	1684	2891	0.798	1.84	5.44
LIFT/SPN/PHI	-	-	-	-	-
AV/D/PHI	8	3972	0.815	1.78	3.79
AV/SN/PSI	119	2758	1.06	1.58	3.24
LIFT/AV/SN/PSI	119	1713	0.679	4.40	12.7
LIFT/SN/PSI	-	-	-	-	-
LIFT/SPN/PSI	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-

Table 6.22: Performance for Water

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0.6	8326	0.3	4.5	0.45	787023	753221
LIFT/SN/PHI	0.6	7789	0.1	3.0	0.3	1466681	867146
LIFT/SNED/PHI	0.7	3855	0.5	6.5	0.75	503358	616369
LIFT/SPN/PHI	0.6	8358	0.3	4.5	0.6	983898	1024246
AV/D/PHI	-	-	0.6	2.0	0.9	4816719	3700555
AV/SN/PSI	-	-	0.6	6.5	1.2	902967	1612670
LIFT/AV/SN/PSI	0.5	9514	0.2	2.5	0.3	670624	1088150
LIFT/SN/PSI	-	-	-	-	-	-	-
LIFT/SPN/PSI	-	-	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-	-	-

Table 6.23: Monte Carlo Parameters and Effects for Carbon

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	5004	5.32	-	0.07
LIFT/D/PHI	8	3762	0.369	12.8	19.5
LIFT/SN/PHI	74	5831	0.305	15.1	18.4
LIFT/SNED/PHI	888	2309	0.413	15.9	25.4
LIFT/SPN/PHI	412	2902	0.450	12.6	17.0
AV/D/PHI	7	2742	0.672	4.27	8.09
AV/SN/PSI	82	835	1.38	4.77	6.30
LIFT/AV/SN/PSI	78	3374	0.418	11.3	16.9
LIFT/SN/PSI	-	-	-	-	-
LIFT/SPN/PSI	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-

Table 6.24: Performance for Carbon

We recall that all multigroup calculations were carried out on IBM RISC-6000/590's rather than on the Sun SPARCstation 20's used for one-group calculations. The IBM's are roughly four times faster than the Sun's, and have much more memory. The Sun's used for the one-group problem did not have enough memory to handle the multigroup problems. Thus the figures of merit are not really higher for multigroup problems than for one-group problems, if corrected for hardware. Correcting for hardware is not necessary though, since one-group and multigroup comparisons are difficult anyway, due to the group-dependent scattering ratios.

The water problem appears to be the most problematic, with lower figures of merit compared to concrete or carbon, and one deterministic failure. The SP_N calculation failed to produce usable fluxes for the adjoint solution. Some of the fluxes were essentially zero, and we were unable to discover the cause of this problem within the time constraints of this thesis. The water cross sections were difficult for all of the deterministic methods, and may be why the SP_N method failed. Referring to Table 6.21, we see that the ratio of the largest total cross section to the smallest is very large compared to the same ratios for concrete or carbon. This presents one with a trade-off. Either the spatial discretization for the deterministic methods has to be made small, in order to keep each cell's dimensions equal to about one mean free path in group 5, or the system size has to be greatly increased to keep particles in group 1 from leaving on first flight. Either way, memory requirements and calculation time are increased significantly. Forcing the SP_N method to solve the problem with insufficient spatial discretization or excessive leakage might have caused the its failure. It also may have reduced the accuracy of the other deterministic methods. The other problem with water cross sections is the extremely high scattering ratio in group 5. This results in minimal amounts of biasing of particles in the last group in the LIFT methods. Unfortunately, the last group is probably where particles spend most of their time.

The most significant difference between the cross sections for concrete and carbon

is their scattering ratios. Carbon's higher scattering ratios are probably responsible for the lower efficiency of the LIFT methods, compared to concrete. Higher scattering ratios result in less biasing. Both problems should be solved accurately by the deterministic methods, thus avoiding the decrease in efficiency caused by lower scattering ratios in the one-group problems. Low scattering ratios did not become a problem in one-group, until they became 0.5 or lower. The lowest scattering ratio in the concrete or carbon problems is 0.65. Ray effects are also minimized by high scattering ratios. Thus, we should not be surprised that the highly accurate Exponential Discontinuous method resulted in the highest LIFT figures of merit for concrete and carbon. It is hard to say why regular S_N had so much trouble, causing angularly-dependent AVATAR to perform more poorly than diffusion-based AVATAR in all of the multigroup problems, and the LIFT/ S_N combination to perform more poorly than the LIFT/diffusion combination for carbon.

The optimal values of the parameter f_4 are about the same for the multigroup problems as for the one-group problems. The exception is water, where troublesome cross sections probably made the LIFT method more sensitive to overbiasing. As with the one-group problems, the AVATAR methods relied more heavily on Russian Roulette and splitting than did the LIFT methods, and still produced higher statistical errors. Also, as with the one-group calculations, the deterministic computing times were usually much smaller than the Monte Carlo computing times. The exception is the Exponential Discontinuous calculation. In this case, taking the deterministic time into account when calculating the figure of merit would have a significant effect. Taking deterministic times into account, diffusion does very well. The LIFT/diffusion figures of merit are very competitive with the other methods, even without taking into account that the diffusion results were obtained in less than 10 seconds.

Finally, we note that except for a couple of cases in the water problem, the worst figures of merit for the LIFT methods always exceeded the best figures of merit for the AVATAR method. Even in the water case, the best figure of merit for the LIFT-only

methods exceeded AVATAR's best by about a factor of two or more. For water, the best method was the LIFT/AVATAR combination.

Multigroup Heterogeneous Problems

This problem uses the same cube with a lower density duct running through it, as was used for the one-group problem, except that the material is concrete. The same cross sections used for homogeneous concrete are used here. The duct is also concrete, but with a density of 0.01 times the bulk material. The deterministic calculations are identical to the previous section. The Monte Carlo calculations are also identical to the previous section, except that survival biasing was run for 17,000,000 histories. Tables 6.25 and 6.26 provide the results for this problem.

	<i>f4</i>	<i>nadjust</i>	<i>cf</i>	<i>spf</i>	<i>sur</i>	<i>spl</i>	<i>cut</i>
SB	-	-	-	-	-	-	-
LIFT/D/PHI	0.4	9992	0.2	2.0	.4	945006	989989
LIFT/SN/PHI	0.5	6790	0.3	4.0	.9	916103	883625
LIFT/SNED/PHI	0.6	2197	0.5	9.0	.75	277877	489293
LIFT/SPN/PHI	0.5	8716	0.3	3.0	.45	438263	840551
AV/D/PHI	-	-	0.9	2.0	1.35	2079639	2269285
AV/SN/PSI	-	-	0.6	4.5	1.2	1280031	2039082
LIFT/AV/SN/PSI	0.4	8848	0.1	1.5	.2	1238774	1434828
LIFT/SN/PSI	-	-	-	-	-	-	-
LIFT/SPN/PSI	-	-	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-	-	-

Table 6.25: Monte Carlo Parameters and Effects for Concrete With Duct

	<i>D-time</i>	<i>MC-time</i>	<i>Err %</i>	<i>FOM-W</i>	<i>FOM-O</i>
SB	-	4542	3.42	-	0.19
LIFT/D/PHI	10	3000	0.662	5.66	7.61
LIFT/SN/PHI	112	2850	0.437	14.1	18.3
LIFT/SNED/PHI	591	1546	0.554	14.7	21.1
LIFT/SPN/PHI	670	1558	0.846	6.77	8.97
AV/D/PHI	10	993	1.34	3.78	5.64
AV/SN/PSI	112	763	1.23	6.56	8.69
LIFT/AV/SN/PSI	112	3895	0.373	14.4	18.4
LIFT/SN/PSI	-	-	-	-	-
LIFT/SPN/PSI	-	-	-	-	-
LIFT/SN/PSI-E	-	-	-	-	-

Table 6.26: Performance for Concrete With Duct

Again we see that the survival biasing method's efficiency increases with the addition of a duct to the problem. The time saved streaming through the duct, more than makes up for the increased variance in the weights of particles arriving at the detector. This may not be true in a problem with lower scattering ratios, where the number of collisions per particle is more important. We also see that similar to the one-group problems, the LIFT and AVATAR methods suffer a decrease in efficiency, caused by the duct. The reduced accuracy of the deterministic methods is probably responsible.

The addition of the duct helps the angularly-dependent AVATAR method outperform the diffusion-based AVATAR method. It also helps the S_N -based LIFT methods outperform the diffusion and SP_N -based methods. In both cases, the duct requires that particles be biased accurately in angle. The diffusion and SP_N -based methods cannot compete with the S_N -based methods in this respect. Apparently, ray effects did not offset this advantage in this problem.

Summary

Overall, the LIFT methods performed very well in comparison to the AVATAR methods. The highest figures of merit were always produced by LIFT methods. In some cases, it helps to combine LIFT with AVATAR's angularly-dependent weight windows. In the 11 problems considered, the LIFT/AVATAR combination produced 7 of the highest figures of merit, followed by the LIFT/ S_N ED method (4 of the highest figures of merit), and the LIFT/ SP_N method (1 of the highest figures of merit). There was a tie in the second one-group duct problem, accounting for the total of 12 winners in 11 problems. In looking at which methods qualified for the second tier (close in performance to the winners, and significantly higher than the lower performers), we see that the LIFT/AVATAR combination gained 3 more "points", making it one of the best in 10 out of 11 problems. The LIFT/ S_N ED method gains 2 more "points", making it one of the best in 6 out of 10 problems. The LIFT/ SP_N method gains 4 more "points", making it one of the best in 5 out

of 10 problems. Although the LIFT/ S_N combination did not *win* any performance battles, it picked up 6 second tier “points”, making it one of the best in 6 out of 10 problems. Following these methods are the angularly-dependent AVATAR method with 3 second tier “points”, the LIFT/diffusion method and the LIFT/ S_N /PSI method with 2 “points” each, and the LIFT/SN/PSI-E method with one “point”. The non-stellar performances of the LIFT/*/PSI methods were the reason they were not tried on every problem, thus saving a significant amount of computing effort, without losing important comparisons.

CHAPTER 7

CONCLUSIONS

We have derived a transformed transport problem that can theoretically be solved by analog Monte Carlo with zero variance. Lacking the ability to carry out the zero variance Monte Carlo simulation in practice, we have developed a method for approximating it. The resulting Local Importance Function Transform (LIFT) method is an approximation to the zero variance solution. It involves replacing the continuous adjoint transport solution in the transformed transport problem by a discretized approximation. This contains information from a deterministic calculation that is used to uniquely determine biasing parameters that are “local” in space, energy, and angle. The transport and collision processes of the transformed problem are used to bias distance-to-collision and selection of post-collision energy groups and trajectories in a traditional Monte Carlo simulation of “real” particles. This means that we start with unbiased particles and convert back to unbiased particles after each biased event. A more efficient approximation of the zero variance method would apply a survival biasing Monte Carlo simulation directly to the transformed problem. This approach would also bias each source particle’s energy, angle, and spatial distribution. Both approaches control the weight fluctuations traditionally caused by attempts to bias transport processes. We foresee no barrier to the complete implementation of source biasing, and intend for that to be our next step in the development of the LIFT method.

The LIFT method is a step toward the goal of creating a “black box” or automatic variance reduction technique. Such a technique would allow a user to define a problem to be solved, and would enable the code to determine the most efficient biasing parameters. By utilizing deterministic calculations to provide information for a Monte Carlo

simulation, we have reduced the amount of time that must be spent by a user to obtain accurate answers. In fact, for many problems, the LIFT method should produce solutions more efficiently than users could produce by trial and error optimization of other variance reduction techniques.

We have demonstrated numerically that the LIFT method is more efficient than AVATAR³⁶, one of the best variance reduction techniques currently available in a state-of-the-art Monte Carlo code. In many source-detector problems, the LIFT method should produce higher figures of merit than AVATAR, even when LIFT is used as a “black box”. Like most other variance reduction techniques, the LIFT method requires some fine-tuning to produce optimal results. However, it performs well without fine tuning, and many users should be able to obtain efficient solutions without any knowledge of the method, and without the need for trial and error runs. There are some problems that cause trouble for most variance reduction techniques. For example, we have demonstrated that problems with voids, or low density regions, can cause a reduction in the efficiency of the LIFT method. However, LIFT still performs more efficiently than survival biasing and AVATAR in these difficult cases.

We have also seen that the LIFT method suffers a decrease in efficiency as scattering ratios approach zero or unity. The benefit factor compared to survival biasing approaches unity as the scattering ratio approaches unity. This is because the amount of biasing in the LIFT method reduces to zero as the removal of particles from an energy group approaches zero. Fortunately, the removal of particles from an energy group can only approach zero in a one-group problem, or the last group of a multigroup problem. Thus, the benefit factor for the LIFT method should be greater than unity for most problems. Despite inaccuracies in deterministic calculations causing the efficiency of the LIFT method to decrease slightly as the scattering ratio approaches zero, the benefit factor compared to survival biasing increases greatly. Thus, problems with high absorption, that are traditionally difficult to solve with Monte Carlo, become relatively easy with the LIFT

method. The benefit factor of LIFT compared to survival biasing could easily exceed 100,000 for highly absorbing problems. This means that a given statistical error can be achieved in one $100,000^{\text{th}}$ of the time taken by a survival biasing calculation, or given the same amount of time, the LIFT method can reduce the error by a factor of over 300.

Overall, the LIFT method has been proven to perform very well in some fairly realistic problems. Being a newly-developed method, we expect that performance will increase as new strategies are implemented to further enhance the implementation of the LIFT method's approximation to the zero variance solution. However, this does not necessarily mean that more accurate adjoint solutions are required. We have seen in Chapter 4 that the method with the greatest efficiency is not always the method that uses the most accurate adjoint solution. Higher accuracy entails obtaining more information about the solution. Too much information can result in too much algebra within the code, thus disadvantageously increasing computation time.

The main point is that by implementing a very accurate approximation to the adjoint solution, one can make reductions in the variance, but at such a high computational cost (due to the increase in algebraic complexity) that the figure of merit is decreased. The zero variance method is one that minimizes the variance, not (necessarily) the figure of merit. Thus, one probably should not take *too* seriously the concept of very accurately approximating the zero variance solution. Figure 7.1 represents the potential scenario that one might discover through experiments with various methods.

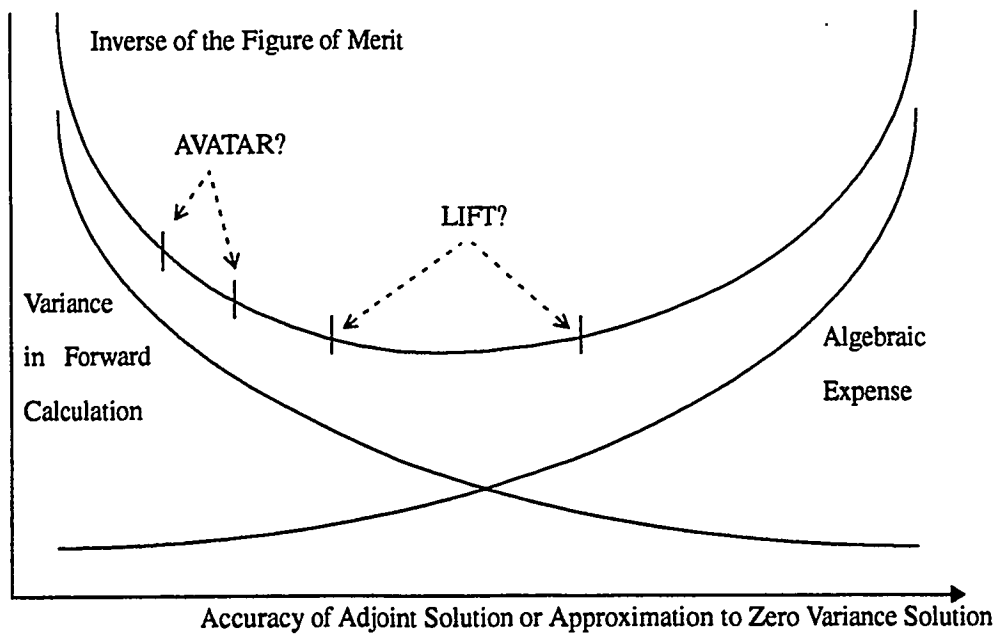


Figure 7.1: Method Efficiency

CHAPTER 8

FUTURE WORK

We present here some ideas for further development of the LIFT method:

1. Implement complete source biasing. The LIFT method, as presented in this thesis, only biased distance-to-collision for source particles. Biasing of source particles' energy, trajectory, and spatial distribution was overlooked. Such biasing would not have improved the results by much for the problems presented, involving small monoenergetic sources in materials with high scattering ratios. However, source biasing would be more important in problems with low scattering ratios, and a large source having a wide energy distribution.
2. Derive alternatives to the analytical approximation of the adjoint angular flux. Other forms may be beneficial in problems with voids, or with scattering ratios approaching unity. Other forms may also be more efficient or more accurate in general. AVATAR's representation of the adjoint angular flux, based on the maximum entropy distribution³⁶ is one possibility. The Exponential Discontinuous method's discrete ordinates representation⁴² is another possibility. The accuracy of the latter method has not been fully utilized in the LIFT method even though the general forms of their approximations to the adjoint angular flux are nearly identical. Taking advantage of the greater accuracy would require a discrete ordinates version of the Monte Carlo code.
3. Implement the LIFT method in a continuous energy Monte Carlo simulation. The continuous energy version should work with input from multigroup

deterministic solutions of the adjoint problem. However, importance sampling in continuous energy could be very difficult.

4. Utilize more information from the S_N calculation. Currently, the LIFT method only uses scalar flux information. However, it may be more efficient to use net current information to determine the biasing parameter in the angular component of LIFT's expression for the adjoint angular flux. Scalar fluxes would still be used to determine the biasing parameter in the spatial component. The potential increase in accuracy could justify the extra cost of the S_N calculations.
5. Investigate self-learning Monte Carlo techniques for improving the accuracy of the biasing parameters for difficult problems. As a Monte Carlo simulation proceeds, information about the adjoint solution could be saved and used to optimize the precalculated, deterministic-based biasing parameters. The additional information may contribute significantly around voids, a traditionally difficult area for deterministic methods to handle.
6. Implement the LIFT method in a state-of-the-art Monte Carlo code, such as MCNP.

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