Chapter 1

Introduction

The work covered in this dissertation includes the implementation of the Lagrange Discrete Ordinates (LDO) equations in the Exnihilo parallel neutral particle radiation transport framework for the purpose of using the equations' solutions in Monte Carlo variance reduction parameter generation via the ADVANTG software to improve the results of simulations run with MCNP5. We start with an analysis of deterministic scalar flux results from solving the LDO equations compared against those of standard discrete ordinates quadrature set types because the LDO equations have never before been implemented in a framework such as Exnihilo. Then, we assess the performance of the Monte Carlo variance reduction parameters generated based on the forward and adjoint solutions from the various quadrature set types in the contexts of both the Consistent Adjoint-Driven Importance Sampling (CADIS) and the Forward-Weighted CADIS (FW-CADIS) methods.

1.1 Motivation

Radiation shielding is an important and interesting problem from various perspectives. Simulation of shielding scenarios is critical for health physics and nuclear security applications, but arriving at a solution for a given response of interest (e.g., neutron flux at a given location) can be computationally difficult in the context of the magnitude of particle attenuation often seen in shielding problems.

The steady-state neutron transport equation (NTE), introduced below in Section 1.3, is typically solved using either deterministic methods or stochastic (Monte Carlo) methods. We will look at each of these solution methods in further detail in Chapter 2, but briefly note here that both solution methods have individual strengths and weaknesses. So-called "hybrid" methods aim to combine the favorable aspects of deterministic and Monte Carlo methods to achieve better results. Although hybrid methods are used to significant effect in radiation shielding problems, they do not entirely mitigate the negative aspects of the combined simulation types.

One particular area of study where hybrid methods tend to fall short is in shielding problems with highly anisotropic particle movement and particle streaming pathways. This is because the standard implementation of the CADIS and FW-CADIS methods is based on scalar particle flux rather than angular particle flux. So, solutions from deterministic calculations exclude information about how particles move toward a response of interest. For problems with strong anisotropies in the particle flux, the importance map and biased source developed using the standard space/energy treatment may not represent the real importance well enough to sufficiently improve efficiency in the Monte Carlo calculation.

This work aims to gauge the performance of Monte Carlo biasing parameters based on scalar flux solutions from solving the LDO equations. We will be employing the LDO equations' solutions in the standard CADIS and FW-CADIS methods to assess how well the LDO representation's unique treatment of scattering and asymmetry in angle incorporate angular information into the resultant scalar flux solutions and corresponding Monte Carlo biasing parameters.

1.2 Goals and Impacts

The primary goal of this work is to assess the forward and adjoint scalar flux solutions of the Lagrange Discrete Ordinates equations as input for Monte Carlo variance reduction parameter generation in the contexts of the CADIS and FW-CADIS methods. Additional research objectives in support of the primary goal for this work include:

- Implement the LDO equations in a neutral particle radiation transport framework designed to solve the traditional discrete ordinates form of the NTE.

- Choose a small variety of test cases in which to assess the various quadrature types' deterministic scalar flux solutions for efficacy in Monte Carlo variance reduction parameter generation.

- Compare forward and adjoint scalar flux solutions resultant from the LDO equations against those generated with standard discrete ordinates quadrature sets for the chosen test scenarios.

- Test the impact of biasing parameters' angular mesh refinement on Monte Carlo results across various quadrature types.

In meeting these objectives as progress towards accomplishing the primary research goal, we verify the relative accuracy of the deterministic solutions of the LDO equations and then examine how they perform as the deterministic solver for hybrid methods. The test problems used are those that challenge hybrid methods in general, and so we have generated a variety of results of interest to the community at large.

1.3 The Neutron Transport Equation

The way in which neutrons move, known as "neutron transport", is governed by the time-dependent neutron transport equation (NTE) [1]:

$$\frac{1}{v}\frac{\partial}{\partial t}\psi(\mathbf{r},E,\mathbf{\Omega},t)+\mathbf{\Omega}\cdot\nabla\psi(\mathbf{r},E,\mathbf{\Omega},t)+\Sigma_t(\mathbf{r},E)\psi(\mathbf{r},E,\mathbf{\Omega},t)=\\ \int_0^\infty\int_{4\pi}\Sigma_s(\mathbf{r},E'\rightarrow E,\mathbf{\Omega}'\cdot\mathbf{\Omega})\psi(\mathbf{r},E',\mathbf{\Omega}',t)d\mathbf{\Omega}'dE'+Q(\mathbf{r},E,\mathbf{\Omega},t), \quad (1.1)$$

where $\mathbf{r}$ is the neutron position, E is the energy of the neutron, $\mathbf{\Omega}$ is the direction of travel of the neutron, and t is the time. The combination of $(\mathbf{r},E,\mathbf{\Omega},t)$ is generally referred to as the "phase space" of the particles. ψ denotes angular neutron flux, Σ represents the cross section of a material, and Q is any additional source (fission, a fixed source, etc.) of neutrons.

We are often interested in situations in which the particle flux is not a function of time. In these cases, we solve the time-independent (steady-state) neutron transport equation, written as

$$\mathbf{\Omega}\cdot\nabla\psi(\mathbf{r},E,\mathbf{\Omega})+\Sigma_t(\mathbf{r},E)\psi(\mathbf{r},E,\mathbf{\Omega})=\\ \int_0^\infty\int_{4\pi}\Sigma_s(\mathbf{r},E'\rightarrow E,\mathbf{\Omega}'\cdot\mathbf{\Omega})\psi(\mathbf{r},E',\mathbf{\Omega}')d\mathbf{\Omega}'dE'+Q(\mathbf{r},E,\mathbf{\Omega}). \quad (1.2)$$

The steady-state neutron transport equation can be thought of as a balance equation in which the neutron losses represented on the left-hand side of the equation are equal to the neutron gains represented on the right-hand side of the equation [1]. The first term on the left-hand side of the steady-state NTE accounts for all neutrons lost by streaming out through the surface of the system being considered. The second term in the left-hand side of the steady-state NTE accounts for all neutrons lost to collisions; this includes neutrons lost via absorption as well as neutrons that exit the phase space of interest by scattering into a different energy and angle. The right-hand side of the equation totals system gains by summing up all neutrons that scatter into the phase space of interest from different energies and angles along with neutrons created from the source. The scattering term depends not on the individual angles $\mathbf{\Omega}$ and $\mathbf{\Omega}'$ but on their dot product.

The derivative in the first term of the steady-state NTE suggests that we must prescribe appropriate boundary conditions for the equation in order to solve the problem. The boundary conditions depend on the given problem of interest and will be discussed in more detail later. The following chapter will provide in-depth explanations of various solution methods for the time-independent NTE.

1.4 Dissertation Outline

The remainder of this dissertation is structured so as to provide a relevant theoretical background and discussion as a prelude to the eventual presentation of the results and analysis arrived at in meeting the sundry and ultimate objectives listed above in Section 1.2. Chapter 2 provides a theoretical basis of the foundation of solution methods for the NTE, followed by a discussion of pertinent work in the area of hybrid methods. Specific attention is given to developments that aimed to incorporate angular information into Monte Carlo biasing parameters; we will see in Section 2.3 that the interest in using the LDO equations' solutions for Monte Carlo variance reduction parameter generation stems from the unique way in which the LDO equations treat particle scattering.

Transitioning from theory to practice, Chapter 3 examines the traditional discrete ordinates equations and the LDO equations from the perspective of implementing both sets of equations in a neutral particle radiation transport software framework. Specific focus is given on the differences in implementing the contrasting equations; a discussion of details regarding the solution of the LDO equations in a framework designed to solve the conventional discrete ordinates equations concludes the chapter. We note that the discussion in Chapters 2 and 3 focuses on neutron transport, but the solution methods can be leveraged for photon transport as well; Chapter 4 presents the test case scenarios examined in this work with results from the various hybrid methodologies for both neutron and photon transport problems. Chapter 5 concludes the dissertation with a summary review of the results and analysis followed by a brief discussion of future work paths.

Bibliography

[1] James J. Duderstadt and Louis J. Hamilton. *Nuclear Reactor Analysis.* New York, NY: John Wiley & Sons, Inc., 1976.