# Thesis Proposal: Development of a Monte Carlo Code System with Continuous Energy Adjoint Transport Capabilities for Neutrons and Photons

Alex P. Robinson
aprobinson@wisc.edu

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## 1 Introduction

The Monte Carlo method has a rich history going back as far back as Babylonian times. However, its use in the field of radiation transport began in the 1940s and can be attributed to the work of von Neumann, Ulam, Metropolis, Kahn, Fermi and their collaborators [1]. The first successful application of the method in the field of radiation transport coincided with the construction of the first digital computers [2]. Because computational resources were relatively scarce and expensive, the computer codes implementing the Monte Carlo method to solve radiation transport problems were full of approximations to both the physical models and the cross section data. As the availability of computer resources increased it became feasible to do high fidelity Monte Carlo simulations with regard to both the physical models and the cross section data [3]. Today, the Monte Carlo method is regarded as the gold standard of computational methods for solving radiation transport problems because all variables of interest (i.e. energy, direction and position) can be treated on a continuous scale and because the problem geometry can be modeled completely. As computers continue to grow in size and speed, the Monte Carlo method will continue to be used for more and more challenging problems [1].

## 2 The Monte Carlo Method

The Monte Carlo method is a stochastic method in which samples are drawn from a parent population through sampling procedures governed by a set of probability

[1] Already, the Monte Carlo method is appearing in full reactor core simulation codes where it was once deemed too costly and inefficient to use [4].

laws. From the samples, statistical data is acquired and analyzed to make inferences about the parent population.

In radiation transport problems, the system of interest is a collection of bounded regions which can contain one or more of the following: a material, a vacuum, a source, a detector. The parent population is the set of all possible radiation histories and the samples are histories drawn from this set. The particle history can be regarded as a random walk from a source region to a problem domain boundary or some other terminating location (i.e. absorption point). Each phase of the random walk is governed by a set of probability laws that are all related to the material interaction cross sections of the particular form of radiation. The portion of a random walk that passes through a finite detector region is recorded or scored.

While radiation transport problems are typically solved by sampling radiation histories that start in what can be regarded as a model of the physical source and recorded in what can be regarded as a model of the physical detector, the opposite can also be true. The process of sampling the starting point of a history in the model of a physical source and recording information in the model of the physical detector is often called a forward process. The probability laws used in a forward process can be derived from the radiation transport equation. The forward process is most effective when the detector region is large relative to the source region. As the detector region decreases in size, the probability of any given history passing through the detector region decreases until, for a point detector, the probability goes to zero [5]. The process of sampling the starting point of a history in the model of the physical detector and recording information in the model of the physical source is referred to in the literature as an adjoint or reverse process [5, 6]. The reverse process is most effective when the source region is large compared to the detector region. When the detector region is a point, only the reverse process can be used without resorting to special procedures. The probability laws that govern the reverse process can be derived from the adjoint transport equation, which will be a major focus of this work.

# 3 Monte Carlo Codes Available Today

Most Monte Carlo codes available today focus on the forward process described before. The forward process has been developed to a level where very few approximations are used. For instance, it is very common to treat radiation histories on a continuous energy scale. This is also made possible by the very accurate cross section data that is available. The reverse process has not been developed to the same level yet. Only a few Monte Carlo codes have implemented the reverse process in a way that is relatively free of approximation. The GEANT4 toolkit has implemented the reverse process on a continuous energy scale for electromagnetic radiation and charged particles. In this implementation there are still some approximations that lead to discrepancies in results compared to the forward process [6]. FOCUS, a research code written by Hoogenboom, was the first code to implement the reverse process for neutrons on a continuous energy scale. This code was not able to model the coupled reverse process for neutrons and photons [7]. Today only the commercial United Kingdom code MCBEND has implemented the reverse process for neutrons on a continuous energy scale [8]. The implementation in MCBEND has some approximations that can be eliminated as well. Like FOCUS, MCBEND can not model the coupled reverse process for neutrons and photons. Table 3 summarizes the continuous energy modeling capabilities of most Monte Carlo codes available today. Please note that two of the most powerful and popular codes, MCNP5 and MCBEND are not open source codes. GEANT4, though a software development kit and not a true code, is the only open source software that has some continuous energy reverse capabilities. Several codes, such as MCNP5 and MORSE have implemented the reverse process on a discrete or multigroup energy scale.

Table 1: **Continuous Energy Capabilities of Monte Carlo Codes Available Today**. *The final column shows the proposed capabilities of the Forward-Adjoint Continuous Energy Monte Carlo (FACEMC) code.*

| Code | $n$ | $\gamma$ | $e^-$ | $p$ | $n^\dagger$ | $\gamma^\dagger$ | $e^{-\dagger}$ |
|---|---|---|---|---|---|---|---|
| EGS4 | - | $\surd$ | $\surd$ | - | - | - | - |
| EGSnrc | - | $\surd$ | $\surd$ | - | - | - | - |
| ITS6 | - | $\surd$ | $\surd$ | - | - | - | - |
| PENELOPE | - | $\surd$ | $\surd$ | - | - | - | - |
| MORSE | - | - | - | - | - | - | - |
| TART2005 | $\surd$ | $\surd$ | - | - | - | - | - |
| MCNP5/6 | $\surd$ | $\surd$ | $\surd$ | - | - | - | - |
| MCNPX | $\surd$ | $\surd$ | $\surd$ | $\surd$ | - | - | - |
| GEANT4 | $\surd$ | $\surd$ | $\surd$ | $\surd$ | - | $\surd$ | $\surd$ |
| MCBEND | $\surd$ | $\surd$ | $\surd$ | - | $\surd$ | - | - |
| FACEMC | $\surd$ | $\surd$ | $\surd$ | $\surd$ | $\surd$ | $\surd$ | $\surd$ |

One of the main reason for the apparent lack of codes that have implemented the reverse process on a continuous energy scale is the lack of available adjoint cross section data necessary for the reverse process. The popular ENDF libraries only supply cross section data for the forward process. In addition, most of the literature only discusses sampling procedures for the forward process based on differential cross sections. Fortunately, Hoogenboom has shown that both the total and differential adjoint cross sections can be derived from the forward cross sections. The calculation of these cross sections is costly, but only needs to be done once and can be done in the popular ENDF format [7].

# 4 The FACEMC Code

To address the limitations of current Monte Carlo codes and to bring the adjoint process up to the level of the forward process, the Forward-Adjoint Continuous Energy Monte Carlo (FACEMC) code will be developed along with any adjoint Monte Carlo cross sections and sampling techniques that are currently lacking. This code will be open source to foster adoption by other researchers. Only fixed source problems will be considered in the development of this code. The energy range over which the forward and adjoint neutron processes will be explored is $10^{-5}$ eV to 20.0 MeV. For the forward and adjoint photon processes, the energy range that will be explored is 1.0 keV to 20.0 MeV. These energy ranges will be sufficient to model a large number of problems important to both the nuclear engineering community and the medical physics community. Several such problems will be used to test the final version of the code.

# 5 Deliverables

This work will deliver the following items:

- Develop and open source framework in C++ for continuous energy Monte Carlo simulations of neutrons and photons (FACEMC).
- Compute the adjoint cross sections and differential cross sections for adjoint neutrons and adjoint photons.
- Develop improvements to the current adjoint models so that reverse simulations are as accurate and as fast as forward simulations.
- Run a series of test problems relevant to the fusion community and the medical physics community.

# 6 Committee

- Douglass Henderson (advisor): Professor, Department of Engineering Physics
- Paul Wilson: Professor, Department of Engineering Physics
- Greg Moses: Professor, Department of Engineering Physics
- Bruce Thomadsen: Professor, Department of Medical Physics
- Bryan Bednarz: Assistant Professor, Department of Medical Physics

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