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Development of a Modular, Concept-Based C++ Monte Carlo Neutral Particle Transport Code with Continuous Energy Adjoint Capabilities

Alex Robinson
Douglass Henderson

University of Wisconsin-Madison: 1500 Engineering Dr., Madison, WI, 53706, aprobinson@wisc.edu
University of Wisconsin-Madison; 1500 Engineering Dr., Madison, WI, 53706, henderson@engr.wisc.edu

INTRODUCTION

Several processes exist for estimating quantities of interest in radiation transport problems using Monte Carlo. The most commonly used process, where radiation histories start in a model of the physical source and are recorded in a model of the physical detector, is called the forward processes. A second processes, where radiation histories start in a model of the physical detector and are recorded in a model of the physical source, is called the adjoint (or reverse) process.

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. Conversely, 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 [1].

Using the above observation, one can come up with many examples of problems relevant to the shielding community where the adjoint process could be useful. Despite the possible uses of the adjoint process, very few codes are available that can conduct the adjoint process with a similar level of fidelity as the forward process (i.e. continuous energy scale, few simplifications to interaction models, etc.).

To address the limitations of current Monte Carlo codes and to bring the adjoint process up to the level of the forward process for photons and neutrons, the Forward-Adjoint Continuous Energy Monte Carlo (FACEMC) code is being developed along with any adjoint cross sections and sampling techniques that are currently lacking. Though the source code is currently private, the ultimate goal is for this code to be an open source project.

Some preliminary verification work has been conducted for the adjoint photon capabilities in the FACEMC code. The results of this verification work will be shown.

ADJOINT MONTE CARLO APPLICATIONS

One of the primary motivations for using the adjoint process is that quantities of interest can be estimated more efficiently (at least in theory) with an adjoint process when the detector is small relative to a source.

While a wide range of shielding problems could benefit from the adjoint process based on this observation, the shutdown dose problem is of particular interest. In a shutdown dose problem, the photon dose in a region of an experiment, fusion device or fission device, which results from neutron activation of the surrounding material, is desired. This information is particularly important for planning maintenance on the experiment or device.

Shutdown dose problems are often solved using a method called the rigorous 2-step (R2S) method [2-4]. In this method the neutron flux throughout the experiment or device is calculated. This neutron flux data is then given to an activation code, which calculates the source of photons due to the decay of activated material. Finally, the dose due to photons is calculated in the areas of interest using a forward process. Often, the amount of activated material is much larger than the region where the dose distribution is desired, which indicates that these problems could potentially benefit from the adjoint process for photons. The use of the adjoint photon process in the rigorous 2-step method has been coined the rigorous 2-step adjoint (R2SA) method [4].

Source distribution optimization problems can also benefit from the adjoint process. The adjoint flux, which can be estimated by using the adjoint process, is commonly interpreted as the importance or sensitivity of a particular point of the source (in phase space) to the detector response [5].

In both brachytherapy and external beam treatment planning optimization, the use of adjoint flux data interpreted as a source importance distribution has been shown to allow for faster and simpler treatment planning optimization algorithms [6-8].

THE FACEMC CODE

FACEMC is a C++ code that is being developed with modern coding practices and tools. The source code is stored in a private git repository, which will be made public as soon as the necessary permissions have been received. The code is in a state where basic verification work is being done for the photon and adjoint photon

capabilities. Some preliminary results of this verification work will be shown in the next section. In this section the motivation for writing the code, along with the code requirements, the design of the code, and the generation of adjoint cross sections will be discussed.

Motivation

Despite the potential usefulness of the adjoint process, most Monte Carlo codes available today focus on the forward process. 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 capability is also made possible by the very accurate cross section data that is available. The adjoint process has not been developed to the same level yet. Only a few Monte Carlo codes have implemented the adjoint process in a way that is relatively free of approximation.

The GEANT4 toolkit has implemented the adjoint process on a continuous energy scale for photons and charged particles. GEANT4 still uses some approximations that lead to discrepancies in results compared to results from the forward process [9].

FOCUS, a research code written by Hoogenboom, was the first code to implement the adjoint process for neutrons on a continuous energy scale [10]. Today, only the commercial United Kingdom code MCBEND has implemented the adjoint process for neutrons [11]. Both FOCUS and MCBEND use a one-group treatment of thermal neutrons.

Table I summarizes the continuous energy modeling capabilities of a sampling of the popular Monte Carlo codes available today.

Table I. Continuous Energy Capabilities of Monte Carlo Codes Available Today.

Code	n	γ	$n^{\dagger}$	$\gamma^{\dagger}$
EGS4	-	√	-	-
EGSnrc	-	√	-	-
ITS6	-	√	-	-
PENELOPE	-	√	-	-
MORSE	-	-	-	-
TART2005	√	√	-	-
MCNP5/6	√	√	-	-
MCNPX	√	√	-	-
GEANT4	√	√	-	√
MCBEND	√	√	√	-

The FACEMC code has been created out of a need for high fidelity adjoint capabilities for adjoint photons and neutrons that are not currently available in any one code.

Code Requirements

The FACEMC code will be able to model photons and adjoint photons in the energy range 1 keV to 20 MeV. It will also be able to model neutrons and adjoint neutrons in the energy range 10^{-5} eV to 20 MeV. Coupled adjoint photon and adjoint neutron transport in this energy range will also be possible.

Users will be able to model spatial domains using either CAD models or more standard combinatorial geometry representations. To accomplish spatial domain modeling using CAD models, the Direct Accelerated Geometry (DAG) tool in the Mesh Oriented Database (MOAB) library is currently being used [12]. The combinatorial geometry representation of spatial domains will be accomplished with the ROOT package [13].

Several popular variance reduction techniques will be available to users: implicit capture, Russian roulette, splitting, forced collisions, and weight windows. A weight window generator will not be included in the initial release.

Because this code is primarily designed for shielding applications, domain replication will be the only type of parallelism that will be implemented.

Code Design

The FACEMC code has been designed to provide a tool with a set of core features for users. In addition, it has been designed as a development platform where new features can be added relatively easily. To that end, the code has been designed in a highly modular way that allows for changes and customizations to be made in a fairly straightforward way. The five core modules that make up FACEMC are the geometry handling module, the source handling module, the estimator handling module, the collision handling module and the random number generation module. Each module consists of a handling concept (C++ template) and a traits class, where additional characteristics of the handling concept are defined. Each handling concept, along with its corresponding traits class, specifies the interface for the particular module.

For users, a default concept model (C++ template instantiation) and corresponding traits class specialization is provided for each module (and ultimately compiled into the default FACEMC executable). Developers that deem a default concept model for a particular module to be lacking in some way can simply write their own concept model. Recompiling the code with the new concept model will then result in a custom version of FACEMC with the different and/or new capabilities provided by the developer.

It should also be noted that developers need not write their own concept model for every module. As long as a concept model for a particular module is implemented

correctly, it will be able to interact with the other (possibly default) modules.

Adjoint Cross Section Generation

Because there are currently no cross section libraries available that contain adjoint cross section data, all adjoint cross sections are generated by FACEMC. Equations 1 and 2, which come about from the derivation of the adjoint random walk process, are used to generate most of the adjoint cross sections [10,14]. The function $c(E)$ represents the average number of secondary particles (of the same type as the primary) that are released from the interaction, given initial particle energy of E.

$$\sigma^{\dagger}\left(E' \to E, \hat{\Omega}' \to \hat{\Omega}\right) = c(E)\sigma\left(E \to E', \hat{\Omega} \to \hat{\Omega}'\right) \qquad (1)$$

$$\sigma^{\dagger}(E') = \iint c(E)\sigma\left(E' \to E, \hat{\Omega}' \to \hat{\Omega}\right) dE d\hat{\Omega} \qquad (2)$$

For continuous energy adjoint photon transport, the interactions of primary interest are adjoint incoherent scattering, adjoint coherent scattering and adjoint pair production. Adjoint incoherent and adjoint coherent scattering are relatively straightforward and have been documented in many references [10,14].

An example integrated adjoint incoherent scattering cross section that is used by FACEMC is shown in fig. 1. Due to the properties of the scattering kinematics for adjoint photons, the total adjoint incoherent scattering cross section is infinite unless a maximum problem energy is set [14]. As mentioned before, the maximum problem energy for FACEMC is 20 MeV.

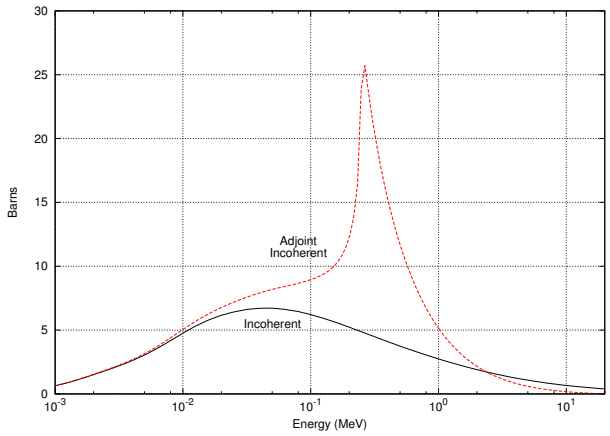

Fig. 1. The integrated adjoint incoherent scattering cross section for Aluminum with the maximum problem energy of 20 MeV.

Adjoint pair production is much more complicated but the methodology for handling adjoint pair production has been documented by Hoogenboom [15].

Two more phenomena that are of interest are Doppler broadening and x-ray production due to atomic relaxation after an incoherent or photoelectric effect interaction. Both of these phenomena can be modeled for photons but cannot currently be modeled for adjoint photons. From equations 1 and 2, it is clear that an equivalent photoelectric effect cross section does not exist for adjoint photons (c = 0 for the photoelectric effect cross section), which is why taking x-ray production into account with adjoint photons currently hasn't been done.

These two phenomena will not have a large effect in high-energy photon problems but will likely have an effect in low-energy photon problems, which are common in the medical physics community. New methods to model these processes will be looked at in more depth in the future.

PRELIMINARY VERIFICATION RESULTS

The preliminary verification work has consisted of checking that results from an adjoint photon simulation match the results from a photon simulation.

A simple sample problem has been constructed[a] that consists of a point source and five concentric spheres. The first sphere has a radius of 10 cm and each successive sphere has a radius that is 10 cm larger than the previous sphere. Fig. 2 shows the simple geometry that is used for both the forward and adjoint simulation.

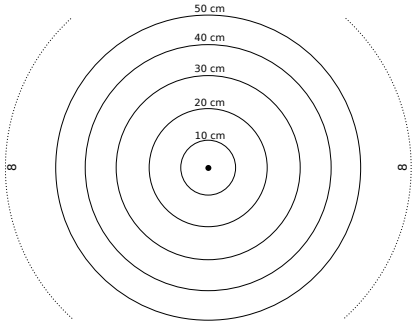

Fig. 2. The simple problem geometry used to conduct the preliminary verification of FACEMC adjoint photon capabilities.

The point source emits photons at energies of 616.66 keV and 321.0 keV. The frequencies of these emissions are 0.8 and 0.2 respectively. A simple surface flux estimator is used on each spherical surface. Water is used as the material throughout the geometry, which is also set up to be infinite. Because the geometry is essentially one dimensional and infinite, the adjoint problem can be set up identically to the forward problem.

Table II summarizes the results of the forward and adjoint simulations after running 10^7 histories for each simulation. The percent differences between the fluxes calculated at each surface of interest are less than one percent, indicating that both the adjoint cross sections and

the adjoint random walk process implementation are likely correct. However, much more verification work must be done before this can be declared with a high level of confidence.

Table II. The photon flux calculated at each spherical surface using 10^7 histories in a forward and an adjoint simulation.

Dist. (cm)	Flux (for. sim.)	Rel. Err.	Flux (adj. sim.)	Rel. Err.
10	1.5748e-3	0.0007	1.5788e-3	0.0014
20	4.1291e-4	0.0007	4.1491e-4	0.0018
30	1.4150e-4	0.0007	1.4235e-4	0.0022
40	5.2255e-5	0.0011	5.2322e-5	0.0033
50	1.9963e-5	0.0014	2.0030e-5	0.0033

FUTURE WORK

As mentioned in the previous section, Doppler broadening and x-ray production due to atomic relation cannot currently be modeled for adjoint photons. One of the primary goals is to develop methods to handle these processes for adjoint photons.

The methods outlined by Hoogenboom for adjoint neutron cross section generation and simulation will be explored and implemented [10]. In addition, a more detailed model for thermal adjoint neutron scattering will be developed that is more similar to the models for thermal neutron scattering.

ENDNOTES

[a]This problem was proposed by Dorothea Sommer at the Technische Universität Dresden.

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