Working Title: Monte Carlo Analysis of Dynamic Systems

by

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Dedicated to...

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0.1 Introduction

The rapid design iteration process of complex nuclear systems has long been aided by the use of computational simulation. Traditionally, these simulations involve radiation transport in static geometries. However, in certain scenarios, it is desirable to investigate dynamic systems and the effects caused by the motion of one or more components. For example, Fusion Energy Systems (FES) are purposefully designed with modular components that can be moved in and out of a facility after shutdown for maintenance. To ensure the safety of maintenance personnel, it is important to accurately quantify the shutdown dose rate (SDR) caused by the gammas emitted by structural materials that became activated during the device operation time. This type of analysis requires neutron transport to determine the neutron flux, activation calculation to determine the isotopic inventory, and finally a photon transport calculation to determine the SDR. While MC calculations are revered to be the most accurate method for simulating radiation transport, the computational expense of obtaining low error results in systems with heavy shielding can be prohibitive. However there are techniques, known as variance reduction (VR) methods, that can be used to increase the computational efficiency. There are several types of VR methods, but the basic theory is to artificially increase the simulation of events that will contribute to the quantity of interest such as flux or dose rate. One class of VR techniques relies upon a deterministic estimate of the adjoint solution of the transport equation to formulate biasing parameters used in the MC transport. The adjoint flux has physical significance as the importance of a region of phase space to the objective function.

The purpose of this work is to create a methodology for the efficient calculation of quantities of interest in dynamic, geometrically complex nuclear systems. For cases involving coupled multi-physics analysis, such as SDR calculations, a new hybrid deterministic/MC VR technique will be proposed. This new method will adapt the Multi-Step Consistent Adjoint Driven Importance Sampling (MS-CADIS) method to dynamic systems.

The basis of MS-CADIS is that the importance function used in each step of the problem must represent the importance of the particles to the final objective function. As the spatial configuration of the materials changes, the probability that they will contribute to the objective function also changes. In the specific case of SDR calculations, the importance function for the neutron transport step must capture the probability of materials to become activated and subsequently emit photons that will make a significant contribution to the SDR. This new VR method will also take advantage of the Groupwise Transmutation (GT)-CADIS method which is an implementation of MS-CADIS that optimizes the neutron transport step of SDR calculations. GT-CADIS generates an adjoint neutron source based on certain assumptions and approximations about the transmutation network. To adapt this method for dynamic systems, the adjoint neutron source will be calculated at each time step and then averaged in order to generate the biasing functions for the neutron transport step.

0.2 Background

This work focuses on the nuclear analysis of systems that include activated, moving components; specifically, parts of fusion energy systems that need to be moved after shutdown for maintenance purposes. Systems that are exposed to intense neutron irradiation become activated and decay via photon emission long after the device has been shut down. In order to accurately protect the maintenance personnel that may be in the vicinity of the activated, moving components, it is important to quantify the biological dose rate in the field.

SDR calculations

Shutdown dose rate (SDR) calculations are necessary to quantify the potential dose to personnel working in facilities exposed to intense radiation fields like fusion energy systems (FES). The dose rate is caused by decay photons that are emitted by materials irradiated by neutrons. Therefore, these calculations involve a neutron transport step, then an activation analysis to determine the decay photon spectrum for a specific irradiation and decay scenario, and finally a photon transport step to determine the dose rate. One methodology for calculating the SDR is known as the Rigorous Two Step (R2S) method. This method relies on a MC code for both neutron and photon transport and a nuclear inventory code for activation analysis. The goal of the neutron transport step is to determine the neutron flux discretized by space and energy. This neutron flux along with an irradiation and decay scenario of interest are used as input into a nuclear inventory code. This code will give the photon flux as a function of decay time which is then used as the source for the photon transport step. A photon flux tally fitted with flux-to-dose-rate conversion factors is used during this step to determine the final SDR [4].

Analog Monte Carlo Calculations

To quantify the dose rate, we need to know th flux of photons produced by the decaying radionuclides in the activated components. The activation is causedd by neutron irradiation. We need to know what the neutron flux looks like in every region of phase space.

We need a detailed distribution of the neutron flux throughout all regions of phase space. The neutron distribution along with and irradiation and decay scheme of interest can then be input for a nuclear inventory code to generate the photon emission density. This photon emission density is used as a source for the photon transport step which ultimately produces the photon flux in every region. The photon flux coupled with a flux-to-dose-rate conversion factor will give us the dose rate.

There are two ways to solve the Boltzmann transport equation: deterministically and stochastically. The most optimal way to perform accurate, full-scale analysis of FES is through Monte Carlo radiation transport *need source*. In general, Monte Carlo (MC) calculations rely on repeated, random sampling to solve mathematical problems. The MC method can be applied to radiation transport by solving the Boltzmann transport equation through the simulation of random particle walks through phase space. In analog operation mode (i.e. no variance reduction), the source particle's position, energy, direction and subsequent collisions are sampled from probability distribution functions (PDFs). Quantities of interest such as flux can be scored, or tallied, by averaging particle behavior in discrete regions of phase space.

Radiation transport simulations in geometries that have thick shielding, such as FES, become challenging for MC codes. The particles have lots of interactions (absorption and scattering) in the shielding regions. This results in low particle fluxes in these discrete regions of phase space.

The statistical error is a function of the relative error, R, which is defined

as

$$R = \frac{S_{\bar{x}}}{\bar{x}} \tag{1}$$

where $\bar{x}$ is the average of the tally scores, and $S_{\bar{x}}$ is the standard deviation of the tally scores. For a well behaved tally, R is proportional to $1/\sqrt{N}$ where N is the number of tally scores [3].

To reliably predict results in these regions, many particle histories need to be simulated which may require large amounts of computer time [1].

MC calculation efficiency is measured by a quantity known as the figure of merit (FOM). The FOM is a function of relative error, R, and computer processing time, T, as given by

$$FOM = \frac{1}{R^2 T} \tag{2}$$

It is desirable to have a high FOM because it means that less computation time is needed to achieve a reasonably low error, less than 0.1 according to the MCNP manual [3]. The relative error is inversely proportional to N. VR methods aim to increase the FOM by increasing N and decreasing $S_{\bar{x}}$ by sampling from biased PDFs; this effectively forces more collisions in regions of phase space that are important to the tally of interest.

VR Methods

Certain MC calculations require the use of variance reduction methods in order to complete or improve the efficiency of the calculation. This is accomplished by preferentially sampling trajectories that are likely to contribute to the tallies of interest. In order to compensate for this biased sampling, the particle statistical weight is adjusted accordingly. The relationship between the particle statistical weight, w, and the PDF that governs particle behavior is as follows

$$w_{\mathrm{biased}}\,\mathrm{pdf}_{\mathrm{biased}} = w_{\mathrm{unbiased}}\,\mathrm{pdf}_{\mathrm{unbiased}} \tag{3}$$

One of the earliest and still commonly used methods of VR is particle splitting and rouletting. This is particularly useful in deep penetration simulations, like FES. Generally speaking, to increase the number of particle histories that can contribute to tallies of interest, it is desirable to split particles as the enter more important regions and roulette particles as the enter less important regions. This requires assigning an importance, I, to every region in the geometry and adjusting the weight, w, of the new particles. When a particle moves from a region A to a region B, the ratio of importances is calculated. If region B is more important than region A such that $I_B/I_A \geqslant 1$, the particle with original weight w_0 is split into $n = I_B/I_A$ particles, each with weight w_0/n. If instead region B is less important than region A such that $I_B/I_A < 1$, the particle will undergo roulette. The particle will survive with a probability n and weight w_0/n [2]. The weight window method in MCNP utilizes both splitting and rouletting. A weight window is a region of phase-space that is assigned an upper and lower bound. The windows can be assigned to cells in the geometry, on a superimposed mesh, and to energy bins. When a particle enters a weight window, its weight is assessed; if its weight is above the upper bound or below the lower bound, it is either split or rouletted, respectively.

Automated VR Techniques

VR techniques require the user to have a priori knowledge of the problem physics in order to assign importance parameters. Many techniques have been developed over the years to automate the selection and assignment of these parameters to reduce the time and expertise required by the user.

One class of VR techniques, known as hybrid deterministic/MC methods, is based upon the solution to the adjoint Boltzmann transport equation having physical significance as the measure of importance of a particle to some specified objective function. Because deterministic solutions to

the transport equation are less precise but require much less computation time, they are useful as an estimate of particle flux throughout the domain which can then be used to determine importance of specific regions. To demonstrate the use of the adjoint solution as an importance function, we will first start with the linear, time-independent Boltzmann transport equation shown below

$$H\Psi = q \tag{4}$$

where Ψ is the angular flux, q is the source of particles, and the operator H is given by

$$H = \widehat{\Omega} \cdot \nabla + \sigma_t(\overrightarrow{r}, E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\overrightarrow{r}, E' \to E, \widehat{\Omega}' \to \widehat{\Omega}) \tag{5}$$

where σ_t is the total cross-section and σ_s is the differential scattering cross-section. The adjoint identity states that

$$\langle \Psi^+, H\Psi \rangle = \langle \Psi, H^+\Psi^+ \rangle \tag{6}$$

where $\langle \cdot \rangle$ refers to the integration over space, energy, and angle and the adjoint operator H^+ is given by

$$H^+ = -\widehat{\Omega} \cdot \nabla + \sigma_t(\overrightarrow{r}, E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\overrightarrow{r}, E \to E', \widehat{\Omega} \to \widehat{\Omega}') \tag{7}$$

The identity can also be written as

$$\langle \Psi^+, q \rangle = \langle \Psi, q^+ \rangle \tag{8}$$

As mentioned, the adjoint solution to the transport equation will be used as an importance function therefore we need to solve

$$H^+\Psi + = q^+ \tag{9}$$

which requires the thoughtful selection of an adjoint source q^+. To demonstrate the physical significance of the adjoint, we will consider the detector response, R

$$R = \langle \Psi, \sigma_d \tag{10}$$

where σ_d is a detector response function. If we choose the adjoint source to be equivalent to the detector response function,

$$q^+ = \sigma_d \tag{11}$$

and substitute this into Eq. 10 and Eq. 8

$$R = \langle \Psi, q^+ \rangle = \langle \Psi^+, q \rangle \tag{12}$$

the adjoint flux Ψ^+ represents the importance of a region to σ_d. This final relation allows us to know the response R for any source q once the adjoint flux Ψ^+ for a detector of interest is known.

The Consistent Adjoint Driven Importance Sampling (CADIS) method is one of the hybrid deterministic/MC VR techniques that uses the adjoint solution to formulate source and transport biasing parameters for MC transport. More specifically, CADIS determines the parameters for source biasing and the weight window lower bounds in a consistent manner. The response, or tally, of interest in a transport calculation can be represented by the following equation

$$R = \int_V d\vec{r} \int_E dE \int_{4\pi} d\widehat{\Omega} \sigma_d(\vec{r}, E, \widehat{\Omega}) \Psi(\vec{r}, E, \widehat{\Omega}) \tag{13}$$

and in terms of the adjoint flux,

$$R = \int_V d\vec{r} \int_E dE \int_{4\pi} d\widehat{\Omega} q(\vec{r}, E, \widehat{\Omega}) \Psi^+(\vec{r}, E, \widehat{\Omega}) \tag{14}$$

The MC solution of the response relies upon the sampling of the particle

source distribution, $q(\overrightarrow{r}, E, \widehat{\Omega})$, represented by a PDF. In an effort to decrease the variance, it is possible to sample from a biased PDF which is given by

$$\widehat{q}(\overrightarrow{r}, E, \widehat{\Omega}) = \frac{\Psi^{+}(\overrightarrow{r}, E, \widehat{\Omega}) q(\overrightarrow{r}, E, \widehat{\Omega})}{R} \tag{15}$$

This biased PDF represents the contribution of particles from phase-space $(\overrightarrow{r}, E, \widehat{\Omega})$ to the total detector response, R. As previously mentioned, when sampling from a biased PDF, the particle weight needs to be adjusted to eliminate systematic bias.

$$w(\overrightarrow{r}, E, \widehat{\Omega}) \widehat{q}(\overrightarrow{r}, E, \widehat{\Omega}) = w_0 q(\overrightarrow{r}, E, \widehat{\Omega}) \tag{16}$$

Substituting in Eq. 15, the corrected particle weight is shown to have an inverse relation to the adjoint flux, or importance function.

$$w(\overrightarrow{r}, E, \widehat{\Omega}) = \frac{R}{\Psi^{+}(\overrightarrow{r}, E, \widehat{\Omega})} \tag{17}$$

In the weight window technique, particles are either split or rouletted as they move from region to region based on the ratio of their importances and their weight is updated accordingly. The weights are used for both the source and transport biasing parameters and are derived from importance sampling in a consistent manner. The transport is biased according to the following relationship

$$w(\overrightarrow{r}, E, \widehat{\Omega}) = w(\overrightarrow{r}\,', E', \widehat{\Omega}') \left[\frac{\Psi^{+}(\overrightarrow{r}\,', E', \widehat{\Omega}')}{\Psi^{+}(\overrightarrow{r}, E, \widehat{\Omega})} \right] \tag{18}$$

The width of the weight windows is determined by a parameter defined to be the ratio between upper and lower bounds $\alpha = w_u / w_l$. MCNP uses

a default value for α and the weight window lower bounds are given by

$$w_l(\overrightarrow{r}, E, \widehat{\Omega}) = \frac{R}{\Psi^+(\overrightarrow{r}, E, \widehat{\Omega})(\frac{\alpha+1}{2})} \tag{19}$$

Automated VR for SDR Calculations

There are two transport steps involved in SDR calculations; the initial neutron trasport to simulate the irradiation and the subsequent photon transport simulating the decaying gammas. The full-scale simulations in large, complex FES models are very computationally expensive at best, and impossible at worst. The R2S method applied to a full-scale, 3D FES become impractical due to the need for accurate space- and energy-dependent fluxes generated by MC codes throughout the geometry. Biasing the photon transport step is a straightforward application of the CADIS method *need source*. The detector response function can be set equal to the photon flux tally fitted with flux-to-dose-rate conversion factors. The adjoint flux can then be used as an importance function to determine source and transport biasing parameters *need source*. Biasing the neutron transport step, however, is not as straightforward. The response function depends on the subsequent computational steps of activation and decay photon transport [5]. The Multi-Step Consistent Adjoint Driven Importance Sampling (MS-CADIS) method was developed to increase the efficiency of the neutron transport step of the SDR calculation process [5]. It uses an importance function to bias the neutron transport that represents the importance of neutrons to the final SDR. As shown before in Eq. *need eqn number*, the detector response can be expressed as the integral of the importance function, I, times the source distribution, q

$$R = \int_V \int_E I(\overrightarrow{r}, E) q(\overrightarrow{r}, E) dV dE \tag{20}$$

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