APPLICATION OF THE DISCRETE ORDINATES ADJOINT FUNCTION TO ACCELERATE MONTE CARLO REACTOR CAVITY DOSIMETRY CALCULATIONS

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ABSTRACT

The deterministic adjoint function is employed to accelerate Monte Carlo reactor cavity dosimetry calculations. Equations for calculating source biasing parameters and weight window lower bounds based on contribution to detector response are developed. The facilities to calculate and use these parameters have been incorporated into the MCNP code. Use of the adjoint function is shown to increase the calculational efficiency of the reaction rate calculation by more than a factor of 4 and improve the statistical convergence, with respect to our best manually optimized model. Further, the use of the adjoint function does not require the intuition, guess work, and/or iterative process typical of current variance reduction techniques.

I. INTRODUCTION

Reactor cavity dosimetry is performed to benchmark models for pressure vessel fluence calculations. These calculations are used to estimate RPV integrity and provide a basis for plant life extension, and therefore, their accuracy is of great importance. In the past, the discrete ordinates method was used, almost exclusively, to perform these calculations. More recently, the Monte Carlo method, which is considered to be the most accurate method available for solving radiation transport problems, has been employed for this application in an effort to better understand the uncertainties associated with the discrete ordinates method and to attempt to benchmark the discrete ordinates calculations.[1-3] However, due to its nature of simulating individual particles and inferring the average behavior of the particles in the system from the average behavior of the individually simulated particles, the Monte Carlo method is extremely computationally expensive. In fact, for many reactor applications, as well as medical and nuclear-well logging applications, the computer time required by the Monte Carlo method is still considered prohibitive and/or impractical. Therefore, for difficult problems such as the cavity dosimeter calculation, where the probability that a particle contributes to the detector of interest is small, some effective means of variance reduction must be used to accelerate the calculation. In fact, for problems of this magnitude the analog Monte Carlo method is not capable of producing results with sufficient precision in a realistic amount of time.

To make Monte Carlo calculations computationally practical we employ our basic knowledge of the physics of the problem and the available variance reduction techniques to coerce *important*

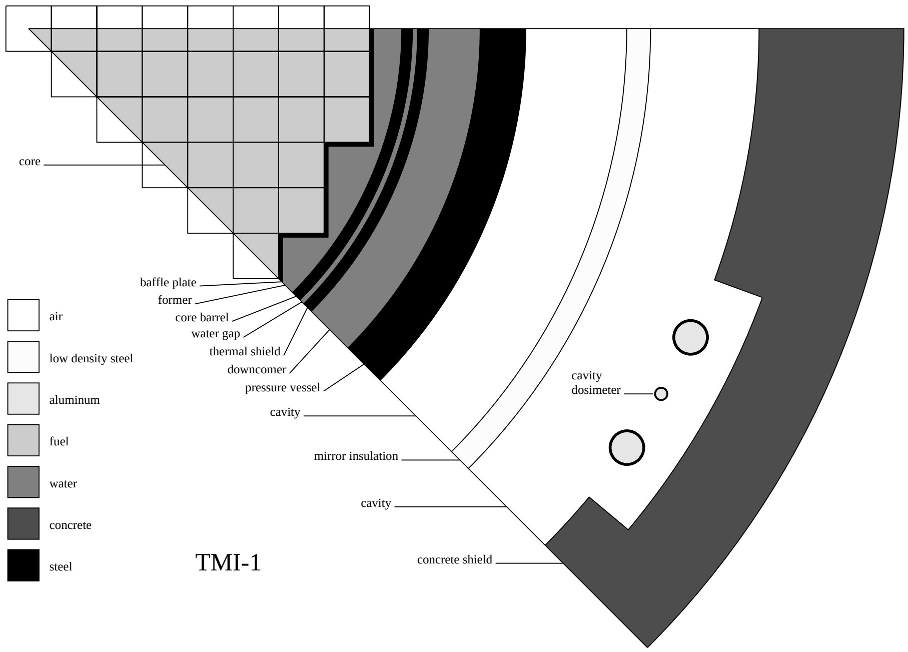

Figure 1: One Octant of the Three Mile Island unit 1 (TMI-1) Reactor

particles to contribute to the quantity of interest (e.g., reaction rate, dose, etc.). Most variance reduction techniques, however, are not straightforward to use since they depend on various parameters which vary significantly with problem type and objective. Thus, one typically engages in an iterative process to develop the variance reduction parameters and arrive at some acceptable level of calculational efficiency. Finally, it should be mentioned that automatic importance generators, such as the weight window generator in MCNP[4], are currently available, but they are restricted by their statistical nature and are of limited use in multi-dimensional deep-penetration problems. Therefore, it is apparent that a deterministic means of generating problem dependent importances would be very beneficial for applying the Monte Carlo method to large problems.

It has long been recognized that the adjoint function (i.e., the solution to the adjoint Boltzmann transport equation) has physical significance as a measure of the importance of a particle to some objective function (e.g., the response of a detector)[5]. It is this physical interpretation that, in theory, makes the adjoint function well suited for use as an importance function for biasing certain types of Monte Carlo calculations. Specifically, problems involving a small detector region(s) at a large distance from the source, such as the reactor cavity dosimetry calculation which attempts to estimate reaction rates at a distance of approximately 350cm from the core centerline. The problem is illustrated in Fig. 1

In this paper, we investigate the procedure and subsequent benefits of using the deterministic adjoint (importance) function to accelerate the reactor cavity dosimetry calculation.

II. THEORY

The adjoint operator $H^\dagger$ is defined by the following identity[5]

$$\langle \Psi^\dagger H \Psi \rangle \;=\; \langle \Psi H^\dagger \Psi^\dagger \rangle$$

where $\langle\rangle$ signify integration over all the independent variables. From this identity, we can show that the response R at some detector with some objective function σ_d is given by

$$R \;=\; \langle \Psi^\dagger q \rangle \;=\; \langle \Psi \sigma_d \rangle, \tag{1}$$

where q is the source density and $\Psi^\dagger$ is the adjoint function.

For the acceleration of the Monte Carlo calculation, we use $\Psi^\dagger$ to more efficiently sample the source of particles as well as the transport of the particles through the medium. To this end, we calculate a biased source energy and spatial distribution $q_b(r, E)$ based on the detector response from the source[6]

$$q_b(r, E) \;=\; \frac{R(r, E)}{\int_V \int_E R(r, E) dE dV} \;=\; \frac{\Psi^\dagger(r, E) q(r, E)}{\int_V \int_E \Psi^\dagger(r, E) q(r, E) dE dV} \tag{2}$$

Physically, the numerator is the detector response from the space-energy element (dV, dE), and the denominator is the total detector response. Therefore, the ratio is a measure of the total contribution to the detector response from the space-energy element (dV, dE).

Since we are biasing the source variables, the statistical weight of the source particles will have to be corrected such that

$$q_b(r, E)\; W(r, E) \;=\; q(r, E). \tag{3}$$

Substituting (Eq. 2) into (Eq. 3) and rearranging, we obtain the following expression for the statistical weight of the particles W

$$W(r, E) \;=\; \frac{\int_V \int_E R(r, E) dE dV}{\Psi^\dagger(r, E)} \;=\; \frac{q(r, E)}{q_b(r, E)}. \tag{4}$$

To use the weight window facilities within MCNP, we need to calculate weight window lower bounds W_l such that the statistical weights defined in (Eq. 4) are at the center of the weight windows (intervals). The width of the interval is controlled by the parameter C_u, which is the ratio of upper and lower weight window values ($C_u = \frac{W_u}{W_l}$). Therefore, the weight window lower bounds W_l are given by

$$W_l(r, E) \;=\; \frac{W(r, E)}{(\frac{C_u+1}{2})} \;=\; \frac{\int_V \int_E R(r, E) dE dV}{\Psi^\dagger(r, E)} \frac{1}{(\frac{C_u+1}{2})} \;=\; \frac{q(r, E)}{q_b(r, E)} \frac{1}{(\frac{C_u+1}{2})}. \tag{5}$$

Since we derived expressions for the source biasing parameters and weight window lower bounds in a consistent manner, the statistical weights of the source particles ($W(r, E) \;=\; \frac{q(r,E)}{q_b(r,E)}$) are within the weight windows as desired.

It is important to note that if the statistical weights of the source particles are not within the weight windows, the particles will immediately be split or rouletted in an effort to bring their weight into the weight window.[4] This will result in unnecessary splitting/rouletting and a corresponding degradation in computational efficiency.

III. METHODOLOGY

As mentioned, utilization of the adjoint function to increase the efficiency of a Monte Carlo calculation is not a new idea,[6] but it is also not typically considered practical for realistic problems. This is due to the fact that the manual procedure for using the deterministic adjoint function to accelerate a Monte Carlo calculation may proceed as follows:

(1) model the problem with a Monte Carlo transport code,

(2) model the problem with a deterministic (e.g., discrete ordinates) code, and calculate the adjoint function for an appropriate response function (adjoint source), and

(3) overlay the spatial and energy dependent adjoint function onto the Monte Carlo model in an appropriate manner.

The first of these three tasks is obviously necessary to perform any Monte Carlo calculation, and is described in some detail for this particular application in Ref. [3]. However, the Monte Carlo modeling in this case is greatly simplified in the sense that it does not require the implementation of any variance reduction techniques. The second task overlaps the first task to some degree, but still requires a significant amount of work related to cross-section and spatial mesh preparation. The details of the discrete ordinates model can be found in Ref. [7]. For many reactor applications, however, deterministic models may already exist, thus eliminating the most tedious of the above steps.

In this paper, we concentrate on performing the third task, and evaluate the benefits of this technique with respect to manually optimizing the calculation. Our *reference*, or manually optimized, model takes advantage of the following variance reduction techniques: energy cutoff, source variable (space, energy, and angle) biasing, weight windows, and exponential transformation. With a crude approximation for the initial weight window values, the weight window generator was used in an iterative process to develop weight window values for two energy groups. Acceptance of the final set of weight window values was dictated by calculational efficiency and proper statistical convergence.

For this application, the ^{63}Cu(n,α), ^{58}Ni(n,p), and ^{54}Fe(n,p) reaction rates (responses), which have thresholds energies of ~5.0, ~1.0, and ~1.0 MeV, respectively, are all of equal interest, and thus we calculate a representative reaction rate as a weighted average of each of the normalized reaction rates based on the width of the energy range affected and the sensitivity to that energy range. Using this representative response function, we can generate an importance function that will simultaneously optimize the calculation for all three reaction rates, and thus avoid calculating an importance function for each individual response that would require three separate Monte Carlo calculations.

With this representative response function as the adjoint source, we calculate a 2-D R-θ adjoint function with the DORT[8] code using the SAILOR[9] P_3 47-group library and a symmetric S_8 quadrature set. Figure 2 shows this adjoint function distribution for energy group 3 (10.00-12.14 MeV). A modified version of MCNP reads the adjoint function from the standard DORT binary flux file, couples the original source distributions with the adjoint function to generate the source biasing parameters and spatially averaged weight window lower bounds, and then performs the

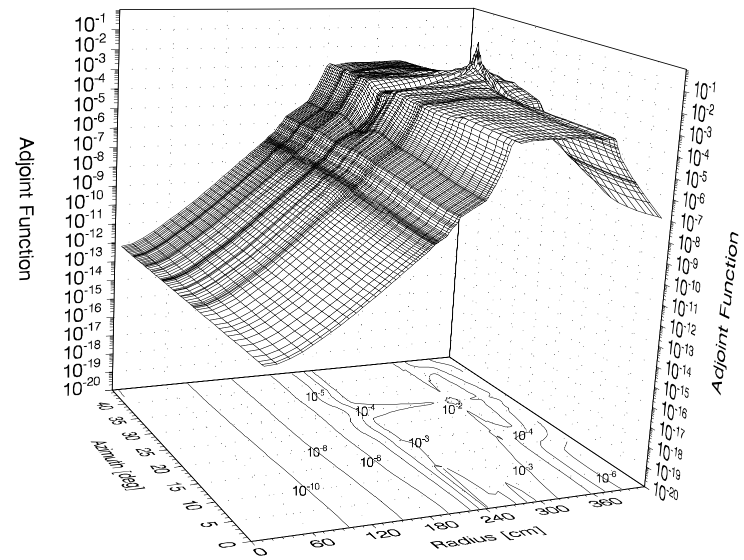

Figure 2: Adjoint Function Distribution for Energy Group 3 (10.00-12.14 MeV)

transport calculation. Within MCNP the source spatial distribution is represented by a probability distribution function at 24 axial locations in each fuel pin of the last two (peripheral) layers of assemblies and the energy distribution is based on an equivalent fission spectrum for the U and Pu fissile isotopes.[10] The following approximations/assumptions are made in this process: (1) the axial behavior for the adjoint function is approximated with a cosine distribution, (2) the MCNP geometry has been previously sub-divided to facilitate the use of spatial weight windows (i.e., cells in areas of rapidly changing importance are less than ∼2 mean-free-paths thick), and (3) to represent the spatial dependence of the energy biasing parameters, the energy dependent adjoint function is averaged over each source cell, and a dependent source energy biasing distribution is calculated for each source cell. No modifications to the source routines are necessary, since the capabilities to handle source variable biasing and dependent source distributions are standard features of the MCNP code.

IV. DISCUSSION OF RESULTS

Since the focus of this paper is on the acceleration of the calculation and not on the calculation itself, the interested reader is referred to the references for discussions regarding the accuracy of results with respect to measurements and discrete ordinates calculations, as well as sensitivity studies related to various aspects of this calculation. However, to provide some idea about the accuracy and to demonstrate that the acceleration technique does not bias the calculation, calculated-to-experimental (C/E) ratios, corresponding to ENDF/B-V transport and SAILOR dosimetry cross-sections, are given in Table 1. The differences between C/E ratios calculated with

Table 1: C/E Ratios at the Cavity Dosimeter for TMI-1

Reaction	Manually Optimized		Adjoint Importance	
	C/E	FOM	C/E	FOM
^{63}Cu(n,α)	0.905 (0.022)[a]	3.7	0.928 (0.015)	18
^{54}Fe(n,p)	0.965 (0.023)	3.5	0.977 (0.013)	21
^{58}Ni(n,p)	0.947 (0.020)	4.5	0.953 (0.013)	24

[a] 1σ uncertainties

the manually optimized model and with the adjoint importance function are within the statistical uncertainties. Table 1 also lists the associated figure of merits (FOM) $[FOM = 1/(RE)^2 T]$, where RE is the relative error, and reveals that the use of the adjoint importance function increases the calculational efficiency by more than a factor of 4 with respect to our *best* manually optimized importance function.

Without the use of variance reduction techniques, the calculation of reaction rates at the cavity dosimeter with sufficient precision is not feasible. However with the use of the adjoint function, the computer time required by the MCNP model to calculate the reaction rates at the ex-vessel cavity dosimeter with 1σ uncertainties of less than 3% is ~1 hour on an IBM RISC/6000 model 370. This behavior is demonstrated in Fig. 3 which plots relative error and $\frac{C}{\sqrt{T}}$ (where C is a constant and T is computer time) versus computer time for the three reaction rates of interest. The two sets of curves in Fig. 3 correspond to calculations performed with different importance functions; namely, the manually optimized importance function generated with the assistance of the weight window generator (2 energy groups) and an importance function derived from a 2-D adjoint function distribution (18 energy groups) using the representative response function.

It is important to note that the relative error RE follows the expected behavior predicted by the Central Limit Theorem ($RE \sim \frac{1}{\sqrt{N}} \sim \frac{1}{\sqrt{T}}$; where N is the number of particle histories), which indicates the validity of the calculated relative errors. Moreover, the use of the adjoint importance function clearly leads to smoother statistical convergence, thereby producing more reliable error estimations.

It should be noted that the aforementioned computer times do not include the discrete ordinates adjoint calculation. Also, for the purpose of comparison, the forward reaction rate calculation (18 group, $E > 1.0MeV$) with discrete ordinates (DORT) requires 3 individual calculations, R-Θ, R-Z, and R; which require approximately 40 minutes of total computer time.

V. CONCLUSIONS

The usefulness of the adjoint function for biasing Monte Carlo reactor cavity dosimetry calculations has been demonstrated, and a procedure for doing so has been briefly discussed. The adjoint (importance) function has been shown to increase the efficiency of the reaction rate calculation by a more than a factor of 4 and improve the statistical convergence. Further, the use of the adjoint function does not require the intuition, guess work, and/or manual intervention typical of current

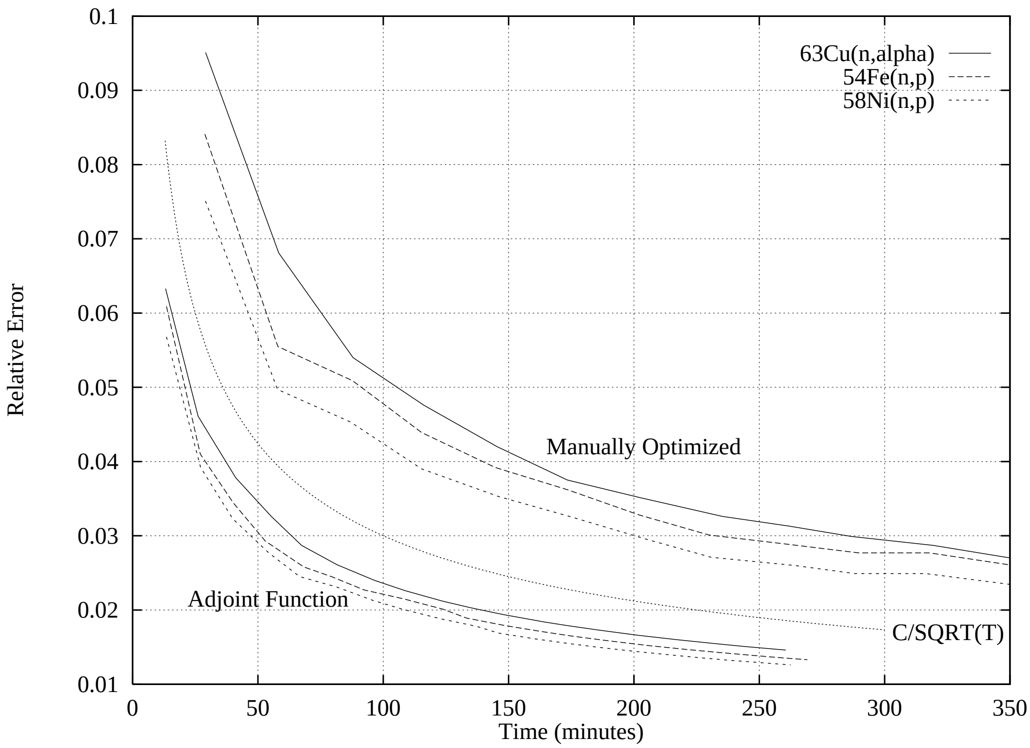

Figure 3: Relative Error vs Computer Time

variance reduction techniques (or importance function generators), thus significantly reducing the analyst's time for performing these calculations.

In reference to the use of variance reduction techniques in Monte Carlo, it is often said that "their use is more of an art than a science." However, the use of the adjoint function, as described in this paper, is based on physics (science), and thus it can reduce and even possibly eliminate the *art* from many Monte Carlo calculations.

VI. ON-GOING DEVELOPMENT

In an effort to develop a useful tool that will take full advantage of the adjoint function for biasing Monte Carlo deep-penetration problems, the following capabilities are being investigated and/or implemented: (1) automatically superimposing the discrete ordinates spatial mesh onto the MCNP problem in a transparent and efficient manner, (2) utilization of the angular dependent discrete ordinates adjoint function, and (3) automatic discrete ordinates mesh generation from the MCNP combinatorial geometric description.

ACKNOWLEDGMENTS

The authors would like to acknowledge the financial support provided by the GPU Nuclear Corporation, the equipment grant (two IRM RISC/6000 workstations) by the IBM Corporation, and the computer resources provided by the Penn State Center for Academic Computing.

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