ACCELERATION OF MONTE CARLO REACTOR CAVITY DOSIMETRY CALCULATIONS WITH THE DISCRETE ORDINATES ADJOINT FUNCTION

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ABSTRACT

The discrete ordinates 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 importance sampling are developed. The facilities to calculate and use these parameters directly have been incorporated into the MCNP code. Use of the adjoint function is shown to increase the 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 characteristic of current variance reduction techniques.

1. Introduction

Reactor cavity dosimetry is performed to benchmark models for pressure vessel fluence calculations. These calculations attempt to estimate reaction rates at a distance of ~350 cm from the core centerline and are used to estimate RPV integrity and provide a basis for plant life extension. In the past, the discrete ordinates (S_N) method was used to perform these calculations. More recently, the Monte Carlo method has been employed for this application in an effort to better understand uncertainties associated with the S_N method and to attempt to benchmark S_N calculations.[1,2]

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 applications the computer time required by the analog Monte Carlo method is prohibitive. Therefore, for difficult problems in which the probability that a particle will contribute to the detector of interest is small, some form of variance reduction or biasing must be applied. Herein, the expressions *variance reduction* and *biasing* refer to *fair-game* techniques used in Monte Carlo calculations to reduce the computer time required to obtain results of sufficient precision.

The application of variance reduction techniques can be quite difficult for realistic problems that are often complex and three-dimensional. The shielding analyst

typically engages in an iterative process to develop the variance reduction parameters; converging at some acceptable level of calculational efficiency. Unfortunately, the appropriate variance reduction parameters vary significantly with problem type and objective. Therefore, the iterative steps must be repeated for calculations with different objectives. Automatic importance generators, such as the weight window generator in MCNP (Ref. 3), are currently available, but are restricted by their statistical nature and are of limited use in multi-dimensional deep-penetration problems. In the absence of more sophisticated methods, however, the weight window generator is a very useful tool in determining the variance reduction parameters.[4]

A further difficultly lies in the statistical convergence of the Monte Carlo results. For large complex applications, it is not uncommon to spend days (and possibly weeks) iterating and adjusting the variance reduction parameters only to achieve reasonable efficiency with unstable statistical behavior. This unstable statistical behavior is caused by improper use of the variance reduction methods (i.e., insufficient detail and/or inappropriate selection of the parameters) and is usually the result of undersampling some important region of the problem phase-space.[5] Further, this undersampling is often difficult to identify and correct.

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 the detector).[6] This physical interpretation, in theory, makes the adjoint function well suited for use as an importance function for biasing Monte Carlo calculations.

In this paper, we demonstrate a procedure for using the S_N adjoint function to accelerate Monte Carlo calculations through source biasing and consistent transport process biasing using the weight window technique. This procedure is applied to a realistic calculation, namely the reactor cavity dosimetry calculation, and the increase in calculational efficiency is quantified.

2. Theory

Problems that can be solved by the Monte Carlo method are essentially equivalent to integrations.[7] For example, the goal of most Monte Carlo particle transport problems is to calculate the response (i.e., flux, dose, reaction rate, etc.) at some location. This is equivalent to solving the following integral

$$R = \int_{4\pi} \int_V \int_E \Psi(r, E, \hat{\Omega}) \sigma_d(r, E) dE dV d\hat{\Omega}, \tag{1}$$

where Ψ is the particle flux and σ_d is some objective function.

From the following identity[6]

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

where $H^\dagger$ is the adjoint operator and $\langle\rangle$ signify integration over all the independent variables, one can show that the response R (under certain boundary conditions) is also given by

$$R = \int_{4\pi} \int_V \int_E \Psi^\dagger(r, E, \hat{\Omega}) q(r, E) dE dV d\hat{\Omega}, \tag{2}$$

where $\Psi^\dagger$ and $q(r,E)$ are the adjoint function and source density, respectively, and (Eqs. 1 and 2) are equivalent expressions for R.

To solve this integral the independent variables are sampled from $q(r,E)$, which is not necessarily the best probability density function (*pdf*) from which to sample. An alternative *pdf*, $\hat{q}(r,E)$, can be introduced into the integral as follows:

$$R \;=\; \int_V \int_E \left[\frac{\Psi^\dagger(r,E) q(r,E)}{\hat{q}(r,E)} \right] \hat{q}(r,E) dE dV, \tag{3}$$

where $\hat{q}(r,E) \geq 0$ and $\int_V \int_E \hat{q}(r,E) dV dE = 1$.

From importance sampling[8], the alternative *pdf*, $\hat{q}(r,E)$, that will minimize the variance for R is then given by

$$\hat{q}(r,E) \;=\; \frac{\Psi^\dagger(r,E) q(r,E)}{R}. \tag{4}$$

Thus to accelerate the Monte Carlo calculation, the source energy and positions are sampled from the biased source distribution $\hat{q}(r,E)$. Physically, the numerator is the detector response from the space-energy element (dV, dE), and the denominator is the total detector response R. Therefore, the ratio is a measure of the contribution to the detector response.

Since the source variables are sampled from a biased *pdf*, the statistical weight of the source particles must be corrected such that

$$\hat{q}(r,E)\; W(r,E) \;=\; q(r,E). \tag{5}$$

Substituting (Eq. 4) into (Eq. 5) and rearranging, we obtain the following expression for the statistical weight of the particles

$$W(r,E) \;=\; \frac{R}{\Psi^\dagger(r,E)} \;=\; \frac{q(r,E)}{\hat{q}(r,E)}. \tag{6}$$

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. 6) 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

$$W_l(r,E) \;=\; \frac{W}{(\frac{C_u+1}{2})} \;=\; \frac{R}{\Psi^\dagger(r,E)} \frac{1}{(\frac{C_u+1}{2})}. \tag{7}$$

It is important to note that we have derived expressions for source biasing parameters and weight window lower bounds in a consistent manner, and thus the statistical weights of the source particles ($W(r,E) = \frac{q(r,E)}{\hat{q}(r,E)}$) are within the weight windows as desired. 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

weights into the weight windows.[3] This will result in unnecessary splitting/rouletting and a corresponding degradation in computational efficiency.

3. Implementation into MCNP

3.1 Overlay of Importance Function

The general version of MCNP provides facilities for energy and cell dependent weight windows. In order to use a fine spatial weight window grid (which is necessary in optically thick regions), the user must subdivide the cell based geometry into many cells. The subdivision of the geometry into a very large number of cells is time consuming and can actually degrade the efficiency of the calculation. Further, there are no general guidelines for this geometric discretization. For this reason, we use the S_N spatial mesh description to construct a separate, but related, geometric grid to facilitate the use of the adjoint distribution. This is done with a modified version of the MCNP code that is able to read the binary flux file (which contains the adjoint function and the spatial mesh and energy group information) from the standard S_N DORT (Ref. 9) code and superimpose the variable spatial mesh and energy grid onto the MCNP problem.

3.2 Weight Checking

Various concepts for minimizing the amount of computational *overhead* associated with this process have been examined. An issue of concern is the determination of the appropriate time (or event) to check the particle's statistical weight. This is important for the following reasons: (1) because the MCNP geometry does not need to be manually subdivided to facilitate the spatial importances, the presently available weight checks (i.e., at collisions and surface crossings) are no longer sufficient to control particle weight and thus large differences in the weight scored by individual particles are possible, (2) there is a computational cost or penalty each time the weight is checked, and this penalty is the time required by the searching routines to determine the importance of the phase-space within which the particle resides, and (3) more frequent checking leads to more reliable results with well-behaved statistical convergence, but at some point the calculational efficiency is sacrificed. Therefore, it is clear that we need to determine an optimum or near-optimum criteria for checking particle statistical weights. Moreover, it is desirable that this criteria be problem independent.

Since the mean free path (*mfp*) is, by definition, the average distance a particle travels between collisions, it is a logical, problem independent parameter by which particle statistical weight can be controlled. Parametric studies analyzing the effect of the increment of *mfp* on problem efficiency and reliability are described in Ref. 10.

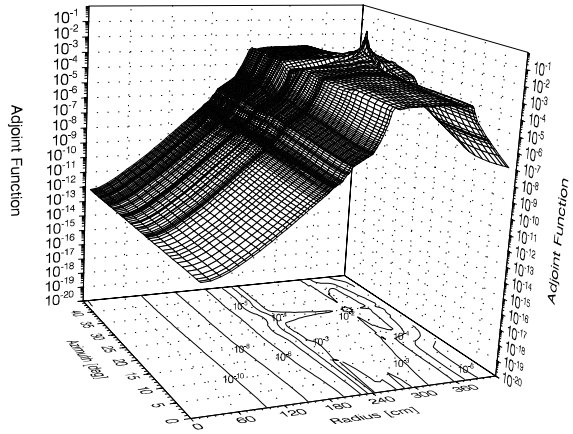

Fig. 1. Adjoint for Energy Group 3

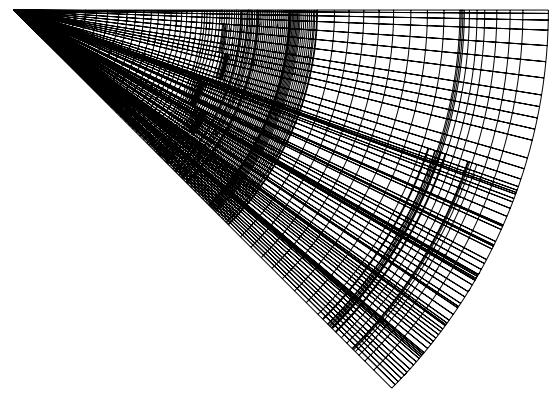

Fig. 2. S_N Spatial Mesh

4. Analysis

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 $\sim$5.0, $\sim$1.0, and $\sim$1.0 MeV, respectively, are all of equal interest, and thus we calculate an effective response function as the normalized sum of each of the normalized response functions. Using this effective 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 effective response function as the adjoint source, a 2-D R-θ adjoint function is calculated with the DORT code using the SAILOR P_3 47-group library[11] and a symmetric S_8 quadrature set. Figure 1 shows this adjoint function distribution for energy group 3 (10.00-12.14 MeV). The modified version of MCNP reads the adjoint function, couples the original source distributions with the adjoint function to generate the source biasing parameters and weight window lower bounds, and then performs the transport calculation. The S_N spatial mesh which is used within MCNP to facilitate the spatial importance distribution is shown in Fig. 2. The following approximations/assumptions are made in this process: (1) the axial behavior for the adjoint function is approximated with a cosine distribution, and (2) to represent the spatial dependence of the energy biasing parameters, the energy dependent adjoint function is averaged over each user defined spatial source cell, and a dependent source energy biasing distribution is calculated for each source cell. For this particular application, each assembly has an associated source energy biasing distribution.

Since the focus of this paper is the acceleration procedure, the interested reader is

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	0.887 (0.038)[a]	16
^{54}Fe(n,p)	0.965 (0.023)	3.5	0.944 (0.033)	20
^{58}Ni(n,p)	0.947 (0.020)	4.5	0.886 (0.032)	22

[a] 1σ uncertainties

referred to the references for discussions regarding the accuracy of results with respect to measurements and S_N calculations, as well as sensitivity studies related to various aspects of this calculation. However, to provide some indication of 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 material cross sections and SAILOR dosimetry cross-sections, are given in Table 1. The differences between C/E ratios calculated with the manually optimized model and with the adjoint importance function are within the statistical uncertainties.

4.1 Calculational Efficiency

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 $\sim$1 hour on an IBM RISC/6000 model 370. To reach the same precision (3%) with the manually optimized model requires nearly 5 hours of CPU time. 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 effective 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 estimated relative errors. Moreover, the use of the adjoint importance function clearly leads to smoother statistical convergence, thereby producing more reliable error estimations. All three reaction rate tallies pass all 10 of the MCNP statistical checks[3], providing an additional indication of proper statistical convergence.

Table 1 lists the figure of merits (FOM) [$FOM = 1/(RE)^2T$] and reveals that the use of the adjoint importance function increases the calculational efficiency by a

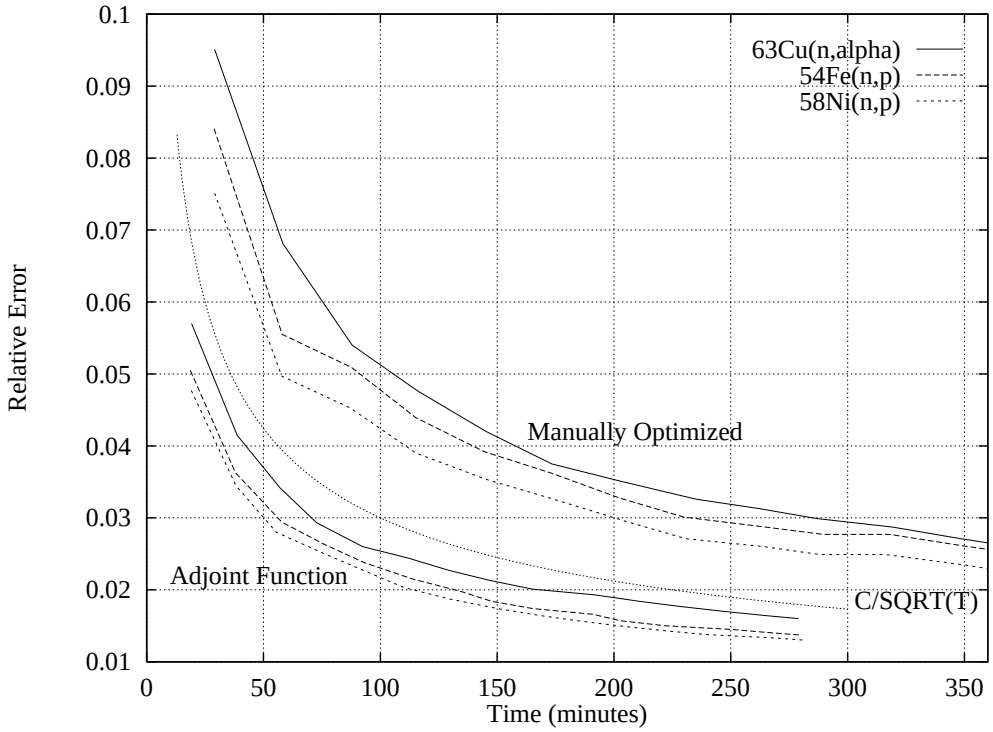

Fig. 3. Relative Error vs Computer Time

factor of 4 with respect to our *best* manually optimized importance function.

The aforementioned computer times do not include the S_N adjoint calculation. Also, for the purpose of comparison, the S_N reaction rate calculation (18 group, $E > 1.0 MeV$) requires 3 individual DORT calculations, R-Θ, R-Z, and R; which require ~40 minutes of total computer time.

5. Summary

A general method for accelerating Monte Carlo transport calculations through source biasing and consistent transport process biasing has been presented. This method is implemented into the general purpose Monte Carlo code MCNP and applied to a realistic calculation, namely the reactor cavity dosimetry calculation. With the use of the adjoint (importance) function, the efficiency of the reaction rate calculation is shown to increase by factor of 4 and the statistical convergence is improved. Further, the use of the adjoint function does not require the intuition, guess work, and/or manual intervention typical of current variance reduction techniques (or importance function generators), thus significantly reducing the analyst's time for performing these calculations.

The limitation to this approach is the requirement of an S_N adjoint solution. Therefore, strategies for generating input files for S_N calculations directly from MCNP

input files are being developed. Coupling the work described in this paper with these strategies will result in the automation of the generation and application of the adjoint function for MCNP calculations.

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