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MONTE CARLO VARIANCE REDUCTION WITH DETERMINISTIC IMPORTANCE FUNCTIONS

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Abstract: Recent trends in Monte Carlo code development have reflected a recognition of the benefits of using deterministic importance functions for Monte Carlo variance reduction. This paper offers a review of the use of deterministic importance functions for variance reduction of Monte Carlo simulations. Adjoint methodology and the concept of "importance" are presented, along with an explanation of their use for variance reduction. Relevant works from a number of different researchers are briefly reviewed. The authors' CADIS methodology for calculating consistent source biasing and weight window parameters based on deterministic importance functions is presented. Efforts to automate the generation and use of deterministic importance functions are briefly described, including an overview of the A^{3}MCNP code. Finally, aspects of interest, including computational benefits, associated with using deterministic importance functions for Monte Carlo simulation of real-world problems are demonstrated.

Keywords: Monte Carlo: variance reduction: radiation transport: adjoint transport

1. INTRODUCTION

The Monte Carlo method is one of the most accurate techniques for particle transport simulation. The method is applied to two major classes of nuclear problems: 1) fixed-source/shielding and 2) eigenvalue/criticality. Fixed source problems mainly involve transport of particles through thick shields that may cause a significant amount of absorption and/or scattering (isotropic/anisotropic), resulting in significant changes in particle energy and direction. This means that particle count in small energy bins

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and/or localized spatial regions may be extremely small, and consequently, a large number of experiments (histories) and long computational times are needed to achieve statistically reliable results. In eigenvalue problems, since the source is not known, there is an added difficulty associated with the need for achieving global source convergence before starting tally accumulation. For loosely coupled and/or sub-critical systems, this may result in false source convergence, impact the reliability of simulations, and ultimately lead to an under-estimation of the eigenvalue - which is a very troublesome safety issue. In recent years, some efforts have been devoted to performing Monte Carlo perturbation and depletion calculations that generally require even longer computing times. Monte Carlo perturbation for both fixed-source and eigenvalue problems has further difficulties associated with being able to distinguish between the statistical errors ($RE = \frac{\sigma_{\bar{x}}}{\bar{x}}$) and the change caused by a perturbation. Moreover, Monte Carlo depletion, because of the need for global results, generally requires impractically large amounts of computer time.

Over the past several decades, a large number of techniques have been developed to reduce the variance of Monte Carlo calculations, referred to as variance reduction and/or biasing techniques. These techniques commonly modify the natural sampling procedure/formulation (related to physical laws of particle transport) to focus computational efforts on the simulation of "important" particles. To compensate for this modification and to conserve particles, each particle is given a statistical weight that is adjusted based on the following equality,

$$w_{biased}\ pdf_{biased} = w_{unbiased}\ pdf_{unbiased}, \tag{1a}$$

where ***pdf*** refers to the probability distribution of the physical process being sampled and ***w*** refers to the particle weight. It is worth noting that in special cases such as integer splitting (i.e., one particle is split into ***n*** particles), one considers a modified form of to Eq. 1a, given by

$$n \times w_{biased}\ pdf_{biased} = w_{unbiased}\ pdf_{unbiased}, \tag{1b}$$

where $\boldsymbol{pdf_{biased} = pdf_{unbiased}} = 1$. In this situation the physical process is changed rather than the probability of its occurrence.

The main difficulty associated with using variance reduction techniques is the determination of the problem-dependent variance reduction parameters present in the biased terms (i.e., $\boldsymbol{pdf_{biased}}$ or ***n***). This paper reviews the use of deterministic importance functions for variance reduction of Monte Carlo calculations, with emphases on fixed-source/shielding problems.

1.1 Background

Variance reduction techniques can generally be classified into the following three categories: modified sampling methods (e.g., source biasing, implicit capture, discrete angle biasing, forced collisions, and exponential transformation), population control methods (e.g., splitting/roulette, weight cutoff, weight-windows, and stratification), and semi-analytic methods (e.g., point detectors and DXTRAN). A number of other techniques and/or modeling choices (e.g., point detectors and energy cutoff) may also be used to improve the efficiency of a Monte Carlo calculation; however these techniques are not generally considered to be variance reduction methods because they do not bias the random walk sampling. Standard "production" Monte Carlo codes such as MCNP (Briesmeister, 2000), MORSE (Emmett, 1975), MCBEND (Chucas et al., 1994), and TRIPOLI (Both et al., 1994) have numerous biasing techniques for different processes. Variance reduction techniques have been developed for optimization of different types of problems, resulting in numerous techniques. Among the variance reduction techniques, the transport biasing method of splitting/roulette has been the most effective and widely used approach for reducing the variance of Monte Carlo calculations (Lux and Koblinger, 1990). The technique of exponential transformation, which stretches the distance to collision in preferential directions, has been linked to the hypothetical zero-variance solution (Goertzel and Kalos, 1958), but is plagued by the potential for large weight fluctuations. Dwivedi

(1982) and Gupta (1984) derived a combined scheme in one-dimensional (1-D) homogeneous slabs in the mono-energetic case with isotropic scattering, consisting of exponential transformation and an appropriate angular biasing for collisions such that the angular biasing nearly cancels the weight fluctuations caused by exponential biasing. From this work, the methods in TRIPOLI (Both et al., 1994; Both et al., 1990; Morillon et al., 1993), and more recently the LIFT method (Turner, 1996; Turner and Larsen, 1997), have been developed that incorporate the concept of a zero-variance solution with angular biasing, exponential transformation, and weight windows. While these methods rest on a solid theoretical base, they assume the spatial component of the solution to be an exponential and impose restrictions on the energy treatment (multigroup) and in some cases, the angular scattering treatment. Further, these methods tend to be more sensitive to the accuracy of the importance function, require additional user input, and are generally less statistically stable and applicable than the splitting/roulette methods alone (Booth, 1992). Nevertheless, when used properly and appropriately these combined methods can be extremely powerful.

All variance reduction techniques require problem specific parameters that are dependent on the importance of particles with respect to the objective function, and therefore require experience and are difficult and time consuming to use. Booth and Hendricks (1984) state, "The selection [of parameters] is more art than science, and typically, the user makes a few short trial runs and uses the information these trials provide to better guess the parameters; that is, the user learns to adjust parameters on the basis of previous experience."

Responding to this difficulty and the concept of learning, a number of strategies for determining variance reduction parameters have been proposed and developed. MacDonald (1975) and MacDonald and Cashwell (1978) demonstrated that through the use of pattern recognition techniques, the calculation could learn and establish Monte Carlo splitting surfaces. The learning mechanics were quite involved, and the method worked with very limited success in complicated geometries. Deutsch and Carter (1977) showed that importances could be estimated at geometry surfaces during a forward Monte Carlo calculation, and subsequently used to assist the analyst in manually selecting variance reduction parameters. Goldstein and Greenspan (1980) developed a recursive (RMC) method for estimating the importance function distribution. The method involved extensively subdividing the geometric regions and solving the forward problem for region importances with varying degrees of accuracy. While this work was reasonably successful, it was concluded that for deep-penetration problems to be efficient, the relevant importance function distribution must be known with sufficient accuracy; insufficient accuracy can lead to significant errors in the prediction of the detector response. Further, Goldstein and Greenspan (1980) concluded that it is far better to invest more time in the importance estimation (the RMC calculation) than in the detector response calculation.

Booth (1982) and Booth and Hendricks (1984) developed an importance estimation technique called the forward-adjoint generator, which has since become known as the weight-window generator (Booth, 1983) because it estimates importances to be used with the weight-window technique. The weight-window technique, which is available in the standard version of MCNP, is simply a spatial- and energy-dependent facility by which splitting and Russian roulette are applied. The importance is estimated as the ratio of the total score due to particles (and their progeny) entering a cell to the total weight entering a cell, in a forward Monte Carlo calculation. At the time, the development and implementation of the weight-window generator represented a significant advancement in automated variance reduction.

Independently, another stochastic optimization method, the Direct Statistical Approach (DSA), was introduced by Dubi et al. (1982, 1990) and later extended by Burn (1990, 1995). In the DSA, expressions for the dependence of the second moment and the calculation time on the splitting parameters are derived. Hence, a unique and significant aspect of this method is that it explicitly attempts to minimize the cost of the calculation by considering both the computer time and the variance. In contrast, importance function based methods do not explicitly consider computer time, and thus the "optimum parameters" generated from importance function based methods can be far from optimal in terms of calculational efficiency. Splitting parameters are optimized based on initial "learning" calculations to estimate the second moment and time function. Similar to the weight-window generator, user intervention is required to adjust importances in regions that are poorly sampled and/or further subdivide the space and energy regions.

These stochastic approaches to estimating importances are basic to the forward learning Monte Carlo methods, and therein lies the fundamental difficulty. To accurately estimate the importance of a space-energy interval, a sufficient number of particles must pass through that space-energy interval and proceed to contribute to the objective. In practice, this condition is typically not met, and as a result, either no importance estimate or an unreliable importance estimate is generated for each space-energy interval (Booth and Hendricks, 1984; Culbertson and Hendricks, 1999). Therefore, current forward Monte Carlo importance generators 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 forward Monte Carlo importance generators, such as the weight-window generator, are very useful in the iterative process of determining variance reduction parameters (Booth and Hendricks, 1984; Booth, 1985a).

As a result of the difficulties associated with statistical importance estimation, many Monte Carlo practitioners and code developers have turned to deterministic methods for generating problem-dependent importances, particularly for large/complex 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) (Bell and Glasstone, 1970). It is this physical interpretation that makes the adjoint function well suited for use as an importance function for biasing Monte Carlo calculations. Kalos (1963) described the importance sampling technique and its relation to an importance function and a zero variance solution. Coveyou et al. (1967) developed several formulations for using the adjoint (importance) function to reduce the variance, and showed the merits of the importance function for transport and source biasing. Following these works, a number of applications of deterministic adjoint solutions and approximate adjoint solutions were made with varying degrees of success. A number of these efforts are discussed individually in a later section of this paper.

Although the idea of using deterministic adjoint (importance) functions for variance reduction of Monte Carlo calculations is not new, several issues related to obtaining and using the adjoint function remained unresolved. Specifically, issues associated with the generation and optimal usage of the deterministic importance function. For example, the creation of an input file for a deterministic transport code to perform a deterministic adjoint calculation requires substantial familiarity with deterministic methods and can be very time consuming. Therefore, automation of the deterministic adjoint calculation is necessary for being able to effectively reduce user and computation time requirements.

To overcome the shortcomings of available variance reduction techniques, the authors have developed: (1) the CADIS methodology, which provides formulations for consistent biasing of the source and transport processes based on deterministic adjoint functions, (2) algorithms for automatic generation of deterministic adjoint functions, and (3) algorithms for generation and usage of space- and energy-dependent source biasing parameters and weight windows. The CADIS methodology and aforementioned algorithms have been implemented into the MCNP code, resulting in a new version of the code, referred to as A^3MCNP (automated adjoint accelerated MCNP). These developments are briefly reviewed in this paper.

1.2 Outline

The remainder of this paper is organized as follows. Section 2 reviews selected important variance reduction techniques used for shielding/fixed source problems. Section 3 discusses the deterministic adjoint methodology and its use in Monte Carlo variance reduction, including a review of independent efforts related to the use of deterministic importance functions for variance reduction. Section 4 describes the authors' CADIS methodology for using deterministic importance functions for variance reduction. Section 5 discusses the automation of the use of deterministic importance functions for variance reduction as implemented in the A^3MCNP code. Section 6 discusses the application and performance of automated variance reduction (A^3MCNP) for the solution of three real-world fixed-source problems of interest to the nuclear industry. Finally, summary and concluding remarks are offered in Section 7.

2. VARIANCE REDUCTION METHODS

Variance reduction (biasing) techniques for Monte Carlo simulations can reduce the amount of computer time required for obtaining results of sufficient precision (Carter and Cashwell, 1975). The goal of all variance reduction techniques is to decrease the relative error,

$$RE = \frac{C}{\sqrt{N}}, \tag{2}$$

where N is the number of samples (particle histories) and $C = \frac{\sigma_x}{\bar{x}}$ is the relative error in the population of samples. Decreasing RE is accomplished by either decreasing C or increasing N, for a fixed amount of computer time. Unfortunately, these goals often conflict with each other because decreasing C requires better information from each history, which typically requires more computer time per history (Booth, 1985a). On the other hand, increasing N (for a fixed computer time) normally increases C because less computer time is spent per history. However, it is often possible to substantially decrease C without significantly decreasing N, and vice versa. Many of the techniques attempt to decrease RE by either producing or destroying particle histories, or both. In general, techniques that produce particles work by decreasing C (ideally much faster than N decreases) and techniques that destroy particles work by increasing N (ideally much faster than C increases).

As mentioned, there are numerous variance reduction techniques/strategies available. However, not all techniques are appropriate for all applications, and some techniques tend to interfere with each other (e.g., create large weight fluctuations when used together), while others tend to compliment each other. Several of the more widely used techniques for fixed-source/shielding applications are briefly reviewed below; the list is by no means exhaustive. More complete discussions may be found in several of the references (e.g., Briesmeister, 2000; Cramer and Tang, 1986; Lux and Koblinger, 1990)

2.1 Source Biasing

The source biasing technique enables the simulation of more source particles, with appropriately reduced weights, in the more important regions of each variable (e.g.. space, energy, and angle). This technique consists of sampling the source from a biased (non-analog) probability distribution rather than from the true (analog) probability distribution, and then correcting the weight of the source particles by the ratio of the actual probability divided by the biased probability according to Eq. 1. Thus, the total weight of particles started in any given interval is conserved, and an unbiased estimate is preserved. Source biasing is widely used to reduce the amount of computer time spent on simulating source particles in regions that do not contribute to the objective. The technique improves the information accumulated per particle history (decreases the average history variance), and thus decreases C.

2.2 Splitting/Roulette

Geometric splitting/Russian roulette is one of the oldest and most widely used variance reduction techniques, and when used properly, can significantly reduce the computational time of a Monte Carlo simulation. The objective of this technique is to spend more time sampling important spatial cells and less time sampling unimportant spatial cells. This is done by subdividing the problem geometry into cells and assigning each cell i an importance I_i. When a particle of weight w_o passes from a cell of importance I_i to a cell with higher importance I_j ($I_i < I_j$), the particle is split into $\nu = I_j/I_i$ identical particles of weight w_o/ν. Conversely, if a particle of weight w_o passes from a cell of importance I_i to a cell with lower importance I_k ($I_i > I_k$), Russian roulette is played and the particle is killed with probability 1 - (I_k/I_i), or followed further with probability I_k/I_i and weight $w_o \times I_j/I_k$.

For the case in which ν in an integer, the splitting process is straightforward. In contrast, when ν is not an integer (*i.e.*, $n<\nu<n+1$), the splitting is more complicated. There are two common approaches to noninteger

splitting, which are referred to as "sampled splitting" and "expected-value splitting" (Booth, 1985b). In sampled splitting, n particles of weight $w=w_o/v$ are selected with probability $q(n) = n+1-v$, or $n+1$ particles of weight $w=w_o/(n+1)$ are selected with probability $q(n+1)=v-n$. Sampled splitting conserves the total weight, but the weight of the individual split particles varies depending on the number of split particles chosen. In expected-value splitting, the expected number of particles, v, is always used to determine the weight of the split particles. The number of split particles are selected from the same probabilities used in sampled splitting, but the weight of the split particles is always taken to be $w=w_o/v$. Consequently, an expected-value split may result in a total after-split weight of either $n(w_o/v)$ or $(n+1)(w_o/v)$, and the weight is only conserved in the expected sense. However, unlike sampled splitting, there is no fluctuation in particle weight with an expected-value split. A theoretical comparison of the two techniques by Booth (1985b) concluded that the expected-value splitting is generally superior to sampled splitting, and hence the MCNP code uses expected-value splitting.

Energy splitting/roulette is similar to geometric splitting/roulette except that the splitting/roulette is performed on the energy domain rather that on the spatial domain. Splitting generally decreases the history variance (decreases C) but increases the time per history (decreases N for a fixed amount of computer time), whereas Russian roulette decreases the time per history (increases N for a fixed amount of computer time).

2.3 Weight-Window Technique/Weight-Window Generator

The weight-window technique (Booth and Hendricks, 1984), as implemented in the MCNP code, is a space- and energy- (or time) dependent splitting/roulette technique. The weight-window technique splits or roulettes particles based on space- and energy- (or time) dependent importances. The user supplies a lower weight bound and the width of the weight window for each energy interval of each spatial cell. If a particle's weight is below the lower weight bound, Russian roulette is performed, and the particle's weight is either increased to be within the weight window or the particle is terminated. On the other hand, if the particle's weight is above the upper weight bound, the particle is split such that the split particles have weights within the weight window. No adjustment is performed if the particle's weight is within the weight window.

Although weight windows and a combination of geometric splitting/roulette and energy splitting/roulette are both means of describing space- and energy-dependent importances and involve splitting and roulette, there are several important differences (Booth and Hendricks, 1984). These include: (1) the weight window discriminates based on particle weight before any action is taken, whereas geometric and energy splitting/roulette are performed without regard for particle weight, (2) the weight window utilizes absolute weights rather than ratios of importances, (3) the weight window can be applied at surfaces, collision sites, or both, whereas splitting/roulette is performed at space and energy boundaries only, (4) the weight window can assist in controlling weight fluctuations introduced by other variance reduction techniques by attempting to force all particles within a given space/energy region to have an associated weight within the weight window for that space/energy region, (5) the weight window can be turned off in selected space and energy regions, and (6) the weight windows can be generated via the weight-window generator.

The weight-window generator attempts to calculate the importance of each cell in the problem description. This is done by noting that the importance of a particle at a point in phase space is equal to the expected score a unit weight particle would generate. The importance of a cell can then be defined as the expected score generated by a unit weight particle after entering the cell. Thus, the cell's importance can be estimated as (Booth and Hendricks, 1984)

$$\textit{Importance} = \frac{\text{total score due to particles entering the cell}}{\text{total weight entering the cell}}. \tag{3}$$

The main difficulty associated with using this statistical importance generator comes from poor estimates of the importance function caused by the statistical nature of the generator. In other words, if a phase space is not properly sampled, either an unreliable importance estimate or no importance estimate will be generated.

As a result, the weight-window generator tends to require a crude approximation of the importance function in order to estimate a better one for subsequent calculations (Booth, 1985a). This typically leads to an iterative process, which ideally converges to an optimum importance function. A further difficulty has been the subdivision of the problem geometry to represent the variation of importance with the spatial weight windows (which were assigned to geometric cells). However, recent work (Liu and Gardner, 1997) has eliminated this difficulty by developing a geometry-independent weight-window generator. This capability has since been incorporated into the latest standard version of MCNP (Briesmeister, 2000).

From the above discussion it should be clear that the weight-window technique is superior to the use of both geometric and energy splitting/roulette. The most notable advantages of the weight-window technique are the discrimination of particle weight before any action is taken, the control of weight fluctuations introduced by other biasing techniques, and the generation of the space-and energy-dependent importances (i.e., the weight-window values). The most notable disadvantage of the weight-window technique is that the generator requires considerable user understanding and intervention to work correctly and effectively (Booth, 1985a).

2.4 Implicit Capture

Implicit capture, survival biasing, and absorption by weight reduction are synonymous. Implicit capture is a variance reduction technique that ensures that a particle always survives a collision (i.e., the particle is never absorbed). When implicit capture is used, rather than sampling for absorption with probability σ_{ai}/σ_{ti} (where σ_{ai} and σ_{ti} are the absorption and total microscopic cross sections for nuclide i, respectively), the particle always survives the collision and is followed with a new weight, $w_0 \times (1-\sigma_a/\sigma_t)$, where w_0 is the weight of the particle before the collision. Implicit capture can thus be thought of as a splitting process in which the particle is split into absorbed weight (which can be discarded) and surviving weight. The main advantage of implicit capture is that a particle that has reached the vicinity of the tally region is not absorbed just before a score is made. Implicit capture generally decreases the history variance (decreases C) but increases the time per history (decreases N for a fixed amount of computer time).

2.5 Exponential Transformation

Exponential transformation samples the distance to collision from a non-analog probability density function. Specifically, it involves stretching the distance between collisions in the direction of interest and reducing the distance between collisions in directions of little interest by modifying the total macroscopic cross section by

$$\Sigma_t^* = \Sigma_t(1 - p\mu), \tag{4}$$

where Σ_t^* is the modified total cross section, Σ_t is the true total cross section, p is the exponential transform parameter used to vary the degree of biasing $|p| < 1$, and μ is the cosine of the angle between the preferred direction and the particle's direction. The particle weight is adjusted so that the expected weight colliding at any point is preserved. It should be mentioned that the exponential transformation technique can produce large weight fluctuations and subsequently produce unreliable mean and variance estimates. Exponential transformation generally decreases the history variance (decreases C) but increases the time per history (decreases N for a fixed amount of computer time).

2.6 Problem Truncation

Although not generally considered to be a variance reduction technique, modeling assumptions that truncate the scope of a problem can be very effective for variance reduction. A simple example is geometry truncation, in which a finite calculational model with vacuum boundary conditions only includes regions that are important to the problem objective. Another example is when energy truncation is used to eliminate low

energy particles in problems in which the problem objective is not sensitive to low energy particles and the low energy particles have no means to gain sufficient energy to become important to the problem objective.

These problem truncations are not generally considered to be variance reduction methods because they do not involve a modification to the particle weight – a particle history is simply terminated if it exists the problem boundaries (e.g., space, energy, time). Unlike most variance reduction techniques, a poor problem truncation assumption (e.g., that neglects an important part of the problem), will not be apparent via unusual or erratic statistical convergence behavior. However, similar to other variance reduction techniques, problem truncation increases N for a fixed amount of computer time.

3. VARIANCE REDUCTION USING DETERMINISTIC "IMPORTANCE" FUNCTIONS

Variance reduction techniques require the assignment of input parameters by the user. These input parameters are dependent on the importance of particles with respect to the problem objective (i.e., an importance function), and therefore require *a priori* knowledge of the problem physics. Consequently, the use of variance reduction methods in Monte Carlo is not straightforward, and effective use of variance reduction methods typically requires a great deal of knowledge, experience, time, and effort. In practice, a manual iterative process is performed to develop the variance reduction parameters, converging to some acceptable level of calculational efficiency. Unfortunately, the appropriate variance reduction parameters vary significantly with problem type and objective. Therefore, the manual iterative process must be repeated to determine the variance reduction parameters for calculations (even for the same problem) with different objectives (e.g., different dose locations and/or reaction rates). A further difficulty lies in the statistical convergence of Monte Carlo results. For large complex applications, it is not uncommon for a Monte Carlo practitioner to spend days (or longer, depending on the problem, the user's experience, and the desired precision) iterating and adjusting the variance reduction parameters only to achieve reasonable efficiency with unstable statistical behavior. Variance reduction methods can exhibit unstable statistical behavior even when good importance functions are available. This unstable statistical behavior is an indictor of unreliable confidence intervals and potentially erroneous results, which, depending on the user's experience, may or may not be apparent to the user.

Although manually applied variance reduction by expert Monte Carlo practitioners has demonstrated potential for increases in computational performance on the order of thousands, a reliable automated variance reduction capability based on a deterministic importance function could yield superior computational performance and convergence reliability, while at the same time significantly reducing the requirements for user expertise, time, and effort. Generally speaking, one expects increased reliability with the use of accurate importance functions; however, depending on the problem characteristics and the variance reduction techniques involved, increased reliability may not always be achieved.

Recent trends in Monte Carlo code development have reflected a recognition of the benefits of using deterministic importance functions for Monte Carlo variance reduction (Larsen, 1999). In the following subsections, we introduce the adjoint transport equation and the importance function, and review its use for variance reduction of Monte Carlo simulations, including a brief review of research efforts in this area.

3.1 Adjoint Transport Equation

The linear time-independent Boltzmann transport equation for a non-multiplying system (Bell and Glasstone, 1970) expresses the particle balance in a phase space as

$$H\psi = q \text{ in } V, \tag{5a}$$

where

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

σ_s is the differential scattering cross-section, σ_t is the total cross-section, ψ is particle angular flux, q is particle source, and V refers to volume.

For a special case with vacuum boundary condition, i.e., "forward" flux is

$$\psi(r, E, \hat{\Omega}) = 0 \text{ for } \hat{n} \cdot \hat{\Omega} \leq 0 \text{ on A} \tag{6a}$$

and adjoint function is

$$\psi^+(r, E, \hat{\Omega}) = 0 \text{ for } \hat{n} \cdot \hat{\Omega} \geq 0 \text{ on A}, \tag{6b}$$

one can demonstrate the following "adjoint property",

$$\langle \psi^+, H\psi \rangle = \langle \psi, H^+\psi^+ \rangle, \tag{7}$$

is preserved and that the adjoint operator H^+ is given by

$$H^+ = -\hat{\Omega} \cdot \nabla + \sigma_t(\vec{r}, E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\vec{r}, E \to E', \hat{\Omega} \to \hat{\Omega}'). \tag{8}$$

Here $\hat{n}$ refers to the unit outward normal to the surface A and the Dirac signs, $\langle\ \rangle$, refer to integration over all independent variables, including space, energy, and angle. Note that H ("forward" operator, Eq. 5b) and H^+ ("adjoint" operator, Eq. 8) differ in the first and third terms, indicating a reversal of energy and directional transfers. To determine the adjoint function, ψ^+, one solves an equation of the form

$$H^+\psi^+ = q^+ \text{ in } V, \tag{9}$$

where q^+ is the adjoint source.

3.2 Adjoint Methodology

In this section, we introduce the use of the adjoint function ("adjoint methodology") through a simple example. Consider one is interested in determining the response, R, of a detector of volume V_d placed at a position in a volume V, which is placed in a vacuum. Based on the "forward" transport equation (Eq. 5), the formulation for response is given by

$$R = \int_{V_d} dV \int_0^\infty dE \int_{4\pi} d\Omega\ \sigma_d(\vec{r}, E) \psi(\vec{r}, E, \hat{\Omega}), \tag{10}$$

where σ_d is the detector cross-section (i.e., response function).

It is possible to derive an alternate formulation for the detector response in terms of the adjoint function. For this, we form the commutation relation between Eqs. 5a and 9. This means that we multiply the "forward" equation by the adjoint function and the adjoint equation by the flux, integrate both equations over all independent variables, and form their difference as given below

$$\langle \psi^+ H\psi \rangle - \langle \psi\ H^+\psi^+ \rangle = \langle \psi^+ q \rangle - \langle \psi q^+ \rangle \tag{11}$$

As discussed in Section 3.1 for a vacuum boundary condition, the left-hand side of the above equation is equal to zero, thereby reducing to

$$\langle \psi q^{+} \rangle = \langle \psi^{+} q \rangle \tag{12}$$

Now, if we consider

$$q^{+} = \sigma_d , \tag{13}$$

the left-hand side of Eq. 12 is the detector response (i.e. Eq. 10). Consequently we have derived an alternate formulation for the detector response in terms of adjoint function as

$$R = \langle \psi^{+} q \rangle , \tag{14}$$

where the adjoint function is determined via

$$H^{+}\psi^{+} = \sigma_d , \tag{15a}$$

$$\psi^{+} = 0 \text{ for } \hat{n}\cdot\hat{\Omega} \geq 0 \text{ on A.} \tag{15b}$$

The detector response, R, is given by the integral of the adjoint weighted source distribution. Thus, once the adjoint function is calculated for a given detector (or objective), responses from different sources can be determined by simple integration. This characteristic makes the adjoint function very useful for perturbation type studies.

3.3 "Importance" Function and its Relation to the Adjoint Function

If we consider a point source of the form

$$q(\bar{r}, E, \hat{\Omega}) = \delta(\bar{r} - \bar{r}_0)\delta(E - E_0)\delta(\hat{\Omega} - \hat{\Omega}_0) , \tag{16a}$$

in Eq. 14, we obtain

$$R = \psi^{+}(\bar{r}_0, E_0, \hat{\Omega}_0) . \tag{16b}$$

Therefore, the adjoint function is the contribution from particles produced at $\bar{r}_0, E_0, \hat{\Omega}_0$ to the detector response. It is this physical interpretation that makes the adjoint function well suited to variance reduction of Monte Carlo simulations.

In Sections 3.1 and 3.2, we demonstrated that when a vacuum boundary condition is valid, one can derive a formulation for H^{+} and detector response in terms of the adjoint function. This, however, has limited use because it is only true for the vacuum boundary condition.

By using the physical interpretation of the adjoint function, it is possible to derive a balance equation for particle "importance". This balance equation has an operator equivalent to the adjoint operator (Eq. 8), however, it is applicable for any arbitrary boundary condition. Hence, the adjoint function refers to a particle property, which is the "importance" of a particle with respect to some objective. Because of the similarity of the operators, "importance" is commonly referred to as the adjoint function (or flux).

3.4 Use of Adjoint (Importance) Methodology for Monte Carlo Variance Reduction

Recognizing the physical interpretation of the adjoint function as an importance function, a number of works have utilized it for biasing Monte Carlo calculations. Kalos (1963) described the importance sampling technique and its relation to an importance function and a zero variance solution. Coveyou et al. (1967) developed an inverse relation between particle statistical weight and the importance function and showed the

merits of the importance function for transport and source biasing. Recognizing the advantages associated with using deterministically generated adjoint functions for variance reduction, a number of research efforts have applied deterministic adjoint solutions and/or approximate adjoint solutions with varying degrees of success. Early work involved the use of deterministic importance functions for simplified, problem-specific tools with notable success. Following successful demonstration of feasibility, efforts turned toward general multi-dimensional applications and automation. A brief review of a select number of independent efforts to use deterministic importance functions for biasing Monte Carlo calculations is presented below, followed by an introduction to the authors' contributions to this area.

One of the early efforts in this area was by Tang et al. (1976; Tang and Hoffman, 1988), which used two-dimensional (2-D) discrete ordinates (S_N) adjoint functions from the DOT code (Rhoades and Mynatt, 1973) to bias multigroup MORSE (Emmett, 1975) Monte Carlo calculations. With the limitation to multigroup Monte Carlo, the source, transport, and collision processes were all biased. Biasing capabilities that utilized the adjoint function included source energy biasing, energy biasing at collision sites, splitting and Russian roulette, and path-length stretching. The biasing of the collision and transport kernels was possible because of the multigroup formulation. The work was extended to include automation of the biasing procedure for spent fuel cask dose calculations using 1-D S_N adjoint functions, culminating in the SAS4 sequence (Tang, 1998) of the SCALE code package (SCALE, 2001).

Miller et al. (1990) developed an automatic importance generator for space- and energy-dependent geometric splitting and Russian roulette based on adjoint diffusion calculations and have incorporated this feature into the MCBEND code (Chucas et al., 1994). The importances are generated on a user-defined three-dimensional (3-D) orthogonal mesh and the diffusion coefficients are modified to provide a closer approximation to transport theory. The technique has been successfully applied to a number of practical applications (Chucas and Grimstone, 1994; Shuttleworth et al., 2000). The developers note, however, limitations in its ability to produce efficient importance maps in geometries that are dominated by voids and ducts and are pursuing other techniques for such situations (Shuttleworth et al., 2000).

Mickael (1992, 1994) developed a modified version of MCNP that performs an adjoint diffusion calculation to generate weight-window parameters for nuclear well-logging calculations. A short analog Monte Carlo simulation is performed to obtain effective group parameters for a 1-D or 3-D adjoint diffusion calculation. The mesh for the diffusion calculation is user-defined and the solution of the time-dependent adjoint diffusion calculation is used to assign weight-window values. The implementation is focused on the nuclear well-logging application and has been demonstrated for neutron, photon, and coupled neutron-photon problems. A recent complimentary work (Gardner and Liu, 1999) has utilized Mickael's approach for generating a 1-D adjoint function and used the adjoint function as a first estimate for their 3-D geometry-independent weight-window generator (Liu and Gardner, 1997) for the simulation of a neutron oil well-logging tool.

Responding to apparent needs for a more general and efficient Monte Carlo-based tool to simulate computationally challenging nuclear well-logging problems, researchers at Los Alamos National Laboratory developed the AVATAR method (Van Riper et al., 1997). The adjoint function and adjoint current, as calculated by the 3-D S_N THREEDANT code (Alcouffe et al., 1995), are used to generate space- energy- and angular-dependent weight windows. A significant aspect of this work is the angular dependence within the weight-window technique, which is based on the approximation that the angular adjoint function is symmetric about the average adjoint current vector. The lower weight-window boundary in each spatial mesh and energy group is set equal to the inverse of the scalar adjoint function. The weight window lower boundaries are then normalized to a particular source location and energy, and consequently the inherent coupling between source and transport biasing is not taken into account. Incompatibility between source and transport biasing has been shown to be problematic due to calculational inefficiency and false convergence (Hendricks and Culbertson, 2000). Originally, this work utilized an interface code to automate the determination and utilization of the adjoint function, including mesh generation for THREEDANT. However, it is our understanding that difficulties with the automation process/code have not been overcome

and that, while MCNP version 4C (Briesmeister, 2000) can now utilize fine-mesh cell-independent weight-window values (e.g., from a deterministic calculation), the user must generate and supply the weight-window values and corresponding spatial and energy grid. A recent AVATAR-related effort (Evans and Wareing, 1999) has applied a 3-D unstructured-mesh discrete ordinates code to generate the adjoint function on a tetrahedral mesh to solve neutron and gamma oil well-logging problems.

Turner and Larsen (1997) have developed the Local Importance Function Transform (LIFT) method, which uses deterministic adjoint solutions to bias the source distribution, distance-to-collision, and selection of post-collision energy group and direction for multigroup Monte Carlo calculations. Significant aspects of this work are that it approximates a zero-variance method and source, transport, and collision processes are all biased via an analytic expression for the importance function. The analytic expression assumes linearly anisotropic importance and is limited to multigroup.

The TRIPOLI Monte Carlo code includes several advanced biasing schemes, including exponential biasing, quota sampling, and collision biasing, that require an importance function (Both et al., 1994). The importance function may be generated on the user-defined mesh by a method based on graph theory or solution of the adjoint transport equation via collision probabilities. To overcome some limitations/difficulties with these importance generation techniques, recent work (Giffard et al., 1999) has utilized a 2-D discrete ordinates code for generation of importances. The scalar adjoint function is mapped onto a user-defined Monte Carlo importance grid in space and energy. In this work, the deterministic adjoint solution is used to bias the source and transport kernels, including splitting and Russian roulette.

Barrett and Larsen (1999) have recently examined the use of approximate deterministic adjoint functions with variational methods (Bell and Glasstone, 1970) for the purpose of Monte Carlo variance reduction, referred to as Variational Variance Reduction (VVR). In this variational method, approximate or low-accuracy forward and adjoint solutions are combined via a functional to calculate a parameter with higher accuracy. Barrett and Larsen have investigated the potential of this approach for 1-D mono-energetic fixed source and eigenvalue problems using deterministic and Monte Carlo methods for the adjoint and forward solutions, respectively. By itself, this VVR method differs from traditional variance reduction methods in that it does not involve a modification to the particle weight in the Monte Carlo transport process. Barrett and Larsen have, however, employed the VVR method in conjunction with other variance reduction methods that do involve modification of particle weight. Extension of this work to energy-dependent multi-dimensional problems is currently being explored.

The authors' first application of deterministic importance functions (Wagner and Haghighat, 1995; 1996) was motivated by the computational expense associated with performing Monte Carlo reactor dosimetry calculations and the time and effort associated with manual developing variance reduction parameters for this application. The MCNP code was modified to (1) process adjoint functions from the 2-D S_N DORT code (Rhoades and Childs, 1988), with an approximate shape function for the third dimension, into space- and energy-dependent source biasing parameters and weight window lower bounds and (2) superimpose and utilize the fine-mesh (MCNP cell-independent) weight-window values. Due, in part, to the importance of source biasing for the reactor dosimetry calculation, we deviated from the standard inverse adjoint relation for particle statistical weight and used the concept of importance sampling to derive consistent relations for source biasing parameters and weight window lower bounds (Wagner, 1997; Wagner and Haghighat, 1998). We refer to our method as Consistent Adjoint Driven Importance Sampling (CADIS). Following successful demonstration of this method, our efforts turned to automation of the generation and use of 3-D adjoint functions from the TORT code (Rhoades and Simpson, 1997). These efforts led to the development of the A^3MCNP (Automated Adjoint Accelerated MCNP) code (Wagner, 1997). The following sections will describe in greater detail our CADIS methodology, implementation of the methodology, development of A^3MCNP, and finally, applications of the A^3MCNP code for real-world shielding/fixed-source problems.

4. CADIS METHODOLOGY FOR USING DETERMINISTIC IMPORTANCE FUNCTIONS

In this section, we review the theory of the CADIS (Consistent Adjoint Driven Importance Sampling) methodology, which includes formulations for source and transport biasing parameters and their implementation within the weight-window technique.

4.1 Source Biasing

In particle transport, the goal of most Monte Carlo simulations is to calculate the response (i.e., flux, dose, reaction rate, etc.) at some location. This is essentially equivalent to solving an integral of the form

$$R = \int_P dP \sigma_d(P)\psi(P), \tag{17a}$$

or its equivalent in terms of the adjoint function given by

$$R = \int_P dP q(P)\psi^+(P), \tag{17b}$$

where $\boldsymbol{P}$ refers to independent variables $(\vec{r}, E, \hat{\Omega})$. To solve the latter integral with the Monte Carlo method, the independent variables are sampled from $q(P)$, which is not necessarily the best probability density function (*pdf*) from which to sample. An alternative *pdf*, $\hat{q}(P)$ can be introduced into the integral as follows:

$$R = \int_P dP \frac{q(P)\psi^+(P)}{\hat{q}(P)}\hat{q}(P), \tag{18}$$

where $q(P) > 0$ and $\int_P dP\hat{q}(P) = 1$. From importance sampling (Kalos and Whitlock, 1986), the alternative *pdf*, $\hat{q}(P)$ that will minimize the variance for $\boldsymbol{R}$ is given by

$$\hat{q}(P) = \frac{\psi^+(P)q(P)}{R}. \tag{19}$$

If the final result, $\boldsymbol{R}$, is known, then the Monte Carlo integration will return $\boldsymbol{R}$ with zero variance. However, in practice, the adjoint function is not known exactly, $\boldsymbol{R}$ cannot be solved by direct integration, and thus, it is necessary to simulate the particle transport. For this process it is desirable to use the biased source distribution in Eq. 19 that, in the limit of an exact adjoint, leads to a zero-variance solution.

Examining Eq. 19 reveals that the numerator is the detector response from phase-space $\boldsymbol{P}$, and the denominator is the total detector response, $\boldsymbol{R}$. Therefore, the ratio is a measure of the contribution from phase-space $\boldsymbol{P}$ to the detector response. Intuitively, it is useful to bias the sampling of source particles by the ratio of their contribution to the detector response, and therefore, this expression could also be derived from physical arguments.

Since the source variables are sampled from a biased *pdf*, the statistical weight of the source particles must be corrected according to Eq. 1 such that

$$w(P)\hat{q}(P) = w_0 q(P), \tag{20}$$

where $\boldsymbol{w_0}$ is the unbiased particle starting weight, which is set equal to 1. Substituting Eq. 19 into Eq. 20 and rearranging, we obtain the following expression for the statistical weight of the particles

$$w(P) = \frac{R}{\psi^+(P)}. \tag{21}$$

This equation shows an inverse relationship between the adjoint (importance) function and the statistical weight. Previous work (Coveyou, 1967) had assumed this relationship and showed it to be near optimal, and others have verified this relationship through computational analysis. However, we have shown that this relationship may be derived from importance sampling.

4.2 Transport Biasing

To obtain a formulation for transport biasing, we start with the integral form of the linear Boltzmann equation given by

$$\psi(P) = \int K(P' \rightarrow P)\psi(P')dP' + q(P), \tag{22}$$

where $K(P' \rightarrow P)dP$ is the expected number of particles emerging in dP about P from events in dP' about P', and $q(P)$ is the source density. If Eq. 22 is multiplied by

$$\frac{\psi^+(P)}{R},$$

we obtain a formulation for the transport equation with a biased source as

$$\hat{\psi}(P) = \int K(P' \rightarrow P)\psi(P')\frac{\psi^+(P)}{R}dP' + \hat{q}(P), \tag{23}$$

where

$$\hat{\psi}(P) = \frac{\psi^+(P)\psi(P)}{R}$$

and $\hat{q}(P)$ is the biased source given by Eq. 19. Further, if we rewrite the integral term in the above equation in terms of the new function $\hat{\psi}(P)$, Eq. 23 reduces to

$$\hat{\psi}(P) = \int K(P' \rightarrow P)\hat{\psi}(P')\frac{\psi^+(P)}{\psi^+(P')}dP' + \hat{q}(P)$$

or

$$\hat{\psi}(P) = \int \hat{K}(P' \rightarrow P)\hat{\psi}(P')dP' + \hat{q}(P) \tag{24}$$

where $\hat{K}$ is the biased transport operator (kernel) given by

$$\hat{K}(P' \rightarrow P) = K(P' \rightarrow P)\frac{\psi^+(P)}{\psi^+(P')}. \tag{25}$$

The above equation is the formal expression of the biased transport operator, which is derived from the biased source formulation. This expression, generally, is of little practical use, because the $K(P' \rightarrow P)$ operator is not known. However, it suggests an approach for altering the number of particles that are transferred from one phase space to another. For example, if the phase space **P** has a higher importance than the phase space P', particles are split based on the ratio of the importance function (i.e., $\frac{\psi^+(P)}{\psi^+(P')}$), while if the opposite is true, the particles are rouletted. Following this split/roulette process, to preserve the expected number of particles, the particle statistical weight following the transport is modified according to

$$w(P) = w(P')\left[\frac{\psi^+(P')}{\psi^+(P)}\right]. \tag{26}$$

In the CADIS methodology, we utilize Eqs. 19 and 21 for calculating source biasing parameters and transport biasing parameters (for the weight-window technique), respectively. To administer the splitting and rouletting of particles, we use the weight-window technique, which deals with particle weights. We have related these weights to particle importance via Eqs. 21 and 26. Since these relationships for the particle statistical weights, which are used in source sampling and the particle transport process, were derived from importance sampling in a consistent manner, we refer to the use of these formulations as Consistent Adjoint Driven Importance Sampling (CADIS).

4.3 Implementation of CADIS in MCNP

To calculate the source biasing parameters over the phase-space (space, energy, and angle) the source from the forward calculation is coupled with the adjoint function as shown in Eq. 19. Further, the particle transport is biased via Eqs. 21 and 26.

The space, energy, and angular dependent adjoint function may require a significant amount of storage, particularly for large 3-D problems. For example, the adjoint function for a 3-D problem with 100x100x100 spatial meshes, 50 energy groups, and 80 directions (S_8) is 4E+09 values that, for double precision, require 32 gigabytes of storage. The S_N method can determine the angular independent (or scalar) adjoint accurately, but not necessarily the angular dependent adjoint because of the limited number of directions. Therefore, because of the memory requirements and inaccuracies of the angular dependent adjoint, we use the space and energy dependent (scalar) adjoint function,

$$\phi^+(\vec{r},E) = \int_{4\pi} d\Omega \psi^+(\vec{r},E,\hat{\Omega}), \tag{27}$$

for calculating space- and energy-dependent source biasing and weight-window parameters. Note that for problems with significant angular dependence (e.g., problems with ducts and/or voids), the use of angular importances is desirable. However, for such problems, "ray effects" can cause significant inaccuracies, even in the scalar adjoint function. Hence, accurate determination and efficient usage of angular-dependent importances remains an area for future work.

4.3.1 Source biasing. Source biasing allows the simulation of a larger number of source particles, with appropriately reduced weights, in the more important regions of each variable (e.g., space, energy, and angle). This technique consists of sampling the source from a biased (non-analog) probability distribution rather than from the true (analog) probability distribution, and then correcting the weight of the source particles by the ratio of the actual probability divided by the biased probability according to Eq. 1. Thus, the total weight of particles started in any given interval is conserved, and an unbiased estimate is preserved.

To accelerate the Monte Carlo calculation the source energy and position are sampled from the biased source distribution $\hat{q}(\vec{r},E)$,

$$\hat{q}(\vec{r},E) = \frac{\phi^+(\vec{r},E)q(\vec{r},E)}{R} = \frac{\phi^+(\vec{r},E)q(\vec{r},E)}{\int_V\int_E q(\vec{r},E)\phi^+(\vec{r},E)drdE} \tag{28}$$

Physically, the numerator is the detector response from space-energy element ($d\vec{r}$, dE), and the denominator is the total detector response, $\boldsymbol{R}$. Therefore, the ratio is a measure of the relative contribution to the detector response.

4.3.2 Transport biasing. As mentioned, the weight-window technique, as implemented in the MCNP code, is a space- and energy-dependent facility by which splitting/roulette is applied. The weight-window technique provides an alternative to geometric splitting/roulette and energy splitting/roulette for assigning space- and energy-dependent importances. To use the weight-window facility within MCNP, we need to calculate weight window lower bounds w_ℓ such that the statistical weights defined in (Eq. 21) 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 ($C_u = \frac{w_u}{w_\ell}$). Therefore, the space- and energy-dependent weight window lower bounds w_ℓ are given by

$$w_\ell(\vec{r},E) = \frac{w}{\left(\frac{c_u+1}{2}\right)} = \frac{R}{\phi^+(\vec{r},E)\left(\frac{c_u+1}{2}\right)}, \tag{29}$$

and during the transport process the weight-window technique performs splitting or roulette according to Eq. 26. In MCNP, the default value for C_u is 5. Because the calculational efficiency has been observed to be fairly insensitive to small deviations in this parameter, the default value was employed throughout this work. It is important to note that because the source biasing parameters and weight window lower bounds are consistent, the statistical weights of the source particles ($w(\vec{r},E) = \frac{q(\vec{r},E)}{\hat{q}(\vec{r},E)}$) are within the weight windows as desired. Moreover, 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 (Briesmeister, 2000). This will result in unnecessary splitting/rouletting and a corresponding degradation in computational efficiency. For problems in which the adjoint function varies significantly within the source region (space and/or energy), this coupling between source and transport biasing is critical.

5. DEVELOPMENT OF A CODE FOR AUTOMATED VARIANCE REDUCTION USING DETERMINISTIC IMPORTANCE FUNCITONS (A^{3}MCNP - AUTOMATED ADJOINT ACCELERATED MCNP)

The major difficulty associated with using deterministic adjoint (importance) functions for variance reduction of Monte Carlo simulations is the requirement for the deterministic adjoint solution. The determination of the adjoint function requires the generation of input files for the discrete ordinates adjoint calculation, which can be a difficult and time-consuming task that requires the user to be knowledgeable in Monte Carlo and deterministic methods and codes, which is not typically the case. To surmount this difficulty, we have developed strategies for automatically generating input files for discrete ordinates calculations, including mesh generation and material cross section preparation, directly from the MCNP input. This automation of the generation of the discrete ordinates input files not only eliminates the tedious process of manually generating these files; it requires very little experience on the part of the user with respect to discrete ordinates adjoint calculations. The coupling of the implementation of the CADIS methodology described in the previous section and the automatic generation of the deterministic adjoint solution has resulted in complete automation of variance reduction for MCNP shielding/fixed-source calculations. The modified version of the MCNP code that contains these features is designated A^{3}MCNP (Automated Adjoint Accelerated MCNP).

A^3MCNP performs the following tasks (Wagner, 1997):

1) Prepares the necessary input files for a deterministic adjoint calculation
   - Generation of a mesh distribution for a deterministic adjoint calculation. Mesh generator utility first generates a uniform mesh distribution to extract information on material distribution, and then through a back-thinning process prepares a variable mesh distribution.
   - Preparation of input file for the TORT S_N code (Rhoades and Simpson, 1997).
   - Determination of material compositions and preparation of input files for the GIP code (Rhoades, 1978) for generation of multigroup cross sections.
2) Reads the adjoint (importance) function from the standard TORT binary output file and prepares source biasing parameters and space- and energy-dependent weight window lower bounds via Eqs. 19 and 21.
3) Superimposes the detailed weight window values (based on the deterministic spatial-mesh distribution and energy-group structure) onto the Monte Carlo model and uses them in a transparent manner.

The flowchart in Fig. 1 presents the steps performed in an A^3MCNP simulation.

A Monte Carlo (MCNP) model or input file describes a problem in terms of combinatorial geometry and continuous energy, while a deterministic method requires discretization of the geometry, energy, and angle. Therefore, while the Monte Carlo input file contains most of the information necessary to generate a corresponding deterministic input file, further processing beyond simple translation is required. Specifically, the Monte Carlo geometry description must be appropriately discretized, a suitable energy group structure must be specified, the material cross sections must be prepared, and various remaining discrete ordinates input parameters must be defined (e.g., S_8 quadrature order is the default). Of these tasks, the discretization of the problem geometry is the most involved.

The Monte Carlo geometry description must be discretized into a spatial mesh that is fine enough to adequately describe the material boundaries and enable a reliable deterministic calculations, while not being refined to the extent that the computational time and/or memory requirements for the deterministic calculation become prohibitive. It is not the intention of the adjoint calculation to solve the problem exactly, thus a compromise between accuracy and efficiency is required to achieve optimum overall efficiency (i.e., minimize total CPU time, which is a combination of the CPU time required for the TORT adjoint and Monte Carlo calculations). A number of studies (Wagner, 1997; Haghighat et al., 1999) have demonstrated that the effectiveness of adjoint functions for variance reduction is not overly sensitive to the accuracy of the adjoint solution. Further discussion on A^3MCNP functions and features is provided in the references (Wagner, 1997). The following section discusses application of A^3MCNP to three important problems.

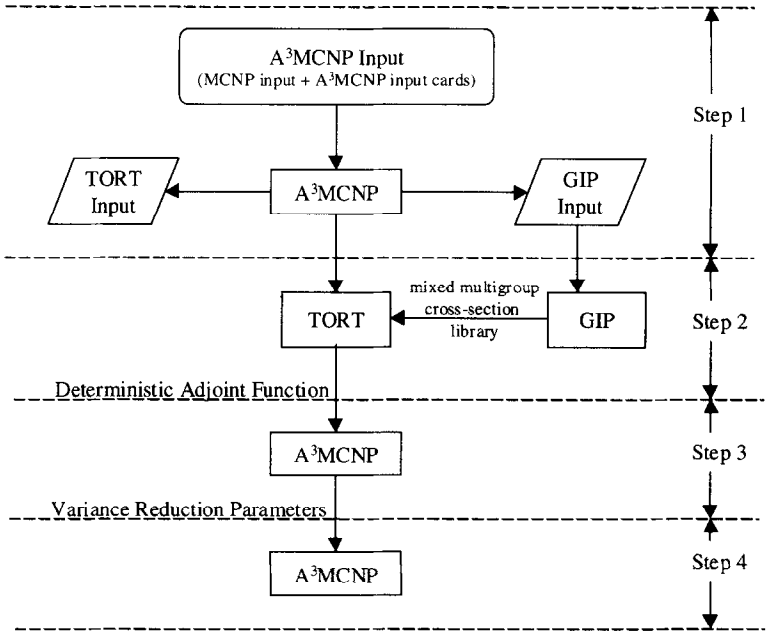


Fig. 1. Automated process for variance reduction with A³MCNP

6. APPLICATION OF AUTOMATED VARIANCE REDUCTION (A³MCNP) TO REAL-WORLD SHIELDING PROBLEMS

In this section we briefly describe the application of automated variance reduction, based on deterministic adjoint (importance) functions, to three real-world shielding problems; including pressurized-water-reactor (PWR) cavity dosimetry, displacement-per-atom (DPA) estimation at a boiling-water-reactor (BWR) core-shroud weld, and gamma dose estimation at the surface of spent nuclear fuel (SNF) storage cask. These problems address major concerns of nuclear utilities and are very important for the continued safe and economical operation of nuclear power plants.

The authors' earliest application of deterministic importance adjoint functions for variance reduction was for the PWR cavity dosimetry problem. This initial work used 2-D adjoint functions, and the process of generating the adjoint function was not automated. Following successful demonstration, the process was automated and applied to several other problems. The problem applications discussed below were chosen to describe/highlight characteristics of using deterministic importance function for variance reduction. The cavity dosimetry problem was used to examine the effect of adjoint accuracy on the effectiveness of variance reduction and compare calculational efficiency and reliability between manually developed variance reduction parameters and those based on a deterministic adjoint function. The BWR core-shroud analysis further explored the impact of adjoint accuracy on the effectiveness for variance reduction. Finally, the storage cask problem was used to investigate issues associated with using localized versus global adjoint sources to calculate dose profiles.

6.1 Cavity Dosimetry and Pressure Vessel Fluence for a PWR

6.1.1 Problem description. The embrittlement of a reactor pressure vessel (RPV) is primarily due to the bombardment of high-energy neutrons and cannot be directly determined from measured quantities. Cavity dosimetry calculations attempt to estimate reaction rates in a small volume outside of the RPV at a distance

of ~350 cm from the core centerline. These reaction rates are used to validate methods/models that are subsequently used to estimate the RPV neutron fluence. The problem is illustrated in Fig. 2, which shows one octant of the Three Mile Island Unit 1 (TMI-1) reactor.

6.1.2 Performance. Without the use of variance reduction techniques, one could allow MCNP to run this problem continuously for weeks and still not obtain statistically significant/reliable results (Wagner and Haghighat, 1998). In fact, this particular problem motivated the authors' usage of deterministic importance functions for variance reduction. Before the CADIS methodology and the A^{3}MCNP code were developed, this problem was manually optimized (Wagner et al., 1996) with existing variance reduction methods, including source biasing, weight windows, exponential transformation, implicit capture, and energy cutoff. This manual optimization required a great deal of time and effort to develop, but proved to be successful in terms of both computational performance and calculational reliability (i.e., enabled problem objectives to be accomplished with available computational resources). During the development of the automated variance reduction methodology, the problem was used to evaluate the efficiency of the automated variance reduction approach (Wagner, 1997; Wagner and Haghighat, 1998). Initial application of the CADIS methodology, which was based on a 2-D adjoint function, increased the calculational efficiency by a factor of 4 with respect to our best manually optimized model and by a factor of ~50,000 with respect to the unbiased case. Furthermore, the automated variance reduction approach required very little user time, effort, or experience.

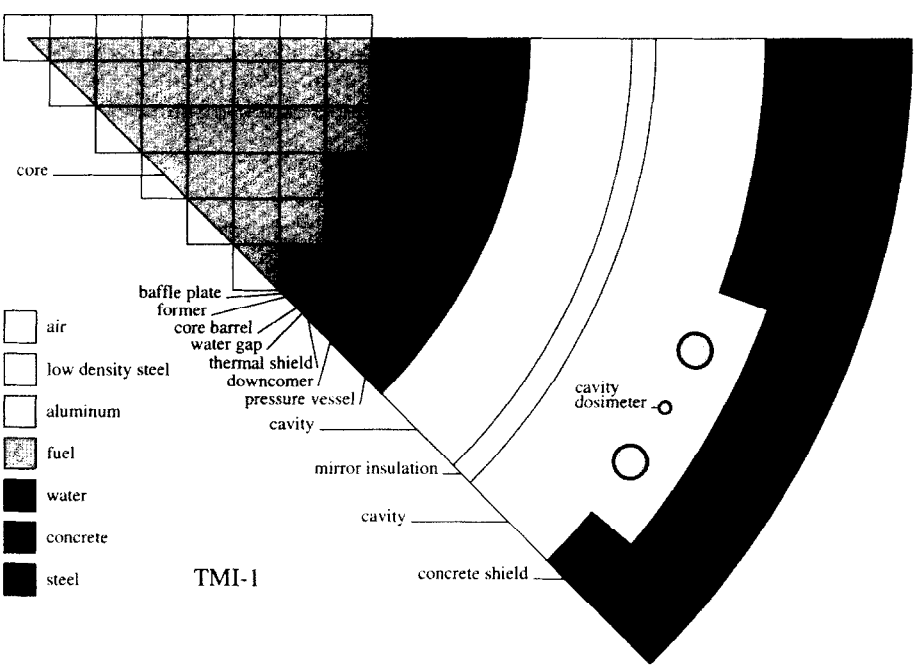


Fig. 2. One octant of the TMI-1 reactor

Since this was the first application of the CADIS methodology, a number of studies were performed to evaluate the relationship between the accuracy of the adjoint function and its effectiveness for variance reduction of the Monte Carlo calculation. The effect of reduced accuracy through the use of adjoint calculations based on reduced spatial, energy, and angular discretization were examined (Wagner, 1997; Wagner and Haghighat, 1998). The effectiveness of the adjoint function for variance reduction was found to

be rather insensitive to the accuracy of the adjoint function, and in some cases, due to the reduction in data volume and CPU time required for the discrete ordinates calculation, less detailed adjoint functions actually yielded greater overall efficiency. Similar findings have also been observed for another real-world problem discussed in next section.

6.2 Simulation of a BWR core shroud

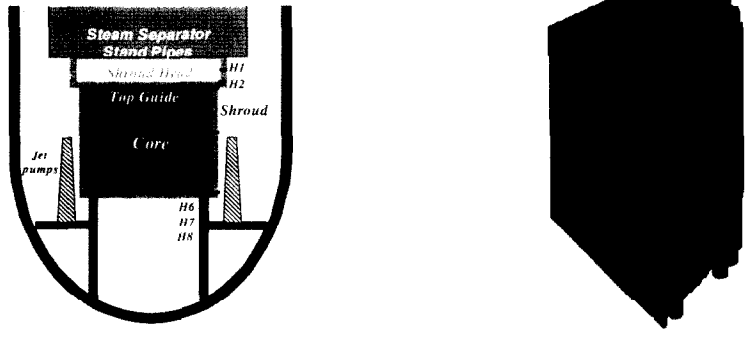
The objective of this simulation is to investigate the role of radiation in the observed cracks in a BWR core-shroud welds.

6.2.1 Problem description.

The core shroud is an ~5 cm thick stainless steel annulus located between the core and the vessel of a BWR. Fig. 3a shows the axial locations of the core-shroud welds (H1 to H8) relative to the reactor core and other structural components. Fig. 3b shows the radial position of the core shroud relative to the core and the jet pumps.

The objective is to determine neutron and gamma flux distributions and DPA at the H2, H3, and H4 welds. Since welds are located above and below the core, and gamma rays are generated within the structural materials through (n,γ) interactions (mainly from thermal neutrons), it is necessary to simulate neutrons of all energies (0 to 20 MeV) and gamma rays in a 3-D model. In this paper, we limit the discussion to our simulations for the H4 weld, which is located ~63.5 cm above the core mid-plane (see Fig. 3a). We have developed a model of size 300×300×381 cm^3.

We determine the DPA at a small segment (2×2×2 cm^3) of the H4 weld. (Note that we consider that the weld width (axially) is 2 cm.) To prepare multigroup cross sections for adjoint calculations, we utilize the BUGLE 96 multigroup [47 neutron and 20 gamma] library (White et al., 1996). Further, for tallying, we use this library's group structure. For the neutron source, we consider a uniform source distribution with a typical BWR spectrum.



(a) Axial view of shroud, locations of welds (b) Radial position of shroud

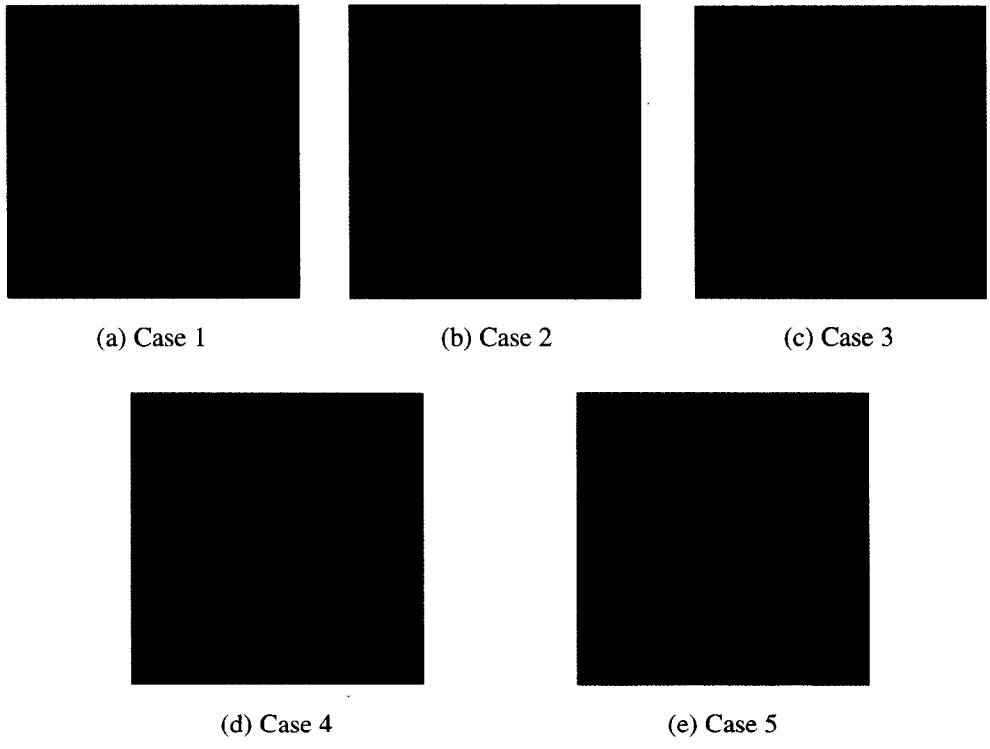
Fig. 3. Schematic of a BWR core shroud

6.2.2 Performance.

The performance of A^3MCNP for different importance functions, corresponding to different spatial mesh distributions used for the deterministic S_N calculations, has been examined. We have tested numerous cases (Haghighat et al., 1999), but for brevity, we will discuss only five cases with uniform meshes. As indicated in Table 1, the mesh sizes for these cases vary from 5-cm to 60-cm. Figs. 4a-4e show the x-y mesh distributions for each of the five cases. Note that in some of these cases, because of large mesh sizes, material regions are either approximated in size/position, or omitted altogether.

Table 1. Characteristics of the spatial mesh distributions for cases considered

Case	*Total # of meshes (# of axial meshes)*	*Mesh size (x, y, z) [cm]*
1	86400 (24)	5, 5, 15.875
2	10800 (12)	10, 10, 31.75
3	2700 (12)	20, 20, 31.75
4	1200(12)	30, 30, 31.75
5	300 (12)	60, 60, 31.75



(a) Case 1 (b) Case 2 (c) Case 3

(d) Case 4 (e) Case 5

Fig. 4. Mesh distributions for different cases

Fig. 5 compares the group-nine adjoint function distributions for different cases. As expected, due to the coarse meshing, the differences are very large (more than a few orders of magnitude). However, as it will be shown shortly, these very approximate distributions still yield significant speedups.

Table 2 compares the DPA values, FOM values, relative errors, and speedups for the different cases after 100 CPU minutes to the unbiased case after 2000 CPU minutes. As expected the cases with finer deterministic spatial mesh achieve better FOM values because their adjoint function distributions are more accurate. These results, however, do not include the effect of the S_N TORT calculations. Hence, we have estimated the amount of CPU time necessary for achieving a relative error of 1% in each case, and then combined it with the corresponding S_N CPU time. Table 3 compares the total CPU times for the biased cases to that of the unbiased case.

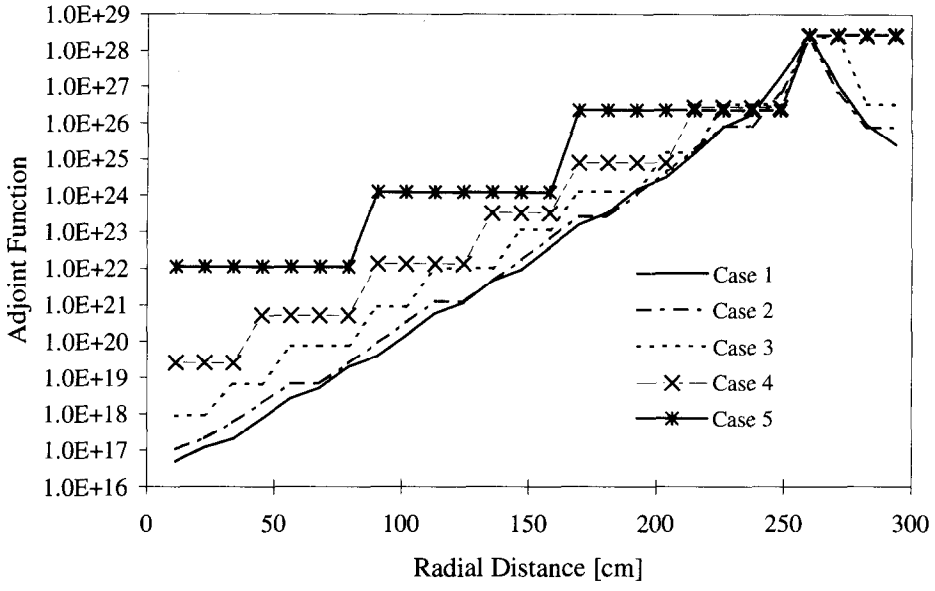


Fig. 5. Radial adjoint function distributions for different cases, group 9 (3.01-3.68 MeV)

Table 2. Estimated DPA and associated statistics after 100 CPU minutes for the unbiased and biased cases

Case No.	*# of meshes (# of axial meshes)*	*DPA [dpa/sec]*	*Relative Error [%]*	*FOM*	*MCNP Speedup* $FOM_{biased}/FOM_{unbiased}$
Unbiased	N/A	3.877E-10*	14.97*	0.022*	1
1	86400 (24)	3.571E-10	1.05	90.7	4123
2	10800 (12)	3.440E-10	1.35	54.9	2945
3	2700 (12)	3.513E-10	2.46	16.5	750
4	1200 (12)	3.512E-10	2.56	15.3	696
5	300 (12)	3.470E-10	5.88	2.89	131

* result after 2000 CPU minutes

Table 3. Comparison of total CPU time (TORT + A^{3}MCNP) to achieve 1.0% (1σ) statistical uncertainty for the unbiased and biased cases

Case No.	*No. of meshes (# of axial meshes)*	*TORT [minutes]*	*A^{3}MCNP [minutes]*	*Total [minutes]*	*Overall Speedup*
Unbiased	N/A	N/A	448,201	448,201	1
1	86400 (24)	424.6	110.3	534.9	838
2	10800(12)	40.8	182.7	223.5	2005
3	2700 (12)	10.2	604.8	615.0	729
4	1200 (12)	5.0	655.2	660.2	679
5	300 (12)	1.3	3461.4	3462.7	129

All the biased cases result in significant speedups over the unbiased case. Case 1 (with the most detailed mesh distribution) yields the shortest time for A^{3}MCNP (because it uses the most accurate adjoint importance function), but the longest time for the TORT calculation. These results indicate that an approximate adjoint may yield a large speedup. For example, case 2 with ~88% fewer meshes shows the best performance, and even case 5 which uses a very inaccurate adjoint function yields a net overall speedup of ~130 as compared to the unbiased case.

6.3 Simulation of a Storage Cask

Here, we discuss the determination of gamma dose over the surface of a SNF storage cask. Further, we compare the effectiveness of A^{3}MCNP for small, localized regions and large surfaces.

6.3.1 Problem description. To expand storage capacity and prevent premature plant shutdown, utilities are storing their SNF on-site in dry casks. Demonstration of compliance with the regulatory limits requires detailed multi-dimensional neutron and gamma transport simulations. Multi-dimensional Monte Carlo codes such as MCNP are used for this application. Because of the large size of the physical model (concrete casks are approximately 3.3 meters in diameter and 6 meters tall) and the need for detailed information with high precision, variance reduction methods are necessary. Here, we consider a model (Redmond and Anton, 2000) of size 178.3×178.3×838.2 cm^3 that includes a quarter of a concrete cask plus some volume of air as shown in Fig. 6. For this discussion, we evaluate the gamma dose on the outer surface of the cask as a whole, and over 19 axial segments between 30.48 cm and 592.5 cm. The first 18 segments are 30.48 cm each, and the last segment is 13.38 cm. Figs. 7 show the gamma source distribution within a quarter of the storage cask.

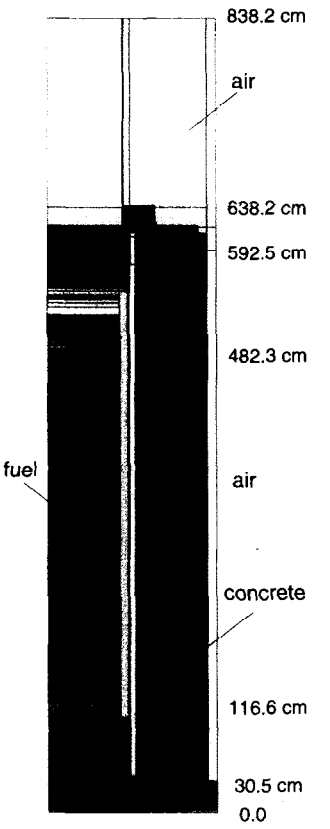
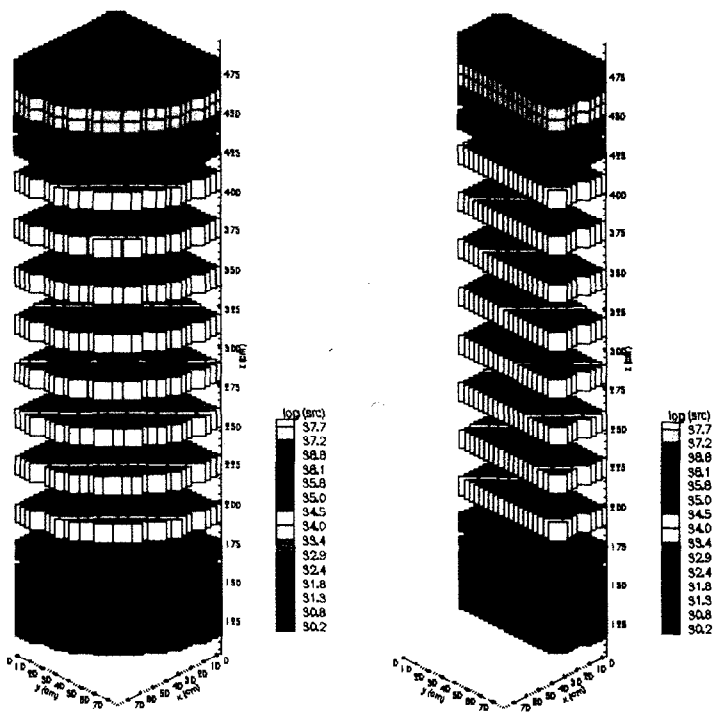


Fig. 6. MCNP model of storage cask

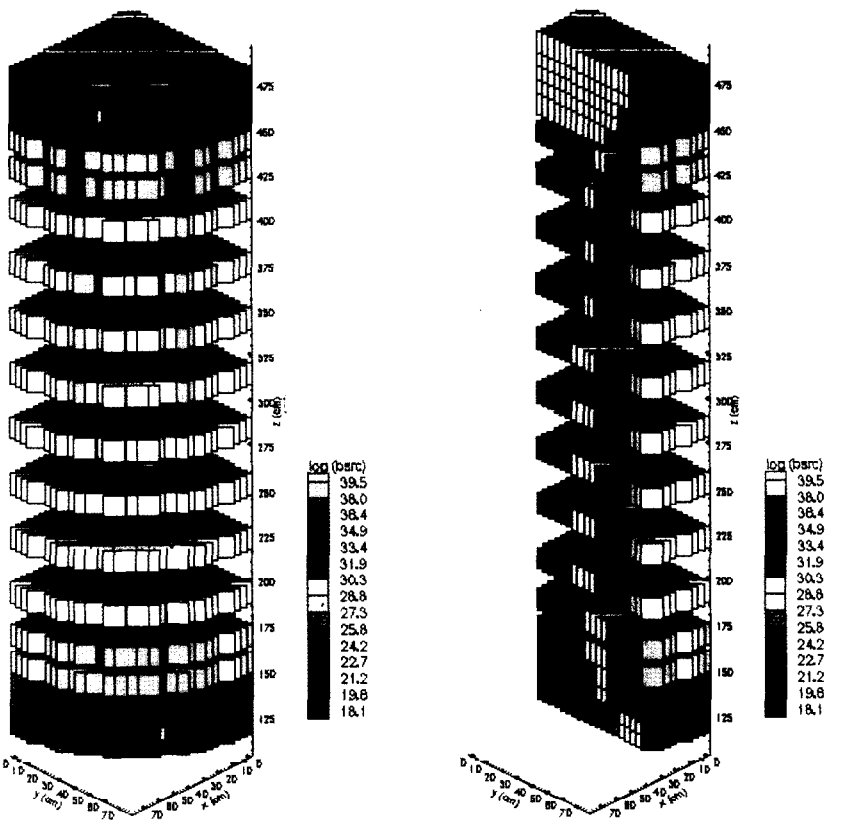


(a) Full (b) Axial projection

Fig. 7. Unbiased spatial source distribution in the storage cask

Note that the source distribution is assumed to be flat radially and axially within the active fuel region, and only changes axially above and below the active fuel.

6.3.2 Performance. In order to assess the performance of A^{3}MCNP, we ran the unbiased MCNP case for 6000 CPU-min to achieve a 1σ uncertainty of 0.0376 with a FOM of 0.12. Then, A^{3}MCNP prepared a biased source distribution and weight-window lower bounds as discussed in Section 4.3. Figures 8 shows the biased source distribution, which differs significantly from the original, unbiased source distribution (shown in Figs. 7). As expected the intensity of the biased source decreases significantly as one moves toward the radial center of the storage cask; therefore, mainly the source particles on the cask periphery are sampled. To obtain the importance function, the TORT calculation required ~20 min of CPU time. For the biased case, we ran A^{3}MCNP for ~180 min and achieved a 1σ uncertainty of 0.0047 and a FOM of 254. This means that to evaluate the dose over the whole cask surface, A^{3}MCNP performs ~2117 times faster than the unbiased case.



(a) Full (b) Axial projection

Fig. 8. Biased spatial source distribution in the storage cask

We also examined the A^{3}MCNP performance for evaluation of the axial dose profile (i.e., dose in localized axial regions). Note that we are using only one adjoint source that is uniformly distributed along the cask axis. In other words, particles are biased for reaching the surface rather than any specific axial segments. Fig. 9 shows the ratio of the FOM values (A^{3}MCNP to unbiased MCNP) and the FOM values for unbiased MCNP as a function of the axial position. As expected, the performance of A^{3}MCNP improves significantly as one moves away from the fuel assembly mid-plane; this is especially evident at the regions above and below the fuel assemblies (i.e., >482.3 cm and <116.55 cm). For example, for the segment in the range of 60.96 to 91.44 cm, A^{3}MCNP, after 200 min (including 20 min for TORT), yields a relative error of 0.072, while the unbiased case after 6000 min yield a relative error of 0.83; this indicates that the unbiased MCNP requires ~569 CPU-days (1.6 years) in order to reduce the error to ~7%. Note that for each axial segment, A^{3}MCNP increases the FOM by a factor of more than 2000, as compared to the unbiased case.

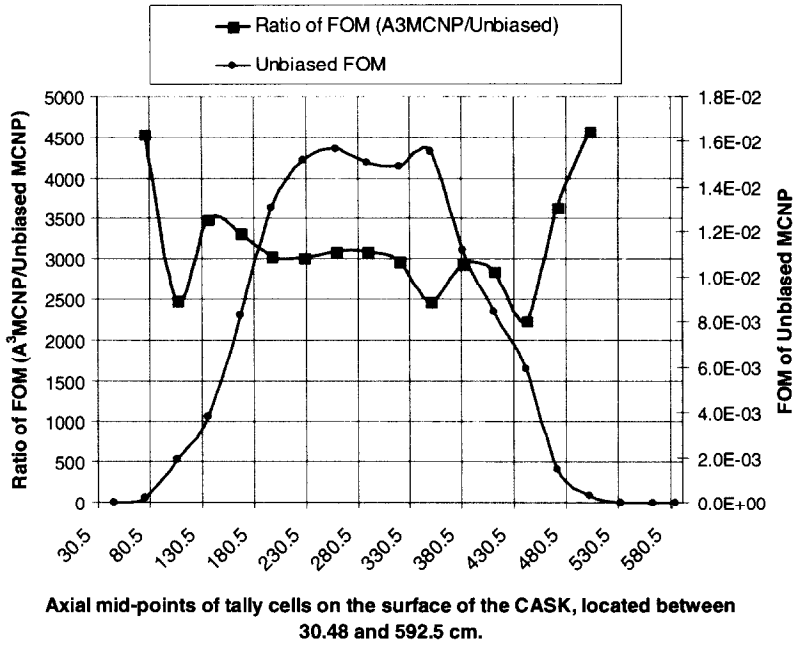


Fig. 9. Comparison of A^{3}MCNP performance to unbiased MCNP for determination of surface gamma dose of a storage cask

7. SUMMARY AND CONCLUSIONS

In this review paper, the use of deterministic "importance" functions for variance reduction of Monte Carlo simulations has been discussed. To illustrate the need for "importance" functions in general, several variance reduction techniques are described. In the absence of an appropriate importance function, effective use of these variance reduction techniques depends on the user's ability to estimate particle importance and subsequently translate into appropriate VR parameters. While reasonable estimation of importance, based on experience and limited knowledge of the problem physics, is possible for simple problems (e.g., 1-D and/or mono-energetic), it is generally impractical and inefficient for complex real-world problems.

Adjoint methodology and the concept of "importance" are presented, along with an explanation of their use for Monte Carlo variance reduction. Relevant works from a number of different researchers are briefly described. These works generally differ in the methodology used for generation of the "importance" function and/or the formulation used for variance reduction. It is noted that the majority of these efforts have focused on shielding/fixed-source problems, while very few investigations have addressed variance reduction for criticality/eigenvalue problems.

A few groups have developed automated techniques and software for generation of the importance function. Among these, MCBEND, AVATAR, and A^{3}MCNP have been used effectively for solving several complex real-world fixed-source problems. A^{3}MCNP has been used to simulate the three problems discussed in this paper, which include cavity dosimetry for a PWR, DPA estimation at a BWR core shroud, and gamma dose estimation over the surface of a storage cask. These simulations have demonstrated that the automated use of deterministic importance functions (with A^{3}MCNP) can yield speedups of several orders of magnitudes, that approximate "importance" functions are adequate, and that, as expected, the methodology is more effective for localized objectives. In addition, because of the consistency between source and transport biasing, the CADIS methodology has proven to be very effective for variance reduction of deep-penetration problems with a distributed source.

The authors believe that the use of deterministic "importance" functions for variance reduction of Monte Carlo simulations is very helpful, especially when dealing with large complex problems. The authors have demonstrated that automated tools can significantly reduce computation and engineer's time. Further, the use of such tools can improve the use and reliability of Monte Carlo simulations. One aspect that has not been emphasized in this paper is the potential for unreliable or erroneous results due to improper use of variance reduction techniques, and the possibility that the incorrect results are not exposed. The use of automated tools for the generation and use of deterministic importance functions for variance reduction has notably reduced this problem for the classes of problems we have investigated. All of these aspects/benefits can have a significant impact on the economics and safety of nuclear systems.

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