International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3–7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

FORWARD-WEIGHTED CADIS METHOD FOR VARIANCE REDUCTION OF MONTE CARLO CALCULATIONS OF DISTRIBUTIONS AND MULTIPLE LOCALIZED QUANTITIES

John C. Wagner, Edward D. Blakeman, and Douglas E. Peplow
Oak Ridge National Laboratory
P.O. Box 2008, Bldg. 5700, MS-6170, Oak Ridge, Tennessee 37831, USA
wagnerjc@ornl.gov; blakemaned@ornl.gov; peplowde@ornl.gov

ABSTRACT

This paper presents a new hybrid (Monte Carlo/deterministic) method for increasing the efficiency of Monte Carlo calculations of distributions, such as flux or dose rate distributions (e.g., mesh tallies), as well as responses at multiple localized detectors and spectra. This method, referred to as Forward-Weighted CADIS (FW-CADIS), is a variation on the Consistent Adjoint Driven Importance Sampling (CADIS) method, which has been used for some time to very effectively improve the efficiency of Monte Carlo calculations of localized quantities, e.g., flux, dose, or reaction rate at a specific location. The basis of this method is the development of an importance function that represents the importance of particles to the objective of uniform Monte Carlo particle density in the desired tally regions. Implementation of this method utilizes the results from a forward deterministic calculation to develop a forward-weighted source for a deterministic adjoint calculation. The resulting adjoint function is then used to generate consistent space- and energy-dependent source biasing parameters and weight windows that are used in a forward Monte Carlo calculation to obtain approximately uniform statistical uncertainties in the desired tally regions. The FW-CADIS method has been implemented in the ADVANTG/MCNP framework and has been fully automated within the MAVRIC sequence of SCALE 6. Results of the application of the method to enabling the calculation of dose rates throughout an entire full-scale pressurized-water reactor facility are presented and discussed.

Key Words: Monte Carlo, variance reduction, hybrid transport, CADIS

1. INTRODUCTION

Recent applications' needs have motivated efforts to develop approaches for optimizing Monte Carlo calculations for distributions, such as flux or dose rate distributions (e.g., mesh tallies), as well as responses at multiple localized detectors and spectra. Recent efforts at Oak Ridge National Laboratory (ORNL) have led to the development of a variation on the Consistent Adjoint Driven Importance Sampling (CADIS) method for effective global variance reduction. This method, referred to as Forward-Weighted CADIS (FW-CADIS), and an example of its application are presented in this paper. To the authors' knowledge, this is a new method and novel use of the adjoint methodology for biasing Monte Carlo simulations.

It has long been recognized that the adjoint function (i.e., the solution to the adjoint form of the Boltzmann transport equation) has physical significance [1] as a measure of the importance of a particle to some objective function (e.g., the response of a detector) and that this physical

interpretation makes the adjoint function well suited for biasing Monte Carlo simulations. Accordingly, recent trends in Monte Carlo code development have reflected a recognition of the benefits of using deterministic adjoint (importance) functions for Monte Carlo variance reduction [2]. The CADIS methodology [2, 3], which has been incorporated into codes such as ADVANTG [4] (based on MCNP) and the MAVRIC (Monaco with Automated Variance Reduction using Importance Calculations) [5] sequence of SCALE [6], has been used to accelerate three-dimensional (3-D) Monte Carlo simulations for a number of real applications (see for example Refs. 2, 4, 7 and 8).

Although the CADIS methodology has proved to be very effective for automated optimization of localized quantities, until very recently, efforts to optimize distributions (e.g., mesh tallies and/or spectra) have not been nearly as successful. A number of heuristic approaches, such as specification of the adjoint source (response function) throughout the problem phase space, have been tested and found to be ineffective. Specification of the adjoint source at the outer boundaries of a problem in an attempt to encourage particles to move outward through the entire system was found to be reasonably effective, but it raised concerns regarding convergence reliability in inner regions of the problem. Previous work by Cooper and Larsen, which used the inverted forward flux as an importance function (no adjoint calculation) in an attempt to distribute particles uniformly throughout a system, has demonstrated benefit [9]. Although this approach does encourage particles toward regions of lower flux and discourage particles from moving toward regions of higher flux, the forward flux does not represent the expected contribution to the desired response, which is postulated to be uniform particle density (or response) throughout the system. When applied to a large realistic application, this method was not found to be effective, particularly in cases where the desired tally regions are a subset of the total problem space. Hence, a need remained for an effective method for variance reduction of Monte Carlo calculations of distributions and multiple localized tally regions.

2. THEORY

The goal of many "traditional" Monte Carlo simulations is to calculate the response (i.e., flux, dose, reaction rate, etc.) at some location(s), which can be expressed as

$$R = \int_P \psi(P)\sigma_d(P)dP \quad , \tag{1}$$

where ψ is the particle flux, σ_d is some objective function (e.g., dose response function), and P refers to the independent variables $\vec{r}, E, \hat{\Omega}$.

From the forward and adjoint forms of the transport equation [1],

$$H\psi = q \quad , \tag{2}$$

$$H^+\psi^+ = q^+ , \tag{3}$$

and the following adjoint identity

$$\langle \psi^+, H\psi \rangle = \langle \psi, H^+\psi^+ \rangle \quad , \tag{4}$$

one can show that

$$\langle \psi, q^+ \rangle = \langle \psi^+, q \rangle \ , \tag{5}$$

where H and H^+ are the forward and adjoint transport operators, ψ^+ is the adjoint function, q and q^+ are the forward and adjoint sources, and $\langle\,\rangle$ signify integration over all the independent variables. If one lets $q^+ = \sigma_d$, the left-hand side of Eq. (5) is the detector response [i.e., Eq. (1)] and the right-hand side is an alternate formulation for the response in terms of the adjoint function, resulting in the following two expressions for response:

$$R = \int_P \psi\ (P) q^+(P) dP \tag{6a}$$

$$R = \int_P \psi^+(P) q(P) dP \ . \tag{6b}$$

From Eq. (6b), the adjoint function, ψ^+, has physical meaning as the expected contribution to the response R from a particle in phase-space P, or, in other words, the importance of a particle in that phase space to the response. It is this physical interpretation that is used in the CADIS methodology to optimize local quantities. Specifically, the user defines a response (at some location) for optimization, which is used as the source in the deterministic adjoint calculation.

2.1 CADIS Method

The CADIS methodology is briefly reviewed in this section to provide background for the FW-CADIS discussion in the following section.

In the CADIS methodology, which evolves from Eq. (6b) and the concept of importance sampling [10], the biased source distribution is given by

$$\hat{q}(\vec{r},E,\hat{\Omega}) = \frac{\psi^+(\vec{r},E,\hat{\Omega})\, q(\vec{r},E,\hat{\Omega})}{\int_{4\pi}\int_E\int_V \psi^+(\vec{r},E,\hat{\Omega})\, q(\vec{r},E,\hat{\Omega})\, d\vec{r}\, dE\, d\hat{\Omega}} = \frac{\psi^+(\vec{r},E,\hat{\Omega})\, q(\vec{r},E,\hat{\Omega})}{R} \ , \tag{7}$$

where the numerator is the detector response from a particle in $(\vec{r},E,\hat{\Omega})$, and the denominator is the total detector response, R. Therefore, the ratio is a measure of the contribution from $(\vec{r},E,\hat{\Omega})$ to the total detector response. Intuitively, it is useful to bias the sampling of source particles by the ratio of their contribution to the detector response; therefore, this expression could also be derived from physical arguments.

Since the source variables are sampled from a biased probability density function, the statistical weight of the source particles must be corrected so that

$$w(\vec{r},E,\hat{\Omega})\, \hat{q}(\vec{r},E,\hat{\Omega}) = w_0 q(\vec{r},E,\hat{\Omega}) \ , \tag{8}$$

where w_0 is the unbiased particle starting weight, which is set equal to 1. Substituting Eq. (7) into Eq. (8) and rearranging, we obtain the following expression for the statistical weight of the particles:

$$w(\vec{r},E,\hat{\Omega}) = \frac{R}{\psi^{+}(\vec{r},E,\hat{\Omega})} \ . \tag{9}$$

This equation shows the inverse relationship between the adjoint (importance) function and the statistical weight. The relationships for the particle statistical weights, which are used in source sampling and the particle transport process, are consistent. Consequently, particles are created with weights that reside within their corresponding weight windows. This is an important characteristic of the CADIS methodology because it eliminates the incompatibility between source and transport biasing that has been problematic in other approaches as a result of poor computational efficiency and/or false convergence. For example, if the statistical weights of the source particles are not within the weight windows, the particles are immediately split or rouletted in an effort to bring their weights into the weight window. This results in unnecessary splitting/rouletting and a corresponding degradation in computational efficiency. Furthermore, for problems in which the adjoint function varies significantly within the source region (space and/or energy), the source biasing is very effective for improving computational efficiency.

2.2 FW-CADIS Method

For global variance reduction, one is typically interested in determining a space- and/or energy-dependent flux or response (e.g., dose rates) with uniformly low statistical uncertainty. To achieve this objective in a Monte Carlo simulation, it has been suggested [9] that the distribution of Monte Carlo particles should be uniform throughout the system. Although this is not a "physical" response, it does intuitively represent a desirable objective for obtaining uniform uncertainty and indicates that it may be possible to develop an adjoint importance function that represents the importance of particles to achieving this desired objective, i.e., uniformly distributed Monte Carlo particles. To do so, we cast the problem of calculating Monte Carlo particle density into our response formulation:

$$R = \int_{4\pi} d\Omega \int_{V} dV \int_{E} dE \ \psi(\vec{r},E,\hat{\Omega}) \ f(\vec{r},E,\hat{\Omega}) \ ,$$

where $f(\vec{r},E,\hat{\Omega})$ is some function that converts flux to Monte Carlo particle density. Since the physical particle density, $n(\vec{r},E,\hat{\Omega})$, is related to the Monte Carlo particle density, $m(\vec{r},E,\hat{\Omega})$, by the average particle weight, $\overline{w}(\vec{r},E,\hat{\Omega})$,

$$n\left(\vec{r},E,\hat{\Omega}\right) = \overline{w}\left(\vec{r},E,\hat{\Omega}\right) m\left(\vec{r},E,\hat{\Omega}\right), \tag{10}$$

and

$$\psi\left(\vec{r},E,\hat{\Omega}\right) = n\left(\vec{r},E,\hat{\Omega}\right) v\left(\vec{r},E,\hat{\Omega}\right) \ , \tag{11}$$

where $v(\vec{r},E,\hat{\Omega})$ is the particle velocity, the Monte Carlo particle density can be estimated by

$$m\left(\vec{r},E,\hat{\Omega}\right) = \frac{n\left(\vec{r},E,\hat{\Omega}\right)}{\overline{w}\left(\vec{r},E,\hat{\Omega}\right)} = \frac{\psi\left(\vec{r},E,\hat{\Omega}\right)}{\overline{w}\left(\vec{r},E,\hat{\Omega}\right) v\left(\vec{r},E,\hat{\Omega}\right)} \tag{12}$$

and the *total* Monte Carlo particle density can be estimated by

$$R = \int_{4\pi}\int_{E}\int_{V} \psi(\vec{r},E,\hat{\Omega}) \left[\frac{1}{\bar{w}(\vec{r},E,\hat{\Omega})\, v(\vec{r},E,\hat{\Omega})} \right] d\vec{r}\, dE\, d\hat{\Omega} \ . \tag{13}$$

Recalling from Cooper and Larsen [9] that if the average particle weight is set proportional to the physical particle density, then the Monte Carlo particle density should be approximately uniform (constant), as desired, i.e.,

$$\begin{aligned} &\textit{for } m \approx \textit{cont.}, \\ &\bar{w} \propto n, \textit{ and} \\ &\bar{w} v \propto \psi. \end{aligned}$$

Therefore, by substituting the forward flux, $\psi(\vec{r},E,\hat{\Omega})$, for $[\bar{w}(\vec{r},E,\hat{\Omega})\, v(\vec{r},E,\hat{\Omega})]$, Eq. (13) becomes

$$R = \int_{4\pi}\int_{E}\int_{V} \psi(\vec{r},E,\hat{\Omega}) \left[\frac{1}{\psi(\vec{r},E,\hat{\Omega})} \right] d\vec{r}\, dE\, d\hat{\Omega} \ . \tag{14}$$

Recognizing the similarities between Eqs. (14) and (6a), we see that by defining the adjoint source as the bracketed term in Eq. (14),

$$q^{+}\left(\vec{r},E,\hat{\Omega}\right) = \frac{1}{\psi\left(\vec{r},E,\hat{\Omega}\right)} \ , \tag{15}$$

we can calculate an adjoint importance function that represents the importance of particles to achieving the desired objective, i.e., uniformly distributed Monte Carlo particles, which should correspond to approximately uniform statistical uncertainties. Physically, this corresponds to weighting the adjoint source with the inverse of the forward flux. Hence, where the forward flux is low, the adjoint source will be high, and vice versa. Once the adjoint is determined, the standard CADIS methodology is used to calculate consistent source biasing parameters and weight windows [see Eqs. (7) and (9)]. Therefore, we refer to this new method as the Forward-Weighted CADIS method.

Following these same steps, it is also possible to determine an importance function for optimizing other responses. For example, if dose rate throughout a model is the desired objective of the Monte Carlo calculation and σ_d represents the dose response function, the adjoint source can be defined as

$$q^{+}(\vec{r},E,\hat{\Omega}) = \frac{\sigma_d(\vec{r},E,\hat{\Omega})}{\iint \sigma_d(\vec{r},E',\hat{\Omega}')\psi(\vec{r},E',\hat{\Omega}')dE'd\hat{\Omega}'} \tag{16}$$

so that

$$R'(\vec{r}) = \iint \psi(\vec{r},E,\hat{\Omega}) \frac{\sigma_d(\vec{r},E,\hat{\Omega})}{\iint \sigma_d(\vec{r},E',\hat{\Omega}')\psi(\vec{r},E',\hat{\Omega}')dE'd\hat{\Omega}'} dE d\hat{\Omega} \tag{17}$$

and the individual spatial contributions to the total response are uniform, as desired for variance reduction of the spatial dose distribution. If, on the other hand, the dose rate throughout a portion of the problem volume, V, is the desired objective, then the adjoint source can be defined as

$$q^{+}(\vec{r},E,\hat{\Omega}) = \begin{cases} \dfrac{\sigma_d(\vec{r},E,\hat{\Omega})}{\iint \sigma_d(\vec{r},E',\hat{\Omega}')\psi(\vec{r},E',\hat{\Omega}')dE'd\hat{\Omega}'} & \text{for } \vec{\mathrm{r}} \in V \\ 0 & \text{for } \vec{\mathrm{r}} \notin V \end{cases} . \quad (18)$$

The adjoint source can be defined for whatever objective is desired. If space- and energy-dependent flux is desired, $\sigma_d(\vec{r},E,\hat{\Omega})$ is unity and the adjoint source is the inverse of the space- and energy-dependent forward flux, integrated over angle. Subsequently, the individual space and energy contributions to the total response are uniform (unity), as desired.

From adjoint transport theory, if we consider a point source of the form

$$q(\vec{r},E,\hat{\Omega}) = \delta(\vec{r}-\vec{r}_0)\delta(E-E_0)\delta(\hat{\Omega}-\hat{\Omega}_0) \text{ ,} \quad (19)$$

in Eq. (6b), we obtain

$$R' = \psi^{+}(\vec{r}_0,E_0,\hat{\Omega}_0) \text{ .} \quad (20)$$

Therefore, the adjoint function is the contribution from particles produced at $\vec{r}_0,E_0,\hat{\Omega}_0$ to the detector response, which, from Eq. (14), is uniform throughout the system. It is this physical interpretation that makes this "nontraditional" adjoint function well suited to global optimization of Monte Carlo simulations.

In the FW-CADIS method, forward information (e.g., flux, dose) is used to define an appropriate response (adjoint source) to be used in a deterministic adjoint calculation to generate the adjoint importance function for achieving uniform particle density (or response) throughout the system. With this method it is possible to optimize for distributions, such as flux or dose rate distributions throughout a problem, as well as multiple individual responses, such as response at multiple localized detectors (see for example Ref. 11) or spectra, simply depending on how the adjoint source is defined.

3. IMPLEMENTATION

The FW-CADIS method requires two (one forward and one adjoint) deterministic calculations, prior to the Monte Carlo simulation. Once the adjoint (importance) function is determined, the CADIS methodology is used to calculate consistent source and transport (weight windows) space- and energy-dependent biasing parameters, as has been described in detail elsewhere [2, 3]. This capability is implemented and automated in the SCALE 6 MAVRIC sequence (uses Denovo [12] for the 3-D deterministic calculations and the SCALE Monaco code for 3-D multigroup Monte Carlo calculations). The capability is also implemented and automated in the ADVANTG code (currently uses TORT or Denovo for 3-D deterministic calculations and the MCNP code for 3-D continuous energy Monte Carlo calculations). Note that although the CADIS methodology is general, the implementation is currently limited to space and energy.

4. EXAMPLE PROBLEM

The FW-CADIS method was developed to address the computational challenge associated with calculating the dose rates throughout an entire pressurized-water reactor (PWR) facility, resulting from the core or spent fuel neutron and photon sources. An actual "as-built" PWR facility, including containment, auxiliary, and turbine buildings, was modeled with the MCNP code (see Fig. 1). The model size is approximately 85×125×70 m. As expected, it is not possible to achieve statistically meaningful results in locations other than those very near the source regions without variance reduction. Hence, the ADVANTG code (using the CADIS methodology) was applied with the adjoint source specified at the outer boundaries of the problem in an attempt to encourage particles to move outward through the entire system. This approach did yield meaningful, good results but required manual iteration/intervention to adjust the adjoint source magnitude at the boundaries (e.g., to increase adjoint source on the boundary furthest from the source regions) and raised concerns about the dose being underestimated in regions between the source and boundary as a result of the extensive biasing toward the boundaries. Also, note that this approach would not be well suited for achieving convergence of energy-dependent quantities.

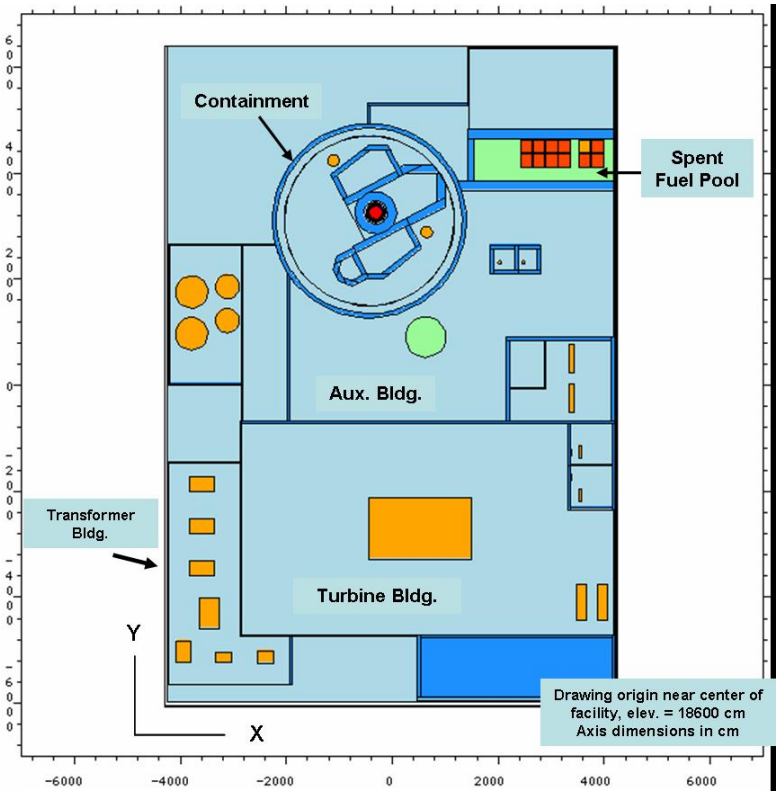

Figure 1. Plan X-Y view of PWR facility MCNP model. The containment, auxiliary, and turbine buildings and major components are shown.

For these reasons, the FW-CADIS method was developed and applied. The objective of this application is uniform statistical convergence of dose (integrated over energy) throughout the facility calculated via the mesh tally feature. With this objective, the energy dependence of the adjoint source is the energy-dependent dose response function; and the spatial dependence is the inverted total dose response for each cell (from a forward deterministic calculation), as shown in Eq. (16). With this approach, the ADVANTG code was used with MCNP5 to calculate the dose map throughout the entire PWR facility [13].

Figure 2 compares dose rate results based on an analog (implicit-capture-only) simulation; the standard CADIS approach, with the adjoint source specified on the exterior boundaries of the problem; and the FW-CADIS method for similar amounts of computational time. It is readily apparent that analog Monte Carlo is not a viable option for this problem. In fact, the analog calculation was subsequently allowed to run five times longer than the time shown in Fig. 2 (i.e., 5E+10 particle histories, ~125 CPU days) and the results look essentially the same (i.e., the same as what is shown in Fig. 2 for the analog case).

Although the CADIS method enables calculation of dose rates (within ~20 CPU days) outside the reactor containment, meaningful results are not achieved in large portions of the problem without the FW-CADIS method. Figure 3 shows the relative errors associated with each case. A comparison of relative error histograms, which illustrates the fraction of mesh tally cells below a certain relative error, is provided in Fig. 4. Figure 5 shows the relative error histogram for tally cells in which the dose rate is $\geq$ 1 mrem/h and reveals that with the FW-CADIS method, ~95% of those tally cells have relative errors of $<$3%.

These figures clearly illustrate that analog Monte Carlo is not viable for this problem and that the FW-CADIS method provides superior convergence. This outcome is expected because the importance function used in the FW-CADIS method corresponds to the actual desired objective. Although regions of large statistical uncertainty still remain with the FW-CADIS method, note that this is an incredibly large problem with dose rates varying by nearly 30 orders of magnitude and that the results are based on only ~20 CPU days. With the use of the FW-CADIS method and multiple processors, this problem becomes quite manageable. Nevertheless, future work is planned to further investigate the performance and convergence behavior of the FW-CADIS method. It is currently hypothesized that the regions of large statistical uncertainty that are present in the FW-CADIS results are associated with deficiencies/inaccuracies in the TORT deterministic calculations, which used very coarse spatial meshing because of the very large size of the problem. However, this has not been confirmed. For the CADIS and FW-CADIS cases, the deterministic calculations required approximately 17 hours of CPU time each.

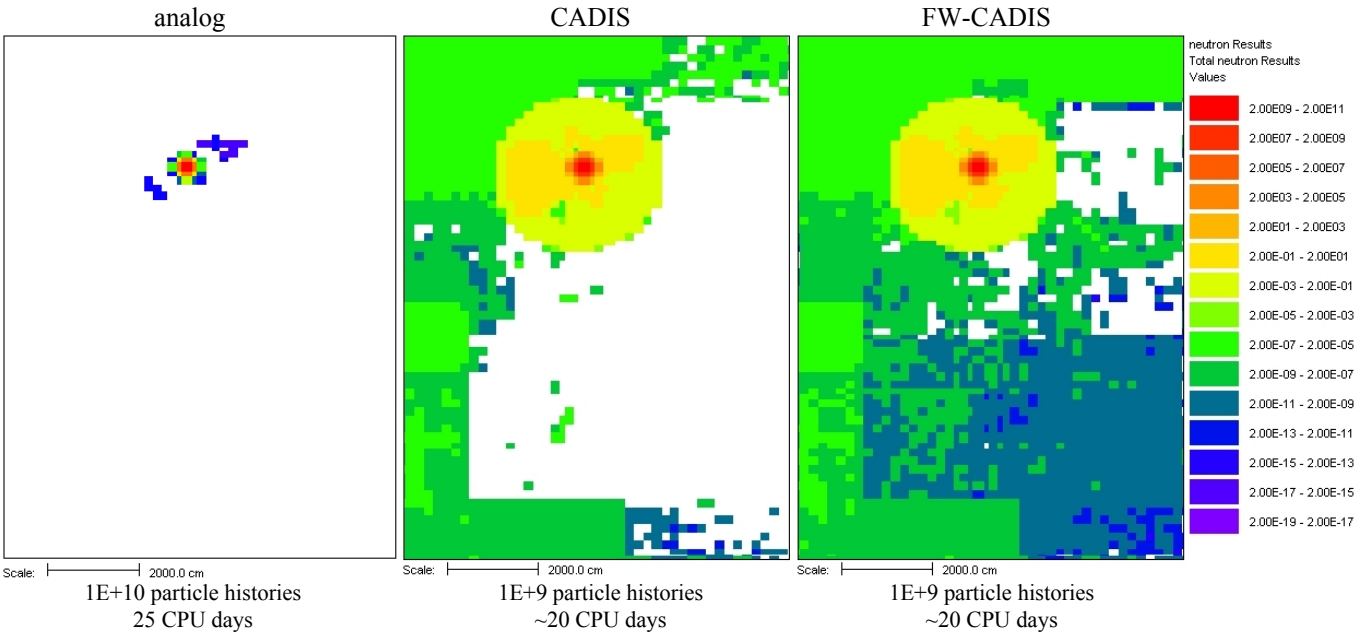

Figure 2. Dose rates (mrem/h) computed using analog (left), CADIS with the adjoint source on the outer boundaries of the model (center), and FW-CADIS (right).

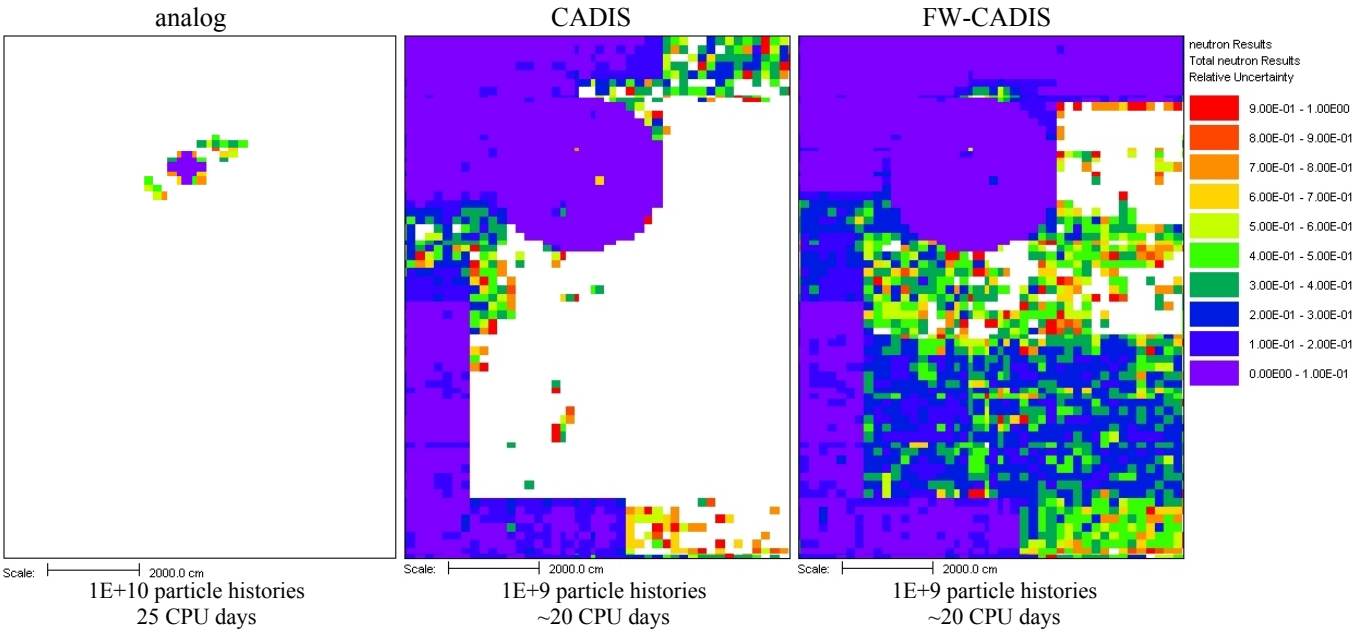

Figure 3. Relative errors computed using analog (left), CADIS with the adjoint source on the outer boundaries of the model (center), and FW-CADIS (right).

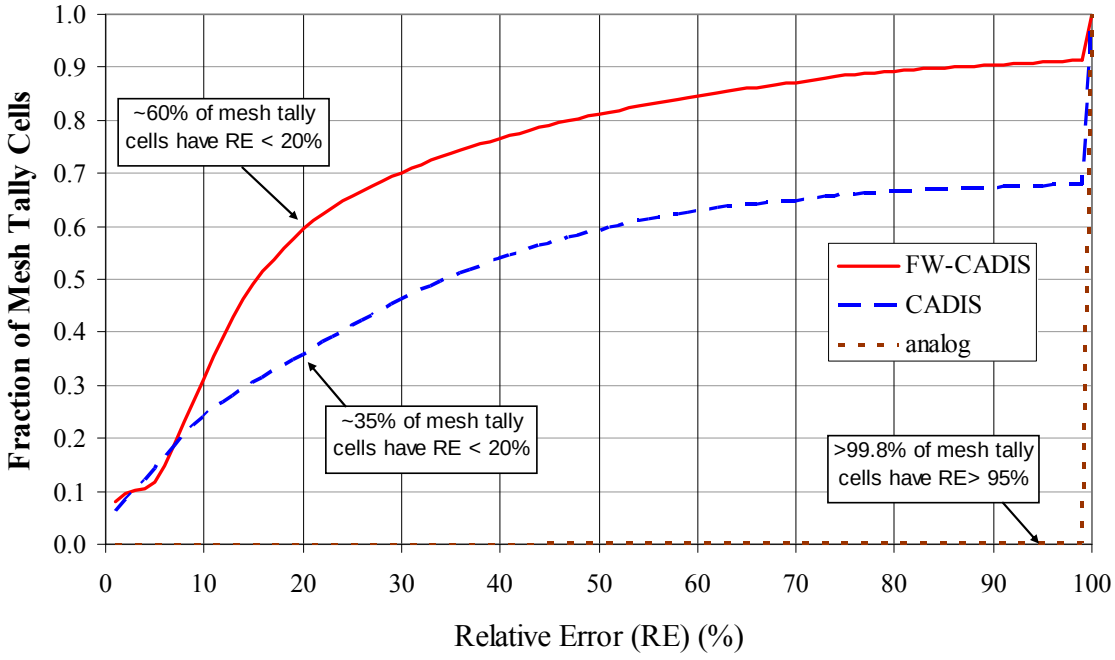

Figure 4. Relative error histograms for the different methods.

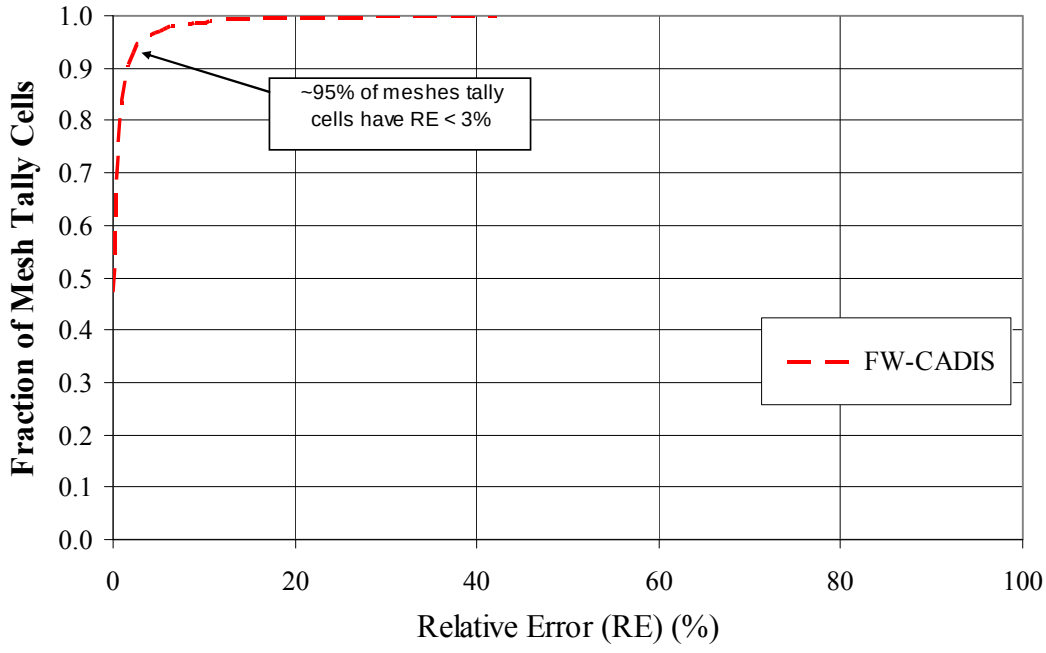

Figure 5. Relative error histogram for tally cells with dose rates ≥ 1 mrem/h.

5. SUMMARY

A new hybrid (Monte Carlo/deterministic) transport method has been developed for increasing the efficiency of Monte Carlo calculations of distributions, such as flux or dose rate distributions (e.g., mesh tallies), as well as responses at multiple localized detectors and spectra. The method was applied to the problem of determining dose rates throughout a full-scale PWR facility and was shown to enable a continuous-energy Monte Carlo-based solution for dose rates throughout the facility, which would otherwise be computationally prohibitive. The method has also been applied to other relevant and challenging problems, including an array of commercial spent fuel storage casks [14, 15], criticality accident alarm system (CAAS) analyses [16], and nuclear well-logging simulations [11]. In all applications to date, excellent results have been achieved. The method requires two approximate discrete ordinates calculations (one forward and one adjoint) to generate consistent source biasing and weight window parameters for the subsequent Monte Carlo simulation and does not require any modifications to existing Monte Carlo codes. A distinguishing characteristic of this method, as compared with other global variance reduction methods [9, 17], is that it can be used to optimize results for a subset (or subsets) of the problem space, as opposed to the entire problem space. Furthermore, this method should be suitable for a large range of problems, including the use of Monte Carlo for depletion calculations and continuous-energy Monte Carlo for generation of problem-dependent multigroup cross sections.

ACKNOWLEDGMENT

This work was sponsored by the Defense Threat Reduction Agency (DTRA). ORNL is managed and operated by UT-Battelle, LLC, for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

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