Forward-Weighted CADIS Method for Global Variance Reduction

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INTRODUCTION

Recent applications' needs/desires have motivated efforts to develop approaches for optimizing Monte Carlo calculations for global distributions, such as flux or dose rate distributions (e.g., mesh tallies), as well as response 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 [5] sequence of SCALE, is being routinely used at ORNL for three-dimensional (3-D) Monte Carlo simulations of real applications.

Although the CADIS methodology has proven to be very effective for automated optimization of localized quantities, until very recently, efforts to optimize global distributions 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. Previous work by Cooper and Larsen, which used the inverted forward flux as the importance function (no adjoint calculation) in an attempt to distribute particles uniformly throughout the system has demonstrated some benefit [6]. While 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 uniform particle density (or response) throughout the system. When applied to a large realistic application, this method was not found to be effective. Hence, a need has remained for an effective method for global variance reduction of Monte Carlo simulations.

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:

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

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],

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

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

and the following adjoint identity

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

one can show that

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

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 alternative formulation for the response in terms of the adjoint function:

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

From Eq. (6), 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 has been used in the application of 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.

For global variance reduction, one is interested in determining a space- and 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 proposed [6] 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. Hence, employing the adjoint transport theory, it is possible to define the adjoint source, q^+, such that the corresponding adjoint function represents the importance of particles to the desired (uniform) objective. 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

$$q^+(\vec{r},E,\hat{\Omega}) = \frac{\sigma_d(\vec{r},E,\hat{\Omega})}{\iint \sigma_d(\vec{r},E',\hat{\Omega}')\psi(\vec{r},E',\hat{\Omega}')dE'd\hat{\Omega}'}, \quad (7)$$

such that

$$R'(\vec{r}) = \iint \psi(\vec{r},E,\hat{\Omega}) \frac{\sigma_d(\vec{r},E,\hat{\Omega})}{\iint \sigma_d(\vec{r},E',\hat{\Omega}')\psi(\vec{r},E',\hat{\Omega}')dE'd\hat{\Omega}'} dEd\hat{\Omega}, \quad (8)$$

and the individual spatial contributions to the total response are uniform, as desired for variance reduction of the spatial dose distribution.

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

$$q(\vec{r},E,\hat{\Omega}) = \delta(\vec{r}-\vec{r}_0)\delta(E-E_0)\delta(\hat{\Omega}-\hat{\Omega}_0), \quad (9)$$

in Eq. (6), we obtain

$$R' = \psi^+(\vec{r}_0,E_0,\hat{\Omega}_0). \quad (10)$$

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. (8), is uniform throughout the system. It is this physical interpretation that makes this "non-traditional" adjoint function well suited to global optimization of Monte Carlo simulations. The use of this "nontraditional" adjoint function with the CADIS methodology is referred to as the FW-CADIS method.

In the FW-CADIS method, forward information (e.g., flux, dose, etc.) 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. From Eq. (8), it is possible to optimize for global quantities, such as flux or dose rate distributions throughout a problem, as well as semi-global responses, such as response at multiple localized detectors or spectra, simply depending on how the adjoint source is defined.

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 elsewhere [2,3]. This capability is implemented and automated in the SCALE MAVRIC sequence (uses TORT for 3-D deterministic calculations and the SCALE Monaco code for 3-D multigroup Monte Carlo calculations), which will be available in the next public release of SCALE. With the exception of the forward deterministic step, which currently requires some user intervention, the capability is also implemented/ automated in the ADVANTG code (uses TORT 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.

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., 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. Also, note that this approach would not be well suited for achieving global convergence of energy-dependent quantities.

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. 7. With this approach, the ADVANTG code was used with MCNP5 to calculate the dose map throughout the entire PWR facility.

Figure 2 shows the dose results based on the standard CADIS approach, with the adjoint source specified on the exterior boundaries of the problem, and the FW-CADIS method for the same amount of computational time. Meaningful results are not achieved in large portions of the problem without the FW-CADIS method. Figure 3 shows the relative uncertainties from both methods. A comparison of relative uncertainty histograms, which illustrates the fraction of mesh cells below a certain relative uncertainty, is provided in Fig. 4. This figure clearly illustrates 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 methods 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 more than 20 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 thoroughly investigate the performance and convergence behavior of the FW-CADIS method.

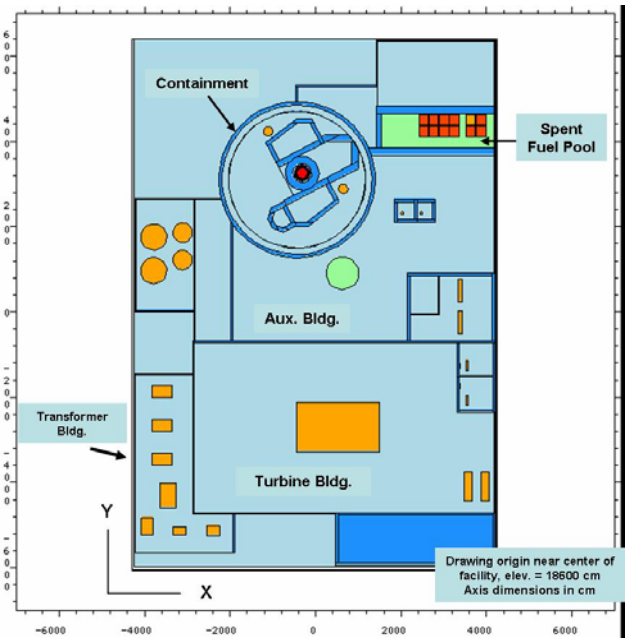

Fig. 1. Plan X-Y view of PWR facility. The containment, auxiliary, and turbine buildings and major components are shown.

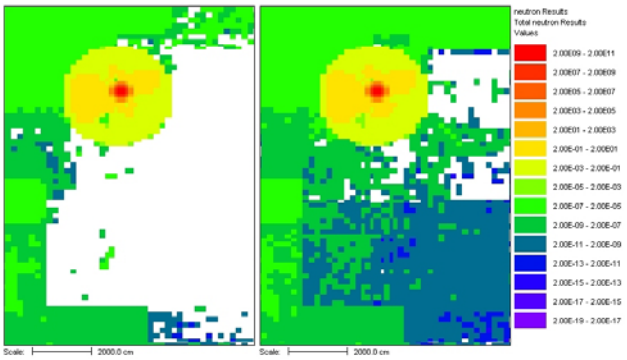

Fig. 2. Dose rates (mrem/h) computed using CADIS with the adjoint source on the outer boundaries of the model (left) and using FW-CADIS (right).

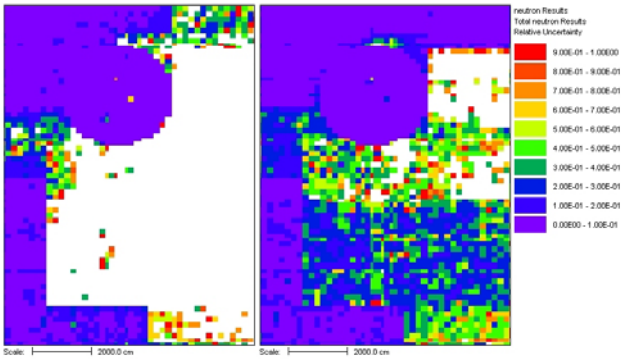

Fig. 3 Relative uncertainties computed using CADIS with the adjoint source on the outer boundaries of the model (left) and using FW-CADIS (right).

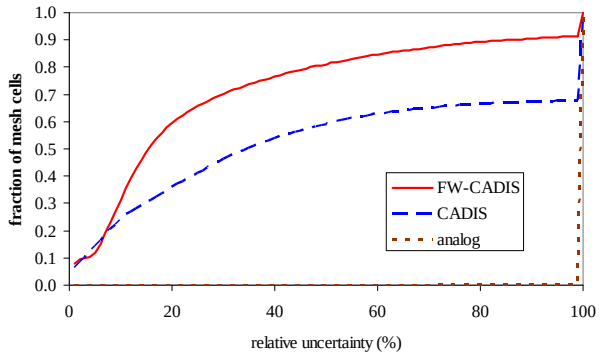

Fig. 4. Relative uncertainty histograms for the different methods.

SUMMARY

The FW-CADIS method for optimizing global distributions has been developed, and initial testing on a model of an entire PWR facility has been performed. The method has also been applied to two other large problems, including an array of spent fuel storage casks, as described in a companion paper [7]. 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. Although more testing and thorough analysis of results is still needed, the potential of this method for optimizing global distributions, including energy-dependent flux distributions, as well as semi-global distributions, such as response at multiple localized detectors or spectra, appears very promising. Furthermore, this method should be suitable for a large range of problems, including the use of Monte Carlo for depletion.

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