FW-CADIS Method for Global and Regional Variance Reduction of Monte Carlo Radiation Transport Calculations

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Abstract—This paper presents a 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 an extension of the Consistent Adjoint Driven Importance Sampling (CADIS) method, which has been used for more than a decade 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 more uniform statistical uncertainties in the desired tally regions. The FW-CADIS method has been implemented and demonstrated within the MAVRIC (Monaco with Automated Variance Reduction using Importance Calculations) sequence of SCALE and the ADVANTG (Automated Deterministic Variance Reduction Generator)/MCNP framework. Application of the method to representative real-world problems, including calculation of dose rate and energy-dependent flux throughout the problem space, dose rates in specific areas, and energy spectra at multiple detectors, is presented and discussed. Results of the FW-CADIS method and other recently developed global variance-reduction approaches are also compared, and the FW-CADIS method outperformed the other methods in all cases considered.

I. INTRODUCTION

Although the stochastic Monte Carlo method is considered to be the most accurate method available for solving radiation transport problems, its applicability has been limited by its computational expense. This is particularly true for deep-penetration shielding problems, involving attenuation of several orders of magnitude between the source and detector, and problems requiring detailed distributions (e.g., flux or dose rate) throughout the system being analyzed. While advanced variance-reduction methods, such as the use of deterministic adjoint importance functions,1 have been applied successfully to the former class of source-detector problems, optimization of Monte Carlo simulations for calculating detailed distributions throughout a system or for calculating the responses of multiple detectors is a relatively new area of research. In fact, it is a generally accepted view in the radiation shielding community that deterministic transport methods (e.g., the discrete ordinates method) are necessary for the analysis of systems for which detailed distributions are required. Nevertheless, desires to capitalize on the accuracy and modeling fidelity associated with the Monte Carlo method, continuing increases in

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available computational resources, and the availability of mesh tally (a set of region tallies defined on a mesh that overlays the geometry) features in modern Monte Carlo codes have motivated users to challenge this status quo and attempt to calculate detailed distributions (e.g., mesh tallies) with the Monte Carlo method. For analyses that require the statistical uncertainty in each mesh cell to be less than some maximum value, the Monte Carlo computation time is dictated by the mesh cell with the slowest statistical convergence (largest statistical uncertainty). Consequently, for problems involving significant radiation attenuation, the computation time required by the Monte Carlo method for calculating detailed distributions is typically prohibitive, and other means (e.g., deterministic methods) must be used for the analysis.

The inability to calculate detailed distributions with available Monte Carlo codes and methods motivated efforts at the Oak Ridge National Laboratory (ORNL) to investigate and develop methods to overcome this inability. These efforts have led to the development of an extension to the Consistent Adjoint Driven Importance Sampling (CADIS) method for global and regional variance reduction. The CADIS method\(^2\) was developed previously and has been shown to be highly effective (see, for example, Refs. 1 through 6) for deep-penetration source-detector–type problems, i.e., problems where a single, localized response is sought, using source biasing parameters and weight windows\(^3\) based on a deterministic adjoint function. The CADIS method is a hybrid method in that it utilizes results from a deterministic calculation to improve the efficiency of a Monte Carlo simulation. The method, referred to as the Forward-Weighted CADIS (FW-CADIS) method,\(^8,9\) involves determining an adjoint importance function that represents the importance of particles to achieving uniform Monte Carlo particle density, which is related to statistical uncertainty, throughout all (global variance reduction) or part (regional variance reduction) of the problem space. The name stems from the fact that the method involves a weighting of the adjoint source with information from a forward solution, i.e., forward weighting. Once the appropriate adjoint (importance) function is obtained, standard CADIS relations are used to calculate consistent source biasing parameters and weight window values. To the authors’ knowledge, the FW-CADIS method represents a novel use of the adjoint methodology for biasing Monte Carlo simulations. This paper provides a detailed description of the FW-CADIS method and examples of its application to relevant problems in the nuclear industry.

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\(^3\)The weight window technique provides a means for assigning detailed space- and energy-dependent importance values and applying geometric splitting/roulette and energy splitting/roulette, while at the same time controlling weight variations. See Ref. 7 for more details.

I.A. Background

Over the past several decades, many techniques, referred to as variance-reduction and/or biasing techniques, have been developed to reduce the variance of Monte Carlo calculations. These techniques commonly modify the natural sampling procedure/formulation (related to the physical laws of particle transport) to focus computational efforts on the simulation of “important” particles (i.e., those particles that contribute to the desired tally). To compensate for this modification and preserve the correct average for the simulation, each particle is given a statistical weight \(w\). At each event where a modified probability density function (pdf) \(f(x)\) is sampled instead of the physical pdf \(\tilde{f}(x)\), the weight is modified by the ratio \(f(x)/\tilde{f}(x)\).

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., \(f(x)\)]. Specifically, all variance-reduction techniques require problem-specific parameters that are dependent on the importance of particles with respect to the tally objective. The challenge to the user has been determining the problem-specific parameters. In the absence of a reliable, physics-based method for developing the needed parameters, Booth and Hendricks\(^10\) aptly describe the situation: “The selection 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 these difficulties, a number of strategies (both deterministic and stochastic) for determining variance-reduction parameters have been proposed and developed.

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\(^11\) 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, trends in Monte Carlo code development have reflected a recognition of the benefits of using deterministic adjoint (importance) functions for Monte Carlo variance reduction.\(^12\) A review of variance-reduction concepts and works related to the use of deterministic importance functions for variance reduction of Monte Carlo simulations is available in Ref. 1. As discussed in Ref. 1, deterministic adjoint functions have been used for Monte Carlo variance reduction of source-detector–type problems for many years with considerable success. The CADIS methodology\(^1,2\) has been implemented and automated into codes such as A\(^3\)MCNP (Refs. 1 and 13) and Automated Deterministic Variance Reduction Generator\(^14,15\) (ADV\(\breve{\text{A}}\)NTG) (more recently), which are based on MCNP (Ref. 7), and the Monaco with Automated
Variance Reduction using Importance Calculations\textsuperscript{16,17} (MAVRIC) sequence released with SCALE 6 (Ref. 18), and is being routinely used at ORNL and elsewhere\textsuperscript{19-23} for three-dimensional (3-D) Monte Carlo simulations of real, complex radiation transport applications.

Although the CADIS methodology has proven to be very effective for automated optimization of localized quantities in source-detector–type problems, efforts to optimize global distributions have not, until very recently, 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\textsuperscript{24,25} but required considerable user understanding of the problem and an iterative approach, which complicates the ability to automate the process. (The ability of any method to be automated is considered by the authors to be critically important to its ultimate use.)

Previous work for global problems by Cooper and Larsen\textsuperscript{26} suggests that in order to obtain uniform relative uncertainties in a Monte Carlo calculation, it is necessary to have uniformly distributed Monte Carlo particle density throughout the system. Recognizing that the physical particle density $n(\vec{r})$ is related to the Monte Carlo particle density $m(\vec{r})$ by the average particle weight $\bar{w}(\vec{r})$,

$$n(\vec{r}) = \bar{w}(\vec{r})m(\vec{r}).$$  \hfill (1)

Cooper and Larsen observed that if the average particle weight is proportional to the physical particle density, the Monte Carlo particle density is approximately constant, as desired [i.e., for $m(\vec{r})$ equal to a constant $c$, then $\bar{w}(\vec{r}) = n(\vec{r})/c$]. Therefore, to make the Monte Carlo particle density $m(\vec{r})$ constant over the geometry, Cooper and Larsen propose the use of weight targets based on an estimate of the forward scalar flux $\phi(\vec{r})$ as

$$\bar{w}(\vec{r}) = \frac{\phi(\vec{r})}{\max(\phi(\vec{r}))}.$$

Intuitively, this method makes sense in that it is desirable to have low weight targets (high importance) where the flux is low, and vice versa. While this approach does encourage particles toward regions of lower flux and discourages particles from moving toward regions of higher flux, the forward flux does not represent the expected contribution to the desired response, which is proposed to be uniform Monte Carlo particle density throughout the system. Using this method, Cooper and Larsen demonstrated good results for one-group test problems. When applied to more realistic applications, however, the method was not found to be satisfactorily effective in many cases.\textsuperscript{24}

Another relevant prior work is that of Becker et al.\textsuperscript{27} which involves a hybrid global variance-reduction method based on a new concept referred to as “correctons.” In this method, a deterministic solution is used to construct an efficient Monte Carlo problem in terms of “correctons” such that the correction flux has considerably less variation across a system than the physical flux. This method has been demonstrated on one-dimensional, one-group problems but has not yet been demonstrated on realistic problems. While many of the methods have focused on creating parameters for use in techniques that are available in the standard codes (e.g., weight windows and source biasing parameters), this method would require changes to existing Monte Carlo codes.

Hence, a need remained for an effective method for global variance reduction of realistic (i.e., geometrically complex, multidimensional, energy-dependent) Monte Carlo simulations. In particular, a method that meets the following criteria is desired:

1. simultaneously optimizes multiple tallies and/or mesh tallies with nearly uniform statistical uncertainties
2. operates in combination with standard Monte Carlo codes through “standard” features and utilizes proven, reliable variance-reduction techniques (e.g., weight windows and source biasing)
3. is automatable so that users without expert knowledge of either deterministic or Monte Carlo methods can still use it effectively on their applications.

The FW-CADIS method was developed in response to this need. Although the FW-CADIS approach was originally conceived to simultaneously optimize near and far detectors in a nuclear well-logging tool,\textsuperscript{28} it was not formalized and initially published until 2007.

In parallel to the work at ORNL, researchers at the University of Michigan were continuing their work to develop a more effective method for global variance reduction. Building on Cooper and Larsen’s method, two approaches have been developed\textsuperscript{29} that create weight windows as functions of space and energy, based on only the forward estimate of flux. These methods differ by the type of global information the user desires from the simulation: global flux weight windows (GFWWs), for obtaining flux in every energy group at every location, and global response weight windows (GRWWs), for obtaining an energy-integrated response at every spatial location. Both of these methods are designed for calculating the “global solution”—everywhere in the geometry of the problem—with nearly uniform statistics. These methods are summarized in Table I.

Becker\textsuperscript{30} has also proposed three methods for developing weight windows based on both forward and adjoint deterministic solutions. The three methods
correspond to the portion of phase-space over which uniform relative uncertainties are desired: a small “detector” region, a region comprising a significant portion of the entire problem, and the global problem. Each of the three methods is designed to provide uniform uncertainties across space and energy or just across space.

I.B. Global Variance-Reduction Terminology

To distinguish between different types of problem objectives, this paper uses the terms “global,” “regional,” and “source-detector” to represent problem objectives that are defined as follows:

1. Global: The goal is to calculate the flux $\phi(r, E)$ or flux-based response throughout the entire problem space with low statistical uncertainty. Examples include calculation of space- and energy-dependent flux and dose rate over the entire spatial domain of a problem.

2. Regional: The goal is to calculate the flux or flux-based response over a portion or portions of the problem space with low statistical uncertainty. Examples include calculation of space- and energy-dependent flux and dose rate throughout one or more spatial regions of a problem.

3. Source-detector: The goal is to calculate the flux or flux-based response at a single location with low statistical uncertainty. For example, to calculate the total dose rate using the flux–to–dose rate conversion factors $\sigma_d(E)$ over a detector volume $V_d$, the specific response of interest is

$$D = \iiint_{4\pi E V_d} \psi(r, E, \hat{\Omega}) \sigma_d(E) d\tilde{r} dE d\hat{\Omega}. \quad (3)$$

I.C. Outline

This paper presents a method that satisfies the above criteria and provides examples of its application. It is an extension of the CADIS method that involves forward weighting of the adjoint source to generate an adjoint function that represents the particle importance to the desired global or regional response. This method, FW-CADIS, has been implemented and demonstrated within the MAVRIC sequence of SCALE 6 and the ADVANTG/MCNP framework. The remainder of this paper is organized as follows. Section II reviews the CADIS methodology for variance reduction of source-detector problems and describes the theory behind the FW-CADIS method for global and regional variance reduction. Section III describes the implementation of the CADIS and the FW-CADIS methodologies in the MAVRIC and ADVANTG codes. Section IV discusses the application and performance of the FW-CADIS method for the solution of example problems that are representative of real-world problems of interest to the nuclear industry. Results of the FW-CADIS method and other recently developed global variance-reduction approaches are also compared in Sec. IV. Finally, summary and concluding remarks are offered in Sec. V.

II. METHODS

As noted in Sec. I.A., it has long been recognized that the adjoint function has physical significance 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. This recognition has led to the development of several methods that utilize deterministic adjoint importance functions for Monte Carlo variance reduction. In this section, we briefly review the adjoint methodology, prior to describing the methods for variance reduction of source-detector, global, and regional problems.

II.A. Adjoint Methodology

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

$$R = \iiint_{4\pi E V} \psi(r, E, \hat{\Omega}) \sigma_d(r, E, \hat{\Omega}) d\tilde{r} dE d\hat{\Omega}. \quad (4)$$

### TABLE I

Global Variance-Reduction Methods Using Forward Estimates

<table>
<thead>
<tr>
<th>Method</th>
<th>To Optimize</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td>GFWW</td>
<td>$\phi(r, E)$</td>
<td>$\tilde{w}(r, E) \propto \phi(r, E)$</td>
</tr>
<tr>
<td>GRWW</td>
<td>$D(r) = \int_E \sigma_d(r, E) \phi(r, E) dE$</td>
<td>$\tilde{w}(r, E) \propto \frac{D(r)}{\sigma_d(r, E)}$</td>
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</tbody>
</table>
where $\psi$ is the particle flux and $\sigma_d$ is some objective function (e.g., dose rate response function).

From the forward and adjoint forms of the transport equation,$^{11}$

$$H\psi = q$$  \hspace{1cm} (5)

and

$$H^+ \psi^+ = q^+,$$  \hspace{1cm} (6)

and the following adjoint identity

$$\langle \psi^+, H\psi \rangle = \langle \psi, H^+ \psi^+ \rangle,$$  \hspace{1cm} (7)

one can show that

$$\langle \psi, q^+ \rangle = \langle \psi^+, q \rangle,$$  \hspace{1cm} (8)

where $H, H^+$ = forward and adjoint transport operators, respectively

$\psi^+$ = adjoint function

$q, q^+$ = forward and adjoint sources, respectively

$\langle \rangle = $ integration over all the independent variables.

If one lets $q^+ = \sigma_d$, the left side of Eq. (8) is the detector response [i.e., Eq. (4)], and the right side is an alternative formulation for the response in terms of the adjoint function, resulting in the following two expressions for response:

$$R = \iiint_{4\pi \ E \ V} \psi(\vec{r}, E, \Omega) q^+(\vec{r}, E, \Omega) d\vec{r}dEd\Omega$$ \hspace{1cm} (9a)

and

$$R = \iiint_{4\pi \ E \ V} \psi^+(\vec{r}, E, \Omega) q(\vec{r}, E, \Omega) d\vec{r}dEd\Omega.$$ \hspace{1cm} (9b)

From Eq. (9b), the adjoint function $\psi^+$ has physical meaning as the expected contribution to the response $R$ from a particle in $(\vec{r}, E, \Omega)$ 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 development of methods, like the CADIS methodology described below, to optimize local quantities for source-detector–type problems. Specifically, the user defines a response (at some location) for optimization, and that response is used to define the adjoint source.

The following sections describe variance-reduction methodologies for source-detector, global, and regional problems, all of which are based on adjoint importance functions.

II.B. Source-Detector Problems: CADIS Method

Although it is certainly not the only deterministic adjoint-based methodology for source-detector–type problems, the CADIS methodology has proven to be very effective for automated optimization of localized quantities in source-detector–type problems and is routinely used at ORNL and elsewhere by SCALE 6 users for 3-D Monte Carlo simulations of real, complex radiation transport applications. The CADIS methodology is briefly reviewed in this section to provide background for the description of the FW-CADIS method for global and regional problems in subsequent sections.

In the CADIS methodology, which evolves from Eq. (9b) and the concept of importance sampling,$^3$ the biased source distribution is given by

$$\hat{q}(\vec{r}, E, \Omega) = \frac{\psi^+(\vec{r}, E, \Omega) q(\vec{r}, E, \Omega) d\vec{r}dEd\Omega}{R} = \frac{\psi^+(\vec{r}, E, \Omega) q(\vec{r}, E, \Omega)}{R},$$  \hspace{1cm} (10)

where the numerator is the detector response from a particle in $(\vec{r}, E, \Omega)$ and the denominator is the total detector response $R$. Therefore, the ratio is a measure of the contribution from $(\vec{r}, E, \Omega)$ 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, and therefore, this expression could also be derived from physical arguments.

Since the source variables are sampled from a biased pdf, $q(\vec{r}, E, \Omega)$, the statistical weight of the source particles must be corrected according to the following equality:

$$w(\vec{r}, E, \Omega) \hat{q}(\vec{r}, E, \Omega) = w_0 q(\vec{r}, E, \Omega),$$  \hspace{1cm} (11)

where $w_0$ is the unbiased particle starting weight, which is set equal to 1. Substituting Eq. (10) into Eq. (11) and rearranging, we obtain the following expression for the statistical weight of the particles:

$$w(\vec{r}, E, \Omega) = \frac{R}{\psi^+(\vec{r}, E, \Omega)}.$$  \hspace{1cm} (12)

Equation (12) 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 window. 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 due to poor computational efficiency and/or false convergence.\textsuperscript{32} For example, if the statistical weights of the source particles are not within the weight windows, the particles are immediately split or roulett in an effort to bring their weights into the weight window. This results in unnecessary splitting/roulettiong and a corresponding degradation in computational efficiency. For problems in which the adjoint function varies significantly (in space and/or energy) within the source region, the source biasing is very effective for improving computational efficiency.


For global variance reduction, one’s interest is not confined to a localized region but rather to determining a quantity (e.g., flux) with uniformly low statistical uncertainty throughout the entire problem space. To achieve this objective in a Monte Carlo simulation, Cooper and Larsen\textsuperscript{26} have suggested 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 particle density. To do so, we cast the problem of calculating Monte Carlo particle density into the response formulation [Eq. (4)]:

\begin{equation}
R' \propto \int_{4\pi \times E \times V} \int \psi (\vec{r}, E, \vec{\Omega}) \sigma_d (\vec{r}, E, \vec{\Omega}) d\vec{r} d\vec{\Omega} ,
\end{equation}

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

\begin{equation}
n (\vec{r}, E, \vec{\Omega}) \propto w (\vec{r}, E, \vec{\Omega}) m (\vec{r}, E, \vec{\Omega}) \quad (14)
\end{equation}

and

\begin{equation}
\psi (\vec{r}, E, \vec{\Omega}) = n (\vec{r}, E, \vec{\Omega}) v (\vec{r}, E, \vec{\Omega}) ,
\end{equation}

where \( v (\vec{r}, E, \vec{\Omega}) \) is the particle velocity. Substituting \( n(\vec{r}, E, \vec{\Omega}) \) from Eq. (15) into Eq. (14) and rearranging, the Monte Carlo particle density can be estimated by

\begin{equation}
m(\vec{r}, E, \vec{\Omega}) = \frac{n (\vec{r}, E, \vec{\Omega})}{w (\vec{r}, E, \vec{\Omega})} \left[ \frac{\psi (\vec{r}, E, \vec{\Omega})}{n (\vec{r}, E, \vec{\Omega}) v (\vec{r}, E, \vec{\Omega})} \right] .
\end{equation}

Integrating over the independent variables, the total Monte Carlo particle density can be estimated by

\begin{equation}
R' = \int_{4\pi \times E \times V} \int \psi (\vec{r}, E, \vec{\Omega}) \left[ \frac{1}{w (\vec{r}, E, \vec{\Omega}) v (\vec{r}, E, \vec{\Omega})} \right] d\vec{r} d\vec{\Omega} .
\end{equation}

Recalling from Cooper and Larsen that if the average particle weight is set proportional to the physical particle density, the Monte Carlo particle density is approximately constant, as desired; i.e.,

\begin{equation}
\text{for } m \approx \text{constant}, \quad \tilde{w} \propto n, \quad \text{and} \quad \tilde{w} v \propto \psi .
\end{equation}

Therefore, by substituting the forward flux \( \psi (\vec{r}, E, \vec{\Omega}) \) for \( w (\vec{r}, E, \vec{\Omega}) v (\vec{r}, E, \vec{\Omega}) \), Eq. (17) becomes

\begin{equation}
R' \propto \int_{4\pi \times E \times V} \int \psi (\vec{r}, E, \vec{\Omega}) \left[ \frac{1}{\psi (\vec{r}, E, \vec{\Omega})} \right] d\vec{r} d\vec{\Omega} .
\end{equation}

Recognizing the similarities between Eqs. (19) and (9a), we see that by defining the bracketed term in Eq. (19) as

\begin{equation}
q^+ (\vec{r}, E, \vec{\Omega}) = \frac{1}{\psi (\vec{r}, E, \vec{\Omega})} ,
\end{equation}

we can calculate an adjoint importance function that represents the importance of particles to achieving the desired objective, i.e., uniform Monte Carlo particle density, 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 importance will be high, and vice versa. Once the adjoint importance function is determined, the standard CADIS methodology is used to calculate consistent source biasing parameters and weight windows.
[see Eqs. (10) and (12)]. Therefore, we refer to this method as the FW-CADIS method.

In some applications the goal is to determine the total (i.e., energy-integrated) flux or flux-based response over the entire problem space with low statistical uncertainty. In such cases, we want to achieve uniform Monte Carlo particle density spatially with respect to the response of interest. For example, if our goal is spatially dependent total flux,

$$ \varphi(\vec{r}) = \int_{4\pi E} \psi(\vec{r}, E, \hat{\Omega}) dE d\hat{\Omega}, $$

then we are interested in making the spatially distributed Monte Carlo particle density, i.e.,

$$ m(\vec{r}) = \int_{4\pi E} m(\vec{r}, E, \hat{\Omega}) dE d\hat{\Omega}, $$

constant. Following the same logic described above, we can develop an adjoint importance function to achieve this objective by defining our adjoint source as

$$ q^+(\vec{r}) = \frac{1}{\int_{4\pi E} \psi(\vec{r}, E, \hat{\Omega}) dE d\hat{\Omega}}. $$

Similarly, if the objective of a calculation is spatially dependent total dose rate,

$$ D(\vec{r}) = \int_{4\pi E} \psi(\vec{r}, E, \hat{\Omega}) \sigma_d(\vec{r}, E) dE d\hat{\Omega}, $$

where $\sigma_d(\vec{r}, E)$ is the dose rate response function, then we can develop an adjoint importance function to achieve this objective by defining our adjoint source as

$$ q^+(\vec{r}, E) = \frac{1}{\int_{4\pi E} \psi(\vec{r}, E, \hat{\Omega}) \sigma_d(\vec{r}, E) dE d\hat{\Omega}}. $$


II.B.2. Regional Problems: FW-CADIS Method

For regional problems the goal is to determine the flux or response over a portion or portions of the problem space with uniform (low) statistical uncertainty. Hence, in such cases, we want to achieve uniform Monte Carlo particle density over one or more spatial regions. For example, if the goal is to calculate dose rate throughout a portion of the problem volume $V$, then the adjoint source can be defined as

$$ q^+(\vec{r}, E) = \begin{cases} \frac{\sigma_d(\vec{r}, E)}{\int_{4\pi E} \sigma_d(\vec{r}, E) \psi(\vec{r}, E, \hat{\Omega}) dE d\hat{\Omega}} & \text{for } \vec{r} \in V \\ 0 & \text{for } \vec{r} \notin V \end{cases}. $$

The adjoint source can be defined for whatever objective is desired. This is a very useful aspect of the method because for many applications results are not needed throughout the entire problem space.

III. IMPLEMENTATION

In the FW-CADIS method, forward information (e.g., flux, dose rate, etc.) is used to define an appropriate response (adjoint source) to generate the adjoint importance function for achieving uniform particle density (or response) throughout the system. It is possible to optimize for global quantities, such as flux or dose rate distributions throughout a problem; regional responses, such as flux or dose rate throughout one or more regions of a problem; and multiple detector responses, such as response or spectra at multiple localized detectors, simply depending on how the adjoint source is defined. A summary of typical cases is provided in Table II.


The first step is generating an estimate of the forward scalar flux $\phi(\vec{r}, E)$, which can be obtained from a discrete ordinates calculation. The adjoint source $q^+(\vec{r}, E)$ is then constructed using one of the forms from Table II. The remainder of the algorithm is the same as that of the standard CADIS method: The adjoint scalar flux $\phi^+(\vec{r}, E)$ is determined, and the biased source distribution is calculated using

$$ q(\vec{r}, E) = \frac{1}{R} q(\vec{r}, E) \phi^+(\vec{r}, E), $$

where $R = \int_{V_s} \int_E q(\vec{r}, E) \phi^+(\vec{r}, E) dE dV$ and where $V_s$ is the volume of the physical source.

Next, the weight window target values are calculated as

$$ w(\vec{r}, E) = \frac{R}{\phi^+(\vec{r}, E)}. $$

Whereas the weight window implementation in MAVRIC uses weight window target values per Eq. (28), the weight window technique implementation in MCNP requires weight window lower bounds $w_L$. The width of the window is controlled by the input parameter $c$, which is the ratio of upper and lower weight window bounds ($c = w_u / w_L$). The space- and energy-dependent weight window lower bounds for use in MCNP are given by
TABLE II
FW-CADIS Options Available in the MAVRIC Sequence*

<table>
<thead>
<tr>
<th>To Optimize</th>
<th>Use an Adjoint Source of</th>
<th>MAVRIC Input</th>
</tr>
</thead>
</table>
| Total dose rate $\int \sigma_d(E)\phi(\vec{r},E)\,dE$ | $q^+(\vec{r},E) = \frac{\sigma_d(E)g(\vec{r})}{\int \sigma_d(E)\phi(\vec{r},E)\,dE}$ | adjointSource 1  
  boundingBox $x_1\,x_2\,y_1\,y_2\,z_1\,z_2$  
  responseID=5  
  end adjointSource  
  respWeighting |
| Groupwise dose rate $\sigma_d(E)\phi(\vec{r},E)$ | $q^+(\vec{r},E) = \frac{\sigma_d(E)g(\vec{r})}{\sigma_d(E)\phi(\vec{r},E)} = \frac{g(\vec{r})}{\phi(\vec{r},E)}$ | adjointSource 1  
  boundingBox $x_1\,x_2\,y_1\,y_2\,z_1\,z_2$  
  responseID=5  
  end adjointSource  
  fluxWeighting |
| Groupwise flux $\phi(\vec{r},E)$ | $q^+(\vec{r},E) = \frac{g(\vec{r})}{\phi(\vec{r},E)}$ | adjointSource 1  
  boundingBox $x_1\,x_2\,y_1\,y_2\,z_1\,z_2$  
  responseID=1  
  end adjointSource  
  fluxWeighting |
| Total flux $\int \phi(\vec{r},E)\,dE$ | $q^+(\vec{r}) = \frac{g(\vec{r})}{\int \phi(\vec{r},E)\,dE}$ | adjointSource 1  
  boundingBox $x_1\,x_2\,y_1\,y_2\,z_1\,z_2$  
  responseID=1  
  end adjointSource  
  respWeighting |

*The function $g(\vec{r})$ has the value 1 where the adjoint source is defined (in the cuboid defined with $x_1\,x_2\,y_1\,y_2\,z_1\,z_2$) and 0 elsewhere; response ID=1 is used to specify the unity function (to compute total flux from the groupwise fluxes); and response ID=5 is used to specify the set of flux–to–dose rate conversion factors $\sigma_d(E)$.

$$w_l(\vec{r},E) = \frac{R}{\phi^+(\vec{r},E)\left(\frac{c+1}{2}\right)}.$$  \hspace{0.5cm} (29)

Both the biased source(s) and the weight window values are used by the Monte Carlo calculation.

The CADIS and FW-CADIS methods have been implemented and automated in the MAVRIC sequence of SCALE 6 and the ADVANTG code (based on MCNP). A discussion of the implementation of the methods in each of these codes is briefly reviewed in Secs. III.A and III.B, followed by a discussion of their usage in Sec. III.C.

### III.A. Implementation in MAVRIC

Since January 2009, SCALE (Ref. 18) has included tools designed for 3-D shielding analysis. These include the Monaco fixed-source multigroup Monte Carlo code, the Denovo Cartesian mesh discrete ordinates code, and the MAVRIC sequence17 for using the CADIS and the FW-CADIS methods.

Monaco uses the same combinatorial solid-body geometry description and multigroup cross-section processing as the KENO-VI/CSAS6 criticality sequence in SCALE. Monaco has an easy-to-use and flexible block and keyword style input, which allows users to define distributions, response functions, and spatial meshes for specifying multiple sources and tallies. Mesh-based weight windows and mesh-based source biasing parameters can also be used by Monaco.

The MAVRIC sequence reads an input very similar to that of Monaco, with one additional block specifying information needed for the automated variance-reduction methods. This additional information consists of one or more adjoint sources (corresponding to the tallies that the user wishes to optimize) and a spatial mesh. MAVRIC constructs a mesh-based version of the geometry and then uses Denovo to calculate forward and/or adjoint fluxes. The mesh-based flux estimates calculated by Denovo are used with either the CADIS or the FW-CADIS methods to construct space- and energy-dependent weight windows and consistent, mesh-based source biasing parameters. These biasing parameters are then passed to Monaco for the Monte Carlo calculation. Note that the tracking and tallies in the Monaco calculation use the combinatorial solid-body geometry, not the mesh-based geometry used in the Denovo calculations. The user’s original source
specifications are replaced by the biased mesh-based source specifications, so care must be taken that the spatial meshing is fine enough in the source regions such that the mesh-based versions of the sources adequately represent the true sources (see Ref. 18 for further details).

MAVRIC can also be executed in parts, so that the results of intermediate steps can be checked before proceeding to the next step. A Java viewer is available to view any of the mesh-based files: the forward and adjoint flux files from Denovo, the space- and energy-dependent weight window values, the final biased mesh sources, and any mesh tallies produced by Monaco. The Denovo flux files, the weight window file, and mesh source files can be used as the starting points in subsequent MAVRIC calculations, eliminating the need to regenerate these files.

With the computational infrastructure in MAVRIC to generate input for, execute, and use results from forward and adjoint deterministic calculations, alternative deterministic importance function–based methods can be implemented and tested with relative ease. The GFWW and GRWW methods, as well as Becker’s methods \(^{30}\) for developing weight windows (for source/detector, source/region and global problems; optimizing either the flux or a response) have been implemented as options in the development version of MAVRIC to support testing and performance comparisons. For the GFWW and GRWW methods, no adjoint sources are required since only forward estimates of the flux over the entire geometry are required. Calculations based on Becker’s methods, using both forward and adjoint flux estimates, are specified in a manner very similar to FW-CADIS calculations with one extra keyword specifying the method to use (source/detector, source/region, or source/global). The current implementation in MAVRIC expands upon the original methods in that biased sources are constructed along with the weight windows for the Monte Carlo calculation.

The metric typically used to evaluate the performance of a variance-reduction method for improving the efficiency of a Monte Carlo simulation is the figure of merit \(^7\) (FOM), which is defined as

$$\text{FOM} = \frac{1}{R^2 T},$$

where \(R\) is the relative uncertainty for a single tally and \(T\) is the total computer time for the Monte Carlo simulation. Although this metric is very useful for evaluating the efficiency of individual tallies, it is not directly useful for comparing the efficiency of calculations of distributions, such as mesh tallies. For the latter purpose, alternative forms of the FOM have been proposed.\(^{34,37}\) In the current development version of Monaco (for SCALE 6.2), the mesh tally FOM is calculated from the mean relative uncertainty of the mesh tally cells with score

$$\text{FOM} = \frac{1}{\bar{r}^2 T},$$

and

$$\bar{r} = \frac{1}{N_i} \sum R_i,$$  \hspace{1cm} (31)

where \(R_i\) is the relative uncertainty of the flux or dose rate in mesh tally cell \(i\) and \(N_i\) is the total number of mesh tally cells. Four statistical tests\(^{34,35}\) have also been added to the development version of Monaco. These tests measure over the simulation: (a) if \(\zeta\), the fraction of voxels that have received a score, is constant (linear slope is \(0 \pm 0.10\)); (b) if the mean relative variance is decreasing as \(1/\sqrt{N}\) (coefficient of determination of a power law fit \(>0.99\)); (c) if the variance of the relative variance is decreasing with \(1/N\) (coefficient of determination of a power law fit \(>0.95\)); and (d) if the FOM is constant (linear slope is \(0 \pm 0.10\)).

### III. B. Implementation in ADVANTG

The ADVANTG code\(^{14}\) was originally developed to implement the CADIS methodology through use of the TORT 3-D discrete ordinates code\(^{36,37}\) for the deterministic adjoint calculation and the MCNP 4C code\(^{38}\) for the Monte Carlo calculation. During the past few years, ADVANTG has been extended to MCNP5 (Ref. 7), the FW-CADIS method has been implemented, and the use of TORT has been discontinued and replaced by Denovo. Denovo implements modern iterative solvers and transport discretization schemes, provides a number of quadrature sets, and includes an embedded first-collision source treatment. ADVANTG has the capability to seamlessly utilize most of the features provided by Denovo, including the execution of parallel calculations, from within its automated sequences.

Input to ADVANTG includes a standard MCNP input file, from which ADVANTG extracts the geometry of the material bodies, material compositions, fixed-source distributions, tally regions, and response spectra. ADVANTG also reads an additional input file that contains a Cartesian structured grid, parameters for the Denovo discrete ordinates calculation(s), and options for the CADIS and FW-CADIS calculations. The spatial mesh grid is used for the deterministic calculations and for the space- and energy-dependent weight windows that are generated by the CADIS or FW-CADIS calculation.

Similar to MAVRIC, when executing an FW-CADIS calculation, ADVANTG performs a sequence of several steps. First, a discretized version of the Monte Carlo problem is constructed for the discrete ordinates calculation. A forward-mode Denovo calculation is then executed, and the scalar flux output is used to construct an adjoint source according to Eqs. (20), (23), or (25), depending on the nature of the response of interest. An adjoint-mode Denovo calculation is then executed, and
the resulting flux distribution (importance function) is used to compute weight window lower bounds according to Eq. (29) and a consistent, biased source distribution according to Eq. (27). The biased source distribution is generated directly on the space and energy bins that were used to describe the source in the MCNP input file.\(^{39}\)

One of the primary tasks required to automate the CADIS and FW-CADIS methods is the construction of a discretized version of the Monte Carlo problem for the discrete ordinates calculation. Since the steps required to accomplish this task are not typically part of conventional transport algorithms, some additional details are provided here. First, the geometry of the MCNP material bodies (cells) and the given source distribution are mapped onto the user-defined grid. The original version of ADVANTG accomplished this in a straightforward way by querying the material defined at the centroid of each mesh cell and assigning that material to the entire cell. A more sophisticated approach is to sample multiple points within each cell and generate a mixed material description.\(^{40}\) The current version of ADVANTG uses ray tracing to estimate the material fractions in each cell. The next step is to translate the MCNP material compositions (nuclide identifiers and number densities) into a form suitable for use with the multigroup cross-section library selected by the user. This library also determines the energy group structure onto which the energy spectra of the sources and responses are mapped. To mitigate the impact of ray effects, Denovo’s embedded first-collision treatment is used for point sources (in forward calculations) and point detectors (in adjoint calculations).

The variance-reduction parameter output by ADVANTG is written in a form that is directly usable by unmodified versions of MCNP. The space- and energy-dependent weight window lower bounds are written as a WWINP file,\(^{b}\) and the biased source distribution is written as SDEF cards that are incorporated into the user’s MCNP input file.

The application of ADVANTG to calculating energy-dependent pulse-height tallies in a simplified radiation portal monitoring scenario is discussed in Sec. IV.B.

III.C. Comments on Usage

Previous studies (Refs. 1, 3, 13, and 14) have demonstrated that the calculational efficiency achievable with the hybrid methods is not overly sensitive to the accuracy of the adjoint function and, therefore, that approximate, fast-running deterministic calculations (e.g., coarse spatial mesh, sparse energy groups, and low quadrature order) are typically sufficient for the purpose of generating effective variance-reduction parameters. This behavior is considered to be desirable, as different users will inevitably take different approaches toward defining mesh resolution for the deterministic calculations and it is desirable to not spend a large fraction of the total computation time on the deterministic calculations. Regarding the mesh distribution, it has been shown that it is important to capture the bulk characteristics of the problem geometry (e.g., material locations and thicknesses) in order to capture the physics characteristics of the problem. Failure to do so can manifest itself in poor computational efficiency and/or convergence behavior. However, because the process is automated, creating and utilizing different mesh distributions is a simple matter.

Both MAVRIC and ADVANTG provide the capability to output 3-D visualization files with the deterministic fluxes and weight window values. Inspecting the quality of the deterministic results (e.g., for expected physical behavior) is an important step to take before proceeding to the Monte Carlo simulation that uses the variance-reduction parameters.

Subsequent to using the results of the Monte Carlo simulation, it is important to carefully study the results of the statistical tests of tally convergence. The trend and magnitude of the variance of variance and the magnitude of the Pareto slope are, in our experience, the primary indicators of statistical convergence issues, which may be the result of an inadequate deterministic solution caused by inadequate spatial mesh or the selection of a cross-section library not applicable to the problem. In challenging simulations the statistical checks may not indicate any issues until several million particle histories have been simulated. For this reason, we advise against relying on very short Monte Carlo runs, even if the initial results appear well converged. Note, this guidance is also applicable to other codes when using variance-reduction parameters.

IV. APPLICATION AND ANALYSES

In this section the hybrid methods discussed in Sec. II are applied to two problems of interest to the nuclear industry. More details on these problems, as well as the application of the FW-CADIS method to other relevant problems, are available in Refs. 5, 9, 17, 24, 25, and 41 through 44.

IV.A. Example Problem 1: Optimizing Mesh Tallies in a Small Building

To evaluate and demonstrate the effectiveness of the FW-CADIS method, we consider in this section a simplified, yet representative, problem involving the calculation of total neutron dose rate throughout a 860-\(\times\)460-\(\times\)460-cm\(^3\) concrete structure holding nuclear fuel, as shown in Fig. 1. The fuel is represented as an 80-\(\times\)80-\(\times\)80 cm\(^3\) of homogenized uranium dioxide and water, surrounded by a 10-cm layer of steel. The concrete...
walls are 30 cm thick, spaced every 1 m in the x direction, leaving air regions that are 70 cm thick. The source is modeled uniformly over the central cube, emitting neutrons from a Watt fission spectrum, with a total strength of 1 Ci. Three cases for optimizing the mesh tally (uniform 10-cm voxel, 86 x 46 x 46) over the building are considered: (a) calculation of the total dose rate $D(r)$, (b) calculation of the flux $\phi(r, E)$, and (c) calculation of the total flux $\Phi(r)$. Five methods of calculation are compared for each case: analog method (with implicit capture on; weight cutoff of $10^{-16}$), Cooper and Larsen’s method, GFWW/GRWW methods, Becker’s method for global optimization (Becker’s Global), and FW-CADIS method. Calculations were all performed with the MAVRIC sequence of SCALE, using the 27-group neutron shielding cross-section library. Denovo calculations used a nonuniform mesh of $106 \times 58 \times 50$, an $S_8$ level-symmetric quadrature, and a Legendre expansion order of 3. Cooper and Larsen’s method calculations used only space-dependent weight windows and an unbiased source (consistent with its original description). The GFWW/GRWW calculations and Becker’s Global were extended beyond their original descriptions to use consistent source biasing parameters.

IV.A.1. Optimizing for Total Dose Rate

For a fair comparison, each method was allowed a total of 120 min on a single processor. For the five methods, detailed timing information (deterministic and Monte Carlo) is shown in Table III, which also shows for each method the statistical quantities relating to the relative uncertainty distribution of the final mesh tally of dose rate (rem/h Ci$^{-1}$) as well as indicates the statistical tests described in Sec. III.A that each method passed. Figure 2 shows a dose rate plot at the midplane ($z=0$) of

Fig. 1. Geometry of the test problem. An 80- x 80- x 80-cm cube of homogenized uranium dioxide and water for the source, surrounded by a 10-cm layer of steel in a system of 30-cm-thick concrete walls and air regions.

<table>
<thead>
<tr>
<th>Method</th>
<th>Time (min)</th>
<th>Relative Uncertainty Mean</th>
<th>Relative Uncertainty Variation</th>
<th>Monte Carlo FOM</th>
<th>Tests</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analog</td>
<td>123</td>
<td>0.8979</td>
<td>5.05 x 10^{-1}</td>
<td>3.18 x 10^{-2}</td>
<td>X</td>
</tr>
<tr>
<td>Cooper and Larsen</td>
<td>94</td>
<td>1.0000</td>
<td>2.96 x 10^{-1}</td>
<td>1.21 x 10^{-1}</td>
<td>X</td>
</tr>
<tr>
<td>GFWW/GRWW</td>
<td>89</td>
<td>1.0000</td>
<td>1.25 x 10^{-1}</td>
<td>7.24 x 10^{-1}</td>
<td>X</td>
</tr>
<tr>
<td>Becker’s Global</td>
<td>64</td>
<td>1.0000</td>
<td>1.16 x 10^{-1}</td>
<td>1.79 x 10^{-1}</td>
<td>X</td>
</tr>
<tr>
<td>FW-CADIS</td>
<td>63</td>
<td>1.0000</td>
<td>8.07 x 10^{-2}</td>
<td>2.87 x 10^{-2}</td>
<td>X</td>
</tr>
</tbody>
</table>

The fraction of voxels with a nonzero score. "X" indicates the test measure was satisfied.
Fig. 2. Dose rates (rem/h Ci⁻¹) and associated relative uncertainties from the analog method, Cooper and Larson’s method, the GRWW method, Becker’s Global, and the FW-CADIS method for the midplane (z = 0) of the small building example.
the building for each method, along with the relative uncertainties associated with the dose rate values. Dose rates and relative uncertainties along a line $(y = z = 0)$ are shown in Figs. 3 and 4. The center of the source in the 3-D geometry representation corresponds to $x = y = z = 0$. The dose rates for all five methods were compared to a very long analog calculation (160 h) to ensure that use of the hybrid variance reduction did not bias the results. Total dose rates from the five methods compared well to the long analog calculation within the first two walls. Beyond the first two walls, the uncertainties of the long analog total dose rates were too large for comparison.

As expected, the dose rates computed in the 120-min analog calculation have low relative uncertainties only where the fluxes are high—near the source region. As the dose rate drops farther from the source region, the relative uncertainties increase significantly. Few particles survive to reach the room farthest from the source.

Since Cooper and Larsen’s method is designed to calculate fluxes for every mesh cell, it is not expected to perform well at calculating the total dose rate, which is more sensitive to the fluxes in the higher-energy groups. Cooper and Larsen’s method does perform better than the analog method, but it should be noted that each history in this method required much more time, by a factor of $>40$, compared to the analog method. With weight windows proportional to the forward flux, particles are repeatedly split as they move outward. While the dose rate results for this problem seem reasonable, the long time per history is a concern because the source is not sampled very often. For a source with a large volume and a distribution over a large range of energies, Cooper and Larsen’s method may not be able to sample the source adequately in reasonable run times, which could result in a significant bias in the calculated results.

As shown in Table III, the GRWW method with a consistent biased source performed well, Becker’s Global performed better, and the FW-CADIS method performed the best for the different mesh tally statistical measurements (lowest mean relative uncertainty, highest mesh tally FOM, etc.). Results for the four mesh tally tests, based on the change of the distribution of relative uncertainties over the last half of the simulation, are shown in Table III for each method. Figures 5 and 6 show the details of the distribution of relative uncertainties of the 181,976 voxels as pdf’s, showing the fraction of mesh cells that has certain values of relative uncertainty, and as
cumulative distribution functions (cdf’s), showing the fraction of mesh cells that has relative uncertainties below certain values. Figures 5 and 6 show that the FW-CADIS method produces a total dose rate mesh tally with more uniform and lower relative uncertainty values than the other methods. The cdf graph is particularly useful in comparing the fraction of voxels below a certain relative uncertainty. For our five methods, the fractions of mesh tally voxels that have $< 10\%$ uncertainty are as follows: analog, 0.1; Cooper and Larsen, 0.006; GRWW, 0.28; Becker’s Global, 0.48; and FW-CADIS, 0.77.

IV.A.2. Optimizing for Space/Energy Flux

Since the goal of this case is to attain low (and uniform) relative uncertainties in every energy group of every voxel, more total run time (24 h) was allowed for each of the five methods. The timing, mesh tally statistical quantities, and results of mesh tally statistical tests described in Sec. III.A are all shown in Table IV. The flux results for the five different methods were similar (where there were reasonable statistics). A comparison of the group 5 (0.9 to 1.4 MeV) fluxes for the line $y = z = 0$ from the five methods is shown in Fig. 7. The corresponding relative uncertainties are shown in Fig. 8. The center of the source in the 3-D geometry representation corresponds to $x = y = z = 0$. As in the previous case, the order of increasing performance was Cooper and Larsen’s method, the GFWW method, Becker’s Global, and the FW-CADIS method. Figures 9 and 10 show the pdf and the cdf of the relative uncertainties of the 4 913 352 space/energy flux values (181 976 voxels, 27 energy groups). Figures 9 and 10 clearly show that the FW-CADIS method provides lower and more uniform relative uncertainties across space and energy than the

<table>
<thead>
<tr>
<th>Method</th>
<th>Discrete Ordinates</th>
<th>Forward (min)</th>
<th>Adjoint (min)</th>
<th>Monte Carlo</th>
<th>Time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analog</td>
<td>16 986 000</td>
<td>31</td>
<td>31</td>
<td>1444</td>
<td></td>
</tr>
<tr>
<td>Cooper and Larsen</td>
<td>375 000</td>
<td>31</td>
<td>31</td>
<td>1415</td>
<td></td>
</tr>
<tr>
<td>GFWW</td>
<td>375 000</td>
<td>131</td>
<td>131</td>
<td>1419</td>
<td></td>
</tr>
<tr>
<td>Becker’s Global</td>
<td>1383</td>
<td>30</td>
<td>30</td>
<td>1417 800</td>
<td></td>
</tr>
<tr>
<td>FW-CADIS</td>
<td>31</td>
<td>26</td>
<td>26</td>
<td>1391</td>
<td></td>
</tr>
</tbody>
</table>

TABLE IV

Details for the Five Methods Used to Optimize the Calculation of Space/Energy Flux for the Small Building Example Problem

- $\text{pdf}$: probability density function
- $\text{cdf}$: cumulative distribution function
- $\text{rms}$: root mean square
- $\text{FOM}$: figure of merit
- $\text{Test}^{b,c}$: statistical tests
- $\text{Monte Carlo}$: Monte Carlo calculations
- $\text{Time (min)}$: total run time
- $\text{Mean of Relative Uncertainty}$
- $\text{Variation of Relative Uncertainty}$

<table>
<thead>
<tr>
<th>Method</th>
<th>Discrete Ordinates</th>
<th>Forward (min)</th>
<th>Adjoint (min)</th>
<th>Monte Carlo</th>
<th>Time (min)</th>
</tr>
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<tbody>
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<tr>
<td>Becker’s Global</td>
<td>1383</td>
<td>30</td>
<td>30</td>
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<td></td>
</tr>
<tr>
<td>FW-CADIS</td>
<td>31</td>
<td>26</td>
<td>26</td>
<td>1391</td>
<td></td>
</tr>
</tbody>
</table>

- $\text{Test}^{b,c}$: statistical tests
- $\text{FOM}$: figure of merit
- $\text{Monte Carlo}$: Monte Carlo calculations
- $\text{Time (min)}$: total run time
- $\text{Mean of Relative Uncertainty}$
- $\text{Variation of Relative Uncertainty}$

Fig. 6. The cdf of relative uncertainties of the dose rates from the analog method, Cooper and Larson’s method, the GRWW method, Becker’s Global, and the FW-CADIS method.

Fig. 7. The cdf of relative uncertainties of the dose rates from the analog method, Cooper and Larson’s method, the GRWW method, Becker’s Global, and the FW-CADIS method.

Fig. 8. The cdf of relative uncertainties of the dose rates from the analog method, Cooper and Larson’s method, the GRWW method, Becker’s Global, and the FW-CADIS method.
other methods for this problem. The fractions of mesh tally voxels with <10% uncertainty are as follows: the analog method, 0.10; Cooper and Larsen’s method, 0.23; the GFWW method, 0.40; Becker’s Global, 0.51; and the FW-CADIS method, 0.67.

As an example of obtaining more uniform relative uncertainties among energy groups, consider just one voxel in the center of the rightmost room of the building. Figure 11 shows the energy-dependent flux computed with different variance-reduction approaches. The analog calculation recorded scores in only the five lowest of the 27 energy groups and is not shown in Fig. 11. The fluxes are very similar among the methods. The relative uncertainties are shown in Fig. 12, with the FW-CADIS calculation achieving the lowest overall uncertainties. These uncertainties are more uniform over the range of energies with slightly higher uncertainties near 1 eV and in the lowest energy group.

IV.A.3. Optimizing for Total Flux

Optimizing for the calculation of the total flux is similar to optimizing a response; in this case the response...
function as a function of energy is simply 1. Results for the five methods are shown in Table V. Optimizing total flux over space was the original intent of Cooper and Larsen’s method, and it does well in this test, performing very similarly to the GRWW method. In fact, since the response being optimized is total flux, Cooper and Larsen’s method should be equivalent to the GRWW method except for the use of the biased source in the GRWW implementation in MAVRIC. The use of the biased source caused the number of source particles sampled by the GRWW method to be larger than with Cooper and Larsen’s method. Becker’s Global and the FW-CADIS method outperform the forward-flux–based methods because the adjoint information is included; the variance-reduction parameters from these methods balance the simulation based on the importance of a particle contributing to the total flux. The pdf and cdf plots of the

![Fig. 11. Neutron flux per unit lethargy for one voxel in the rightmost air region.](image)

![Fig. 12. Relative uncertainties in the neutron flux for one voxel in the rightmost air region.](image)

**TABLE V**

<table>
<thead>
<tr>
<th>Details for the Five Methods Used to Optimize the Calculation of Total Flux for the Small Building Example Problem</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Method</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>GFOM</strong></td>
</tr>
<tr>
<td>Analog</td>
</tr>
<tr>
<td>Cooper and Larsen</td>
</tr>
<tr>
<td>GRWW</td>
</tr>
<tr>
<td>Becker’s Global</td>
</tr>
<tr>
<td>FW-CADIS</td>
</tr>
</tbody>
</table>

 注：

- **a** 表示分数的非零权重。
- **b** 见第 III.A 节的描述这四种测试。
- **c** ‘X’ 表示测试措施被满足。

The fraction of voxels with a nonzero score.

See Sec. III.A for a description of the four tests.

X indicates the test measure was satisfied.
distribution of relative uncertainties over the 181,976 voxels were similar to the corresponding distributions for the dose rate response, with the fractions of mesh tally voxels with <10% uncertainty being as follows: the analog method, 0.16; Cooper and Larsen’s method, 0.25; the GRWW method, 0.32; Becker’s Global, 0.40; and the FW-CADIS method, 0.68.

IV.A.4. Other Types of Optimization with the FW-CADIS Method (Regional Problems)

The FW-CADIS method is quite flexible. The regions that will be optimized in the Monte Carlo calculation are defined by the user’s specification of the adjoint source. Unlike the GFWW/GRWW methods that are global in nature, the FW-CADIS method can be focused on only those regions for which reliable results are needed. In other words, computational time is not wasted on achieving uniform, low statistical uncertainties in regions of the problem where they are not needed. For example, Fig. 13 shows total dose rates and uncertainties from a calculation where the adjoint source definition was restricted to the voxels in the air. Note that the uncertainties in the exterior walls and in the source region are higher than in the air regions. Figure 14 shows the dose rates and uncertainties from a similar calculation where the adjoint source definition was restricted to just the third and fourth large air regions. Notice that those air regions have lower relative uncertainties than the air regions near the source. In MAVRIC (and ADVANTG), the area of optimization can also be set to include areas within a certain range of response (estimated using the Denovo forward-flux estimate). Figure 15 shows an example where the calculation was optimized to the areas for which the estimated dose rates were \(10^{-4}\) to \(10^{-2}\) rem/h Ci\(^{-1}\). Dose rates below \(10^{-4}\) rem/h Ci\(^{-1}\) are not calculated well at all, since particles in those areas have very little chance to contribute to the areas that have a dose rate between \(10^{-4}\) and \(10^{-2}\) rem/h Ci\(^{-1}\).

IV.B. Example Problem 2: Optimizing an Energy-Dependent Pulse-Height Tally in a Radiation Portal Monitor

To evaluate the effectiveness of the FW-CADIS method for obtaining relatively uniform statistical uncertainties in an energy-dependent tally, we consider the radiation detection scenario shown in Fig. 16. This problem is a simplified representation of the use of a radiation portal monitor\(^4\) for screening truck cargos for illicit radioactive materials. Here, the panel detector array is simply represented by four 10.16-\(\times\)10.16- \(\times\)40.64-cm NaI crystals in a staggered arrangement. The 2.44-

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Fig. 13. Dose rates (rem/h Ci\(^{-1}\)) and associated relative uncertainties for the small building example optimized for calculating the dose rates in the air regions.

Fig. 14. Dose rates (rem/h Ci\(^{-1}\)) and associated relative uncertainties for the small building example optimized for calculating the dose rates in the third and fourth large air regions.
2.44-×6.10-m subject cargo container holds an array of 1-×1-×2-m³ blocks of polyethylene (lighter color) and low-density iron (darker color). A point photon source with the emission spectrum of \(^{133}\)Ba (modeled as 13 discrete lines from 4.6 to 383.8 keV) is located at the center of the container, which happens to lie in an air gap between the blocks. The wall of the container is 0.3-cm-thick carbon steel at full density. The detectors and container are placed above a 30.48-cm-thick concrete pad. The objective of the simulation is to estimate the integrated pulse-height spectrum in the four detectors for energies up to 384 keV within 1-keV-width energy bins. The ability to apply variance-reduction techniques, such as weight windows and source biasing, to simulations with pulse-height tallies is a relatively new feature in the MCNP code (released in version 1.50). The implementation of pulse-height-tally variance reduction requires additional bookkeeping and computations that may significantly contribute to run time, especially in simulations where the importance varies over many orders of magnitude.

ADVANTG was used to generate weight windows and a biased source distribution using the FW-CADIS method. Since the objective is to estimate an energy-dependent pulse-height spectrum with relatively uniform uncertainties across the 384 energy bins, the adjoint source was constructed according to Eq. (20), though scalar adjoint fluxes were used. The Denovo run time for completing both calculations was 60 CPU minutes. MCNP5 simulations were performed with and without the ADVANTG-generated weight windows and biased source distribution with run time limits of 5700 and 5760 min, respectively, for the purpose of comparing results on an equal time basis. The pulse-height spectrum mean values and relative uncertainties are plotted in Figs. 17 and 18, respectively. The distribution of tally bin relative uncertainties is shown in Fig. 19.
As expected, the tally mean values exhibit statistical agreement. The differences between the 384 bin mean values estimated with and without the FW-CADIS variance-reduction parameters are approximately normally distributed. In all but one of the bins, the differences were \( < 3\sigma \) from zero. For the outlier, the difference was 3.33\( \sigma \); however, the relative uncertainty of the mean value was 41\% for the case without the FW-CADIS parameters.

The distribution of relative uncertainties, as shown in Fig. 18, is far more uniform when the FW-CADIS variance-reduction parameters are used. Without the FW-CADIS parameters, the relative uncertainties varied between 3.46\% and 100\%, while two of the bins received no scores. With the application of the FW-CADIS method, the uncertainty range was reduced to 0.78\% to 11.28\%, and all tally bins received scores. Moreover, the fraction of tally bins that have relative uncertainties less than a given value, as shown in Fig. 19, was significantly increased. The average per-bin FOM, calculated according to Eq. (30), was increased from 0.045 to 0.830 min\(^{-1}\), which can be interpreted as an average speedup of a factor of 18. The FOM of the total count rate was increased from 18.1 to 173.6. Thus, for this problem, the FW-CADIS method is able to simultaneously increase the number of overall tally contributions, while ensuring that those contributions are distributed relatively uniformly in energy, as was desired.

V. SUMMARY

A novel hybrid Monte Carlo/deterministic transport method, FW-CADIS, has been developed for enabling and/or 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/or regions. The FW-CADIS method has been implemented and demonstrated within the MAVRIC sequence of SCALE and the ADVANTG/MCNP framework. The performance of the method has been demonstrated on representative, real-world problems, including calculation of dose rate and energy-dependent flux throughout the problem space, dose rates in specific areas, and energy spectra at multiple detectors. Results of the FW-CADIS method and other recently developed global variance-reduction approaches have been compared, and the FW-CADIS method was demonstrated to outperform other methods in all cases considered. The method has also been applied to a variety of other relevant and challenging problems, many of which would otherwise be computationally prohibitive, including determining dose rates throughout a full-scale pressurized water reactor facility,\(^{9,23–25}\) site boundary dose rates from an array of commercial spent fuel storage casks,\(^{41}\) criticality accident alarm system analyses,\(^{42}\) nuclear well-logging simulations,\(^{5}\) dose rates throughout a city from a postulated nuclear weapon detonation,\(^{46}\) and fusion neutronics analyses.\(^{44}\) In all applications to date, excellent results have been achieved.\(^{6}\)

Implementation of the FW-CADIS method requires two approximate deterministic 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. An important distinguishing characteristic of this method, as compared with other global variance-reduction methods,\(^{26,30}\) 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. While substantial speedups (hundreds to tens of thou-
sands) are routinely observed with the CADIS method, the FW-CADIS method has proven to be transformational in that it enables high-fidelity Monte Carlo results for distributions (e.g., spatial dose rate distribution) in large phase-spaces—a capability previously attributed only to deterministic methods. Hence, this method has initiated a paradigm shift in the methodology used to obtain accurate, full domain solutions to large, complex radiation transport problems.

Recent work\textsuperscript{47,48} has extended the FW-CADIS method for eigenvalue problems for the purpose of accelerating Monte Carlo reactor analyses. Potential other applications include accelerating continuous-energy Monte Carlo for the generation of problem-dependent multigroup cross sections, and groupwise forward and adjoint fluxes for SCALE sensitivity/uncertainty analyses.

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