A Comparison of the FW-CADIS and MR-CADIS Variance Reduction Methods

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INTRODUCTION

The Consistent Adjoint Driven Importance Sampling (CADIS) method [1, 2], which uses an adjoint deterministic estimate for making variance reduction parameters that optimize Monte Carlo (MC) shielding calculations, was introduced in 1998. This method was designed to optimize a single tally, typically an integrated response such as a detector count rate or a dose rate. Because both deterministic and stochastic methods are employed, CADIS is referred to as a *hybrid method*.

In 2007, the forward-weighted CADIS (FW-CADIS) method [3, 4] was introduced to optimize several tallies at once, giving more uniform relative uncertainties among the tallies for both high-flux and low-flux areas of the problem. This method can be used for several small detectors, for semi-global problems (mesh tally over a large fraction of the problem), or for global problems (mesh tally over the entire problem). Optimization can be done for an integrated response such as a dose rate $D(\vec{r})$ as a function of position, the total flux $\phi(\vec{r})$ as a function of position, or the space/energy flux $\phi(\vec{r},E)$. Both the CADIS and FW-CADIS methods have been in the MAVRIC sequence of SCALE [5] for three versions (6.0 in 2009, 6.1 in 2011, and 6.2 in 2016). The ADVANTG package [6] released in 2015 uses the CADIS and FW-CADIS methods to accelerate MCNP neutron/photon shielding calculations.

In 2014, the multi-response CADIS (MR-CADIS) method [7, 8] was presented as a way to obtain even more uniform relative uncertainties for problems with multiple tallies than those obtained with FW-CADIS. The method does not use a forward deterministic calculation but instead uses one adjoint calculation for every tally to be optimized in the Monte Carlo calculation.

This work compares the above methods.

METHODS

The CADIS Method

For a problem with source distribution $q(\vec{r},E)$ and a detector response function $\sigma_d(E)$ over a small volume $g(\vec{r})$ (where $g=1$ in the tally region and $g=0$ otherwise), the CADIS method optimizes the Monte Carlo solution of the response $\iint \phi(\vec{r},E)\,\sigma_d(\vec{r})\,g(\vec{r})\,dE\,dV$ by developing weight window target values (an importance map) and a biased source distribution. First, a deterministic adjoint calculation is performed using the adjoint source that corresponds to the tally to be optimized, $q^+(\vec{r},E)=\sigma_d(E)g(\vec{r})$. The estimate of the detector response R is made using the resulting adjoint fluxes $\phi^+(\vec{r},E)$ as

$$R=\iint q(\vec{r},E)\,\phi^+(\vec{r},E)\,dE\,dV. \tag{1}$$

The target weight windows $\overline{w}(\vec{r},E)$ and biased source distribution $\hat{q}(\vec{r},E)$ are then computed to be

$$\overline{w}(\vec{r},E)=\frac{R}{\phi^+(\vec{r},E)} \text{ and} \tag{2}$$

$$\hat{q}(\vec{r},E)=\frac{q(\vec{r},E)\,\phi^+(\vec{r},E)}{R}. \tag{3}$$

Because the source particles start with a weight of $q/\hat{q}$ when sampled from the biased source, the source particles match the target weights, so they are neither rouletted nor split just after birth. This is the consistent part of CADIS.

The FW-CADIS Method

To obtain low relative uncertainties across a large portion of the problem, more adjoint source would have to be placed in low-flux areas compared to the amount of adjoint source in high-flux areas. The adjoint source strength is weighted using the inverse of a deterministic estimate of the forward flux, $\phi(\vec{r},E)$. Three types of FW-CADIS can be used depending on the Monte Carlo quantity to optimize. The adjoint source $q^+(\vec{r},E)$ is defined as follows:

To optimize the MC:	Set $q^+(\vec{r},E)=$	
$\phi(\vec{r},E)$	$\dfrac{g(\vec{r})}{\phi(\vec{r},E)}$	(4a)
$\int \phi(\vec{r},E)\,dE$	$\dfrac{g(\vec{r})}{\int \phi(\vec{r},E)\,dE}$	(4b)
$\int \sigma_d(E)\,\phi(\vec{r},E)\,dE$	$\dfrac{\sigma_d(E)\,g(\vec{r})}{\int \sigma_d(E)\,\phi(\vec{r},E)\,dE}$	(4c)

With the adjoint fluxes computed with one of these adjoint sources, the importance map and biased source distribution are then computed just like CADIS, using equations 1–3. The FW-CADIS method compares very

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favorably to other global hybrid methods that only use forward estimates and methods that use a combination of forward and adjoint estimates [9].

The MR-CADIS Method

For every tally i or every voxel of a mesh tally i using response function $\sigma_d(E)$ over volume $g_i(\vec{r})$, the MR-CADIS method computes adjoint fluxes $\phi_i^+(\vec{r},E)$ from an adjoint source of $q_i^+(\vec{r},E) = \sigma_d(E) g_i(\vec{r})$. The adjoint fluxes from each tally are used to estimate the response at each tally R_i and are then combined in a quadrature-type sum as

$$R_i = \iint \phi_i^+(\vec{r},E)\, q(\vec{r},E)\, dE\, dV \tag{5}$$

$$\phi^+(\vec{r},E) = \sqrt{\sum_i \left(\frac{\phi_i^+(\vec{r},E)}{R_i}\right)^2} \tag{6}$$

From this weighted total of adjoint fluxes, a biased source $\hat{q}(\vec{r},E)$ and target weight windows $\overline{w}(\vec{r},E)$ are developed in a manner similar to that used for CADIS, using equations 1–3.

FW-CADIS could be implemented using many adjoint calculations as well, forming the total adjoint flux as

$$\phi^+(\vec{r},E) = \sum_i \frac{\phi_i^+(\vec{r},E)}{R_i} \tag{7}$$

and using estimated response values R_i based on the adjoint fluxes and true source distribution instead of R_i values based on deterministic forward fluxes and the response function. The FW-CADIS method shown in the previous section is more efficient, using a single forward calculation instead of a potentially large number of adjoint calculations.

TEST PROBLEMS

Hollow Concrete Cube

The problem used to demonstrate the MR-CADIS method relative to CADIS and FW-CADIS [7, 8] is the calculation of a mesh tally of total flux across one face of a hollow concrete cube, as shown in Fig. 1. The mesh tally is a 9 × 9 grid, so 81 adjoint calculations will be required by the MR-CADIS method. With a 1 MeV point photon source (3.7×10^{10} /s), source biasing does not come in to play.

Spent Fuel Cask

The simple model of a TN24P fuel cask [10], also shown in Fig. 1, holds two types of assemblies with both photon and neutron sources. Activated hardware at the tops and bottoms of the assemblies emits photons. The goal is to calculate the total dose rate at 2 m from every surface.

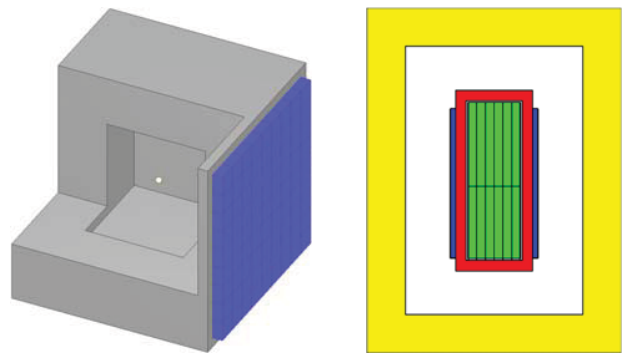

Fig. 1. Test models. Left – cutaway view of the hollow concrete cube test problem (200 cm with 100 cm void), source, and a mesh tally across one face. Right – slice of the simple TN24P cask model with the tally zone (yellow) extending from 1.5 m to 2 m away from the cask surfaces.

RESULTS

Hollow Concrete Cube

This problem was run with all three methods and for three different levels of fidelity in the deterministic estimates. Low fidelity used a 10 cm mesh, a quadruple range (QR) quadrature of 2 azimuthal and 2 polar angles per octant, and a first order (P_1) Legendre scattering expansion. Medium fidelity was a 5 cm mesh, 3/3 QR, and P_3. High fidelity was a 2.5 cm mesh, 4/4 QR and P_5. Each Monte Carlo run time was 4 hours.

The final total fluxes (energy integrated) in each voxel computed by the Monte Carlo calculations were statistically equivalent for the different methods and deterministic fidelities, as they should be; variance reduction should not change the answer, just the figure of merit. Figure 2 shows the mesh tally results. The run times, average relative uncertainties of the voxel fluxes, and the figures of merit, $FOM = (\sigma^2 T)^{-1}$, are listed in Table I. In the table, the MC FOM is calculated with T equal to the run time of the Monte Carlo simulation. The total FOM is calculated with T equal to the sum of the deterministic and Monte Carlo run times.

The relative uncertainties in the total flux mesh tally for CADIS have a broader distribution than for FW- or MR-CADIS, as expected. The MR-CADIS method produces an importance map that is slightly better than FW-CADIS, as illustrated by the FOMs using only the Monte Carlo times. However, when the time required for the 9 × 9 separate adjoint calculations is included, the total FOM for MR-CADIS is lower than FW-CADIS. For the case using the high fidelity deterministic solutions, the total FOM for

MR-CADIS is significantly lower than FW-CADIS and even lower than CADIS, which is not intended for use on semi-global problems.

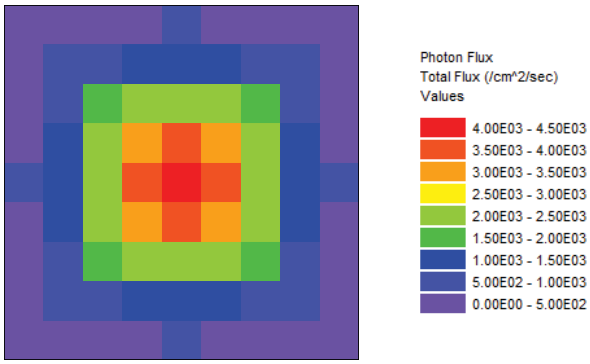

Fig. 2. Total flux (γ/cm^2/s) for the hollow concrete cube problem.

Table I. Hollow Concrete Cube Problem Timing and FOMs

	Deterministic For. (min)	Deterministic Adj. (min)	MC (min)	Mean of Rel. Unc.	MC FOM (/min)	Total FOM (/min)
Analog			4002	1.02E-02	2.4	2.4
Low Fid.						
CADIS		0.1	243.6	3.65E-03	308	308
FW-CADIS	0.1	0.1	241.8	2.86E-03	507	505
MR-CADIS		10.5	241.1	2.83E-03	518	496
Med. Fid.						
CADIS		1.7	241.2	2.72E-03	559	556
FW-CADIS	4.2	1.7	243.0	2.29E-03	783	766
MR-CADIS		132.1	240.6	1.96E-03	1080	698
High Fid.						
CADIS		38.4	241.2	2.74E-03	553	476
FW-CADIS	80.7	33.1	245.4	2.16E-03	878	596
MR-CADIS		3324	242.6	2.05E-03	977	67

Spent Fuel Cask

For this problem, the deterministic calculations used a non-uniform mesh of 48 × 48 × 61 (over the volume of 6.6 × 6.6 × 9 m^3), 4/4 QR and P_5. The dose rates were tallied on a uniform 10 cm mesh, only keeping the 2 × 10^5 voxels in the outer area. For MR-CADIS, the tally region was broken into either 3 adjoint sources (top, bottom, and a cylindrical band) or 9 adjoint sources (top and bottom with inner/outer regions and cylindrical region divided into five bands). The Monte Carlo runs times were all 16 hours. The dose rates computed by the different methods were the same as expected and are shown in Fig. 3. In Monaco/MAVRIC, the neutron (n) and photon (p) dose rates are tallied separately, so the results shown in Table II include entries for both particle types for each calculation method. The distributions of relative uncertainties in the total dose rate mesh tally are shown in Fig. 4, with FW-CADIS showing a tighter distribution (more uniform) and lower mean than the MR-CADIS calculations.

For the TN24P problem, FW-CADIS has higher Monte Carlo–only FOMs than the MR-CADIS calculations, indicating that the importance map and source biasing are better. When including the deterministic times, the total FOM for FW-CADIS is also better than either MR-CADIS calculation. Using more adjoint calculations in the MR-CADIS calculation helped slightly, but it is not clear how many separate adjoints would be required to make an importance map as accurate as FW-CADIS or if that is possible before the time required to calculate all of the adjoints becomes too onerous. This would present a challenge for the user as a parameter that would require some tuning before running a calculation.

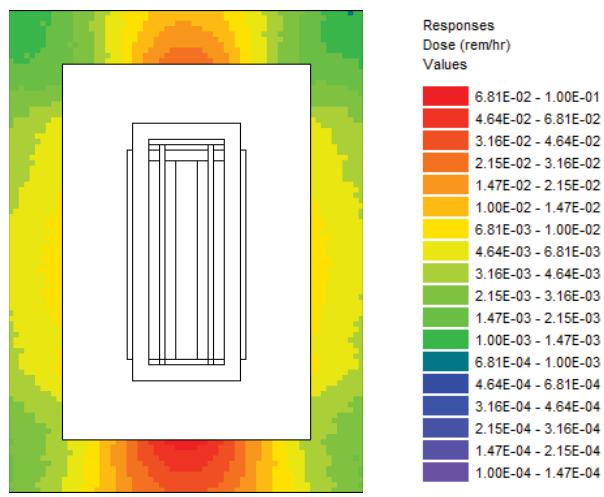

Fig. 3. Total dose rate (rem/hr) for the TN24P problem.

Table II. TN24P Problem Timing and FOMs

	Deterministic For. (min)	Deterministic Adj. (min)		Mean of Rel. Unc.	MC-only FOM (/min)	Total FOM (/min)
FW-CADIS	49	37	n	0.0340	0.895	0.821
			p	0.0236	1.859	1.705
MR-CADIS 3 adjoints		82	n	0.0410	0.616	0.568
			p	0.0282	1.303	1.201
MR-CADIS 9 adjoints		299	n	0.0396	0.663	0.506
			p	0.0265	1.480	1.129

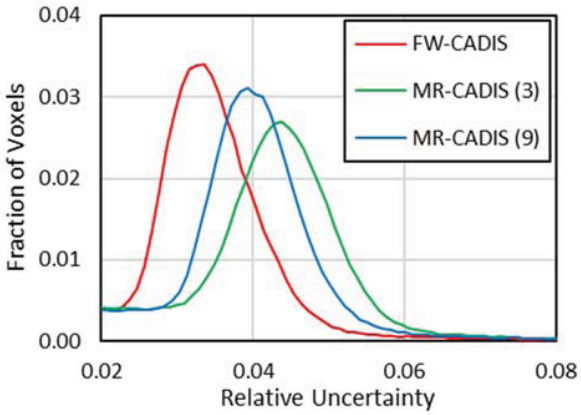

Fig. 4. Distributions of relative uncertainty for the total dose rate 1.5–2 m from the surface of the TN24P cask.

SUMMARY

For some problems with a small number of responses, the MR-CADIS method may be slightly faster than the FW-CADIS method. For global or semi-global problems or for problems with many tallies, the time required to make the variance reduction parameters using the MR-CADIS method may be so large as to lower the overall FOM of the problem. The TN24P problem highlighted the difficulty of determining how many adjoints are needed and how they are selected. Clearly, using 2×10^5 adjoint calculations would not be reasonable, but it is not certain how many calculations would be reasonable. An increase from three to nine adjoints in the MR-CADIS method improved the Monte Carlo performance some, but overall performance decreased.

For global problems with the goal of optimizing the calculation of the space and energy flux $\phi(\vec{r}, E)$, would the MR-CADIS method require an adjoint for every combination of energy group and voxel of the tally? For the TN24P problem using 19 energy groups and 2×10^5 voxels, would 3.8 million adjoint calculations be required? FW-CADIS can make variance reduction parameters for the optimization of $\phi(\vec{r}, E)$ over many groups and large volumes using just two deterministic calculations.

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