Comparison of Hybrid Methods for Global Variance Reduction in Shielding Calculations

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INTRODUCTION

Hybrid methods use quick forward and/or adjoint flux estimates from a deterministic code to create biasing parameters for a detailed Monte Carlo (MC) calculation. One way to incorporate the deterministic estimate is through an importance map that defines target weights, $\overline{w}$, for MC weight windows.

Importance maps can be developed to optimize the MC calculation over different spatial domains. For a source/detector problem, the goal is to maximize the figure-of-merit (FOM) of a single tally. For a source/region problem, the goal is to compute several tallies or a mesh tally over a large portion of the problem with uniform relative uncertainties. For the global case, the goal is to compute a mesh tally over the entire problem space with uniform relative uncertainties – to converge every voxel at the same rate – regardless of the magnitude of the tally in the voxel.

For the source/region and global cases, there are different quantities that the user may wish to optimize with the importance map. These include the spatial flux, $\phi(\vec{r})$; the space/energy flux, $\phi(\vec{r},E)$; and an integrated response, $R(\vec{r}) = \int f(E)\,\phi(\vec{r},E)dE$, where $f(E)$ is a response function (an interaction cross-section or flux-to-dose conversion factors).

Several methods for creating importance maps to optimize the MC calculation of a global quantity have been developed recently and their effectiveness will be compared. These methods are based on either a forward flux estimate or a combination of forward and adjoint flux estimates.

Methods Based on Forward Estimates

To optimize the convergence of the total flux over an entire problem, Cooper & Larsen [1] used weight window targets, $\overline{w}$, proportional to deterministically-estimated values of the forward flux, $\overline{w}(\vec{r}) = \phi(\vec{r})/\max\big(\phi(\vec{r})\big)$. The stated purpose was to obtain a uniform density of Monte Carlo particles over the problem, which should lead to approximately uniform tally convergence. Note that the weight window targets are a function of space only and are normalized so that the point with the highest flux has a target weight of 1.

Becker and Larsen [2] expanded on this with two space/energy methods. For optimizing the MC calculation of space/energy flux, they used the global flux weight window (GFWW) method with $\overline{w}(\vec{r},E) \propto \phi(\vec{r},E)$. For optimizing the MC calculation of a response, they used the global response weight window (GRWW) method with $\overline{w}(\vec{r},E) \propto \int f(E)\,\phi(\vec{r},E)dE/f(E)$. Optimizing total flux used GRWW and $f(E) = 1$. Normalization of these weight window maps was not specified.

In an iterative scheme using the MCNP weight window generator, van Wijk et al. [3] developed weight window targets based on previous MC estimates of either the spatial flux or the relative uncertainty in the spatial flux ($Re(\vec{r}) \propto 1/\sqrt{\phi(\vec{r})}$). The target weights were then normalized using the maximum flux or the minimum relative uncertainty, respectively. The authors state that normalization to the highest flux or lowest uncertainty typically corresponds to the source area of the problem.

Like the other approaches outlined above, weight window targets based on flux or the relative uncertainty in the flux could also be generated from deterministic estimates of those quantities. Note that van Wijk's first method, based on flux, would then be the same as Cooper's method. A potential downfall of the second method, which is based on the relative uncertainties, is that for a problem where the flux spans n orders of magnitude, the weight window targets will only span $n/2$. Particles would have to survive many successive roulettes in order to populate the lowest flux areas of the problem.

Methods Based on Forward and Adjoint Estimates

Wagner and Haghighat [4] developed the Consistent Adjoint Driven Importance Sampling (CADIS) method to develop weight window target values that were consistent with a biased source to optimize the MC calculation of an integrated response R at one detector location. Using an adjoint source equal to the response function, $q^+(\vec{r},E) = f(E)$, located at the detector location, the adjoint flux, $\phi^+(\vec{r},E)$, is computed and an estimate of the response, $R = \iint q(\vec{r},E)\,\phi^+(\vec{r},E)\,dE\,dV$, is made using the true source, $q(\vec{r},E)$. Then the target weights, $\overline{w}(\vec{r},E) = R/\,\phi^+(\vec{r},E)$, and biased source, $\hat{q}(\vec{r},E) = q(\vec{r},E)\,\phi^+(\vec{r},E)/R$, can be developed. Though the idea of using adjoint information to accelerate Monte Carlo was well known for several decades before Ref. 4 was published, the unique feature of the CADIS method is that it ensures that the biased source and importance map are consistent with each other — so that time is not wasted splitting or rouletting particles right after birth.

This method has been extended for optimizing source/region and global problems by incorporating the forward flux estimate into the definition of the adjoint source. The forward-weighted CADIS method (FW-CADIS) [5] uses an adjoint source of $q^+(\vec{r},E) = 1/\phi(\vec{r},E)$ for optimizing the space/energy flux, $q^+(\vec{r},E) = 1/\int \phi(\vec{r},E)\, dE$ for optimizing the total flux, and $q^+(\vec{r},E) = f(E)/\int f(E)\, \phi(\vec{r},E)\, dE$ for optimizing a spatial-dependent response. The FW-CADIS method can be used for source/region problems or global problems by changing the extent of the volume where the adjoint source is defined. From the resulting adjoint fluxes, the weight window targets and biased source are developed similar to CADIS. Also like CADIS, the normalization of the target weights is based on the biased source.

Becker [6] developed methods for three different types of problems: source/detector, source/region and global problems. All three use estimates of the contributon flux, $\phi(\vec{r},E)\, \phi^+(\vec{r},E)$, in the process of creating weight windows. Each of the three methods uses a different adjoint source definition depending on what the weight windows will optimize – either the space/energy flux or an integrated response as a function of space.

It is expected that the adjoint-based methods will perform better than the forward-based methods since the adjoint contains information on the importance of a particle toward the overall objective of the MC calculation.

Implementation in SCALE/MAVRIC

Both SCALE 6.0 and 6.1 [7] contain the MAVRIC sequence, a user-friendly approach to applying CADIS or FW-CADIS to challenging shielding problems. MAVRIC uses the Denovo S_N code [8] for the forward and adjoint flux estimates, creates the importance map (target weights) and biased source, and then uses them in Monaco [9], a fixed-source multi-group Monte Carlo code. All of the methods compared in this summary were added as alternatives to the CADIS/FW-CADIS processing step of the MAVRIC sequence in an internal development version of SCALE. Since they were all run using the same components, the comparisons should be as fair as possible.

Metrics for Mesh Tally Convergence

To compare the effectiveness of different hybrid strategies in computing a global quantity, metrics for the convergence of the mesh tally need to be defined. Four statistical tests based on the distribution of relative variance of the voxels within a mesh tally have been developed for MCNP [10]. These tests have been implemented into Monaco, using the distribution of relative uncertainty instead. For the relative uncertainty R_i in voxel i, the average relative uncertainty over the V voxels is $\bar{r} = (1/V)\sum R_i$, which can be used to compute an FOM for the mesh tally, FOM= $(T\bar{r}^2)^{-1}$, where T is the time. The four statistical tests measured in Monaco are: (1) if the fraction of voxels with score, ζ , is constant; (2) if $\bar{r}$ is decreasing as $1/\sqrt{N}$, where N is the number of MC histories; (3) if the variance of the relative variance is decreasing as $1/N$; and (4) if the FOM is constant.

DESCRIPTION OF THE ACTUAL WORK

Analog MC and five hybrid methods — Cooper's method, van Wijk's Re-based method, GRWW, Becker's global method and FW-CADIS — will be applied to several example problems that compute a global mesh tally of total flux.

The forward-based calculations contained in this study will not use the biased source/importance map normalization, so that the original method is preserved. Becker's forward/adjoint methods will use the biased source/importance map normalization since determining the right normalization without the biased source would be a difficult process.

Example Problem 1

The first example problem is a simple shielding example based on an example problem from van Wijk [3]. This problem consists of a one Curie 14.1 MeV neutron point source at the center of a 40 cm cube of paraffin covered in 10 cm of lead. This source box is located in a two-room building made of 10 cm thick lead walls. The rooms are separated by a borated glass window. The outer dimensions of the problem, shown in Fig. 1, are 420×220×240 cm. The objective of this problem is to compute the total flux everywhere.

Note that this is a fairly simple problem — the ratio of the maximum and minimum fluxes is 1.6×10^6. If all of the materials were voids instead, that ratio would be 1.2×10^4, showing that most of the variation in flux is due to spatial attenuation, not material attenuation.

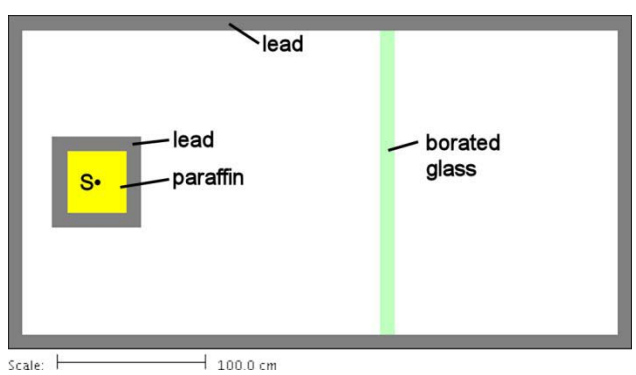

Fig. 1. Geometry of example problem 1.

Example Problem 2

The second example problem is taken from Becker [6]. Consisting mostly of nested cubes, a volumetric UO_2 fission neutron source (10^{16} n/s) is surrounded by layers of steel, concrete and steel. This is located in a large water region, surrounded by concrete, lead, concrete and lead. Several concrete pillars are also contained in the large water region. The overall size of the problem is 300×300×300 cm. Fig. 2 shows a portion of the problem geometry. The objective of this problem is to compute the total flux everywhere.

This is a more difficult shielding problem, covering 14 orders of magnitude in total flux, with only 3 orders of magnitude due to spatial attenuation.

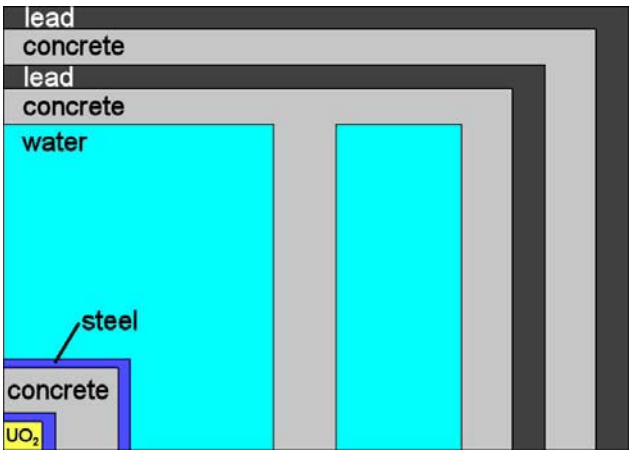

Fig. 2. One octant of the geometry of example problem 2, showing the $x = y$ plane (origin at lower left).

RESULTS

Example Problem 1

The analog (with implicit capture) calculation was allowed 7 hours so that the mesh tally statistical tests could all be satisfied. The target time for the hybrid calculations was a total of one hour on a single processor, with the deterministic calculations requiring 9 minutes (forward) and/or 8 minutes (adjoint). The deterministic calculations used a non-uniform 51×35×37 mesh, a symmetric-level S_8 quadrature and P_3 Legendre scattering expansion.

Results for the final MC mesh tally are summarized in Table I, showing that all of the hybrid methods performed well above the analog. For the statistical tests, "X" is passing, "-" is not. The flux contour plots for each method were all very similar to each other. The FW-CADIS contour plot is shown in Fig. 3. Fig. 4 shows the cumulative distributions of the voxel relative uncertainties for the different methods. This shows that the analog calculation has the smallest fraction of voxels below a given relative uncertainty and FW-CADIS has the most.

Because this problem involves a point mono-energetic source, no biasing of the source distribution in space or energy is possible. The weight window targets created from each method were normalized so that the target at the source location was 1. For the space/energy methods, the target weight at the location of the source in the 14.1 MeV group was set to 1.

TABLE I. Example Problem 1 Results

	ζ	$\bar{r}$	FOM (/min)	Stat. Test 1	2	3	4
Analog	1	8.17E-02	0.35	X	X	X	X
Cooper	1	3.17E-02	16.77	X	X	-	-
van Wijk	1	3.19E-02	16.64	X	X	X	X
GRWW	1	3.14E-02	17.01	X	-	-	-
Becker	1	3.24E-02	19.35	X	-	-	-
FW-CADIS	1	2.27E-02	39.43	X	X	X	X

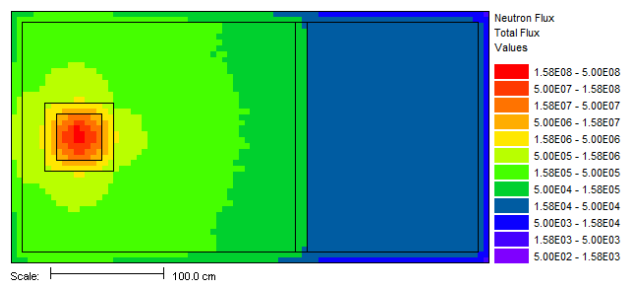

Fig. 3. Total flux (n/cm^2/s) for example problem 1.

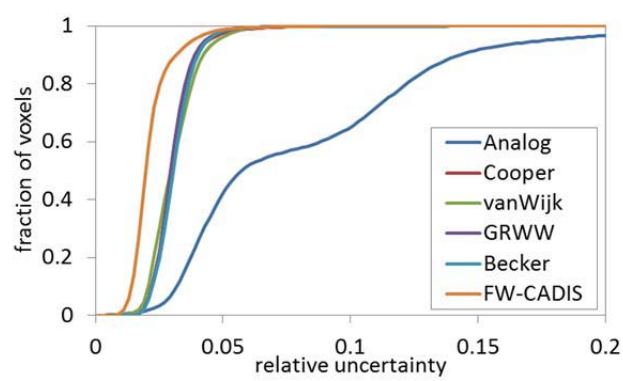

Fig. 4. Fraction of voxels with less than a given amount of relative uncertainty for example problem 1.

Example Problem 2

The analog calculation and the five hybrid methods were each allowed 20 hours, with the forward and adjoint S_N calculations taking 40 and 50 minutes, respectively. The mesh tally results, listed in Table II, show that the forward-based methods did improve the mesh tally by getting particles to every voxel. The adjoint-based methods do much better at reducing the mean relative uncertainty and converging the mesh tally. The total flux computed by FW-CADIS is shown in Fig. 5, and the cumulative distributions of the voxel relative uncertainties for all of the methods are shown in Fig. 6.

TABLE II. Example Problem 2 Results

	ζ	$\bar{r}$	FOM (/min)	Stat. Test 1	2	3	4
Analog	0.3	2.64E-01	0.012	-	-	-	-
Cooper	1	3.49E-01	0.007	X	-	-	-
van Wijk	1	3.54E-01	0.007	X	-	-	-
GRWW	1	3.58E-01	0.007	X	-	-	-
Becker	1	5.26E-02	0.323	X	X	X	X
FW-CADIS	1	3.92E-02	0.582	X	X	X	X

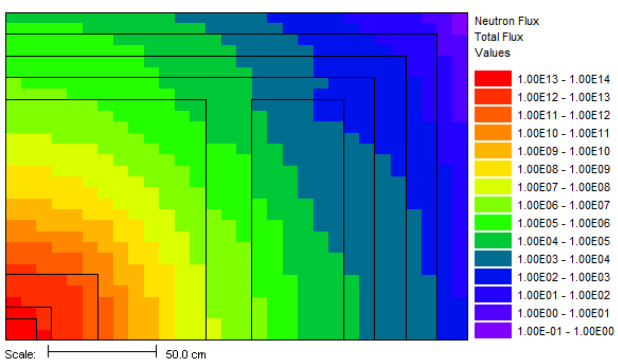

Fig. 5. Example problem 2 total flux in the $x = y$ plane (origin at lower left).

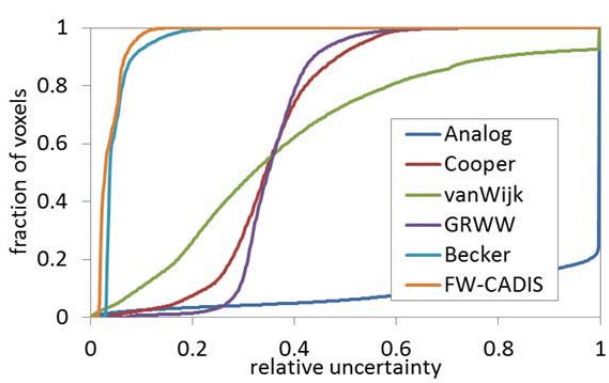

Fig. 6. Example problem 2 fraction of voxels with less than a given amount of relative uncertainty.

In this problem, the three forward-based methods would benefit from using a biasing source and normalizing the importance map to that biased source. FOM's for Cooper's and van Wijk methods improve slightly and the FOM for GRWW improves by a factor of three when using the biased source and normalization.

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