Propagation of Uncertainty from a Source Computed with Monte Carlo

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INTRODUCTION

In multi-step Monte Carlo (MC) problems, where the result of one calculation is used as the source in a subsequent calculation, uncertainty propagation from the first result is usually not included in the uncertainty estimate of the second calculation. The results from the second step, which are dependent on the mean values of the computed source, have associated uncertainties, but they reflect only the statistical uncertainty in the sampling process of the second step – they do not include the uncertainties in the source developed from the first step.

Examples of two-step MC problems where uncertainty propagation may be significant include dose rates from neutron activation, criticality accident dose rates, active interrogation simulations, and reactor fuel depletion calculations.

A common approach to handling the uncertainty propagation is to run the first step of the problem for a sufficiently long time to ensure the statistical uncertainties have all been reduced to a very small level. Any impact the uncertainties in the computed source have on subsequent calculations is then assumed to be small compared to the reported sampling uncertainty. But how long is long enough? How can one be sure?

A very costly method to calculate the uncertainty in the result of the second calculation due to the uncertainty in the first calculation is by using a brute force technique. Multiple clones of the same first- and second-step inputs (with different random number seeds) are run, and the sample standard deviation of all of the final responses is computed and taken to be the total uncertainty of that result, including the uncertainties in the source computed by the first step. The number of clones of the entire problem to run to ensure statistical quality may be large and therefore very costly for difficult problems.

What is needed is an inexpensive method for computing the uncertainty of the final result due to the uncertainties in the source derived from the first MC calculation. In this paper, a method is presented to quickly estimate the uncertainty due to the source uncertainties. This new approach is applied to a simple activation problem yielding good results.

THEORY

Consider a source/detector problem with a single source of strength S which calculates a response R of the form

$$R = \int f(E)\, \phi(\vec{r}, E)\, dE, \tag{1}$$

where $f(E)$ is the response function. The Monte Carlo calculation of R also computes an uncertainty, σ_{MC}, which reflects the statistical uncertainty of the sampling processes used during the transport simulation. If the source strength was determined by a previous Monte Carlo calculation, then the uncertainty in the response due to the uncertainty in the source, σ_S, should also be taken into account when expressing the total uncertainty of the response, σ_{total}. Because the response is directly proportional to the source strength, the total response uncertainty is expressed as

$$\sigma_{\mathrm{total}}^2 = \sigma_S^2 + \sigma_{MC}^2. \tag{2}$$

The brute force method described above could also be used to determine σ_{total} directly.

Now consider the case where the first Monte Carlo calculation computes a mesh tally that will be the basis of the source distribution for the second Monte Carlo. The source distribution consists of many voxels, each with a source strength $S_i \pm \sigma_i$ and a normalized energy distribution $q_i(E)$, where $\int q_i(E)\, dE = 1$. The response computed by the second Monte Carlo calculation can be expressed as the sum of contributions from each voxel i.

$$R = \sum S_i R_i\,, \tag{3}$$

where R_i is the response due to a unit source at i. R_i can be further expanded using the source distribution for each voxel and $R_i(E)$, the response due to a unit source of energy E at voxel i, as

$$R_i = \int q_i(E)\, R_i(E)\, dE. \tag{4}$$

Using the standard propagation of errors, the uncertainty, σ_S, in the total response, R, due to uncertainties in the source strengths can be found as

$$\sigma_S^2 = \sum \left(\frac{\partial R}{\partial S_i}\right)^2 \sigma_i^2 + 2 \sum_{i \neq j} \left(\frac{\partial R}{\partial S_i}\right)\left(\frac{\partial R}{\partial S_j}\right) \rho_{ij} \sigma_i \sigma_j\,, \tag{5}$$

where ρ_{ij} is the correlation coefficient expressing how correlated/uncorrelated/anti-correlated the values of two

source strengths S_i and S_j are. Because the same neutron histories likely contribute to the activation rates in neighboring voxels, the tallies in the neighboring voxels are probably highly correlated ($\rho_{ij} \approx 1$). Voxels farther away from each other are most likely uncorrelated ($\rho_{ij} = 0$), but it is unlikely that any pair of voxels have any degree of anti-correlatation ($\rho_{ij} < 0$). Ignoring the correlation between source voxels (which is the same as assuming each voxel source strength is independent), a lower bound on the uncertainty of the response can then be made using

$$\sigma_S^2 = \sum \left(\frac{\partial R}{\partial S_i}\right)^2 \sigma_i^2 \quad (6)$$

$$= \sum \left(\int q_i(E)\, R_i(E)\, dE\right)^2 \sigma_i^2. \quad (7)$$

Computing the unit responses $R_i(E)$ from each voxel to determine the uncertainty contribution to the final response due to the source uncertainties could be more computationally expensive than applying the brute force method.

The New Approach

The adjoint flux $\phi_i^+(E)$ from a calculation using the response function as the adjoint source represents the response due to a unit source of energy E at voxel i. Using $\phi_i^+(E)$ in place of $R_i(E)$, the result of a single adjoint calculation could be used to calculate the uncertainty in the response from the source with uncertainty as

$$\sigma_S^2 = \sum \left(\int q_i(E)\, \phi_i^+(E)\, dE\right)^2 \sigma_i^2. \quad (8)$$

If importance sampling using the adjoint flux is used for the second calculation [1], the adjoint flux has already been calculated, so this estimate of uncertainty from the "noisy" source is nearly free. Note that for variance reduction uses, the adjoint solution needs only to be approximate. However, for an accurate estimate of uncertainty using this method, a more accurate adjoint flux may be required. The adjoint flux can be used as a replacement for $R_i(E)$ in Eq. (4) as well, which can help evaluate the accuracy of the adjoint solution by comparing this quantity to the MC computed response.

Adjoint solutions have been used to estimate uncertainties in computed fluid-flow parameters due to uncertainties in initial conditions and other input parameters [2]. Reference 2 did not include any correlation between input parameters, which was a reasonable assumption for their problem. The estimates of uncertainty in the final parameters made using their adjoint approach were lower (by up to 20%) than the uncertainties observed in 100 simulations using different random number seeds.

EXAMPLE PROBLEM

An Activation Example

Consider the simplified activation problem shown in Fig. 1, in which 14.1-MeV neutrons to the left of a 100-cm-thick steel shield penetrate the shield and activate the trace impurity of ^{59}Co via an (n,γ) reaction (with a macroscopic activation cross section of $\Sigma(E)$). The radioactive ^{60}Co produced in the shield decays and emits photons. The objective of the problem is to calculate the activation rate throughout the shield and the resulting photon dose rate at a point 100 cm to the right of the shield.

Fig. 1. A 14.1-MeV neutron source (yellow) activates a steel shield (gray), producing an activation photon dose rate at detector D.

The first MC calculation computes the activation rate density in the shield, $\int \Sigma(E)\, \phi_n(\vec{r}, E) dE$, caused by the neutron flux $\phi_n(\vec{r}, E)$. This can be done using a mesh tally. Assuming a long neutron irradiation time, the activity per unit volume, $A(\vec{r})$, of the ^{60}Co produced is equal to the activation rate density,

$$A(\vec{r}) = \int \Sigma(E)\, \phi_n(\vec{r}, E) dE. \quad (9)$$

The photon source can be constructed by combining the activity with the emission spectra, $q(E)$, of the activated product isotope. Because the activity was tabulated on a mesh grid, the source can be expressed as a source strength in each voxel, S_i, with an uncertainty of σ_i. The second MC calculation uses the photon mesh source and computes the dose rate response, R, with an uncertainty of σ_{MC} at the point of interest.

For this example, a neutron source strength of 2×10^9 n/s/cm^3 over a volume of 350×800×800 cm^3 was simulated. The neutron transport step used previously computed variance reduction parameters and a 15 minute MC calculation to compute the activation rate mesh tally, shown in Fig. 2, with a total activation rate of 2.98×10^{13}/s. The mesh tally used a uniform mesh of 50×80×80 over the 100×800×800 cm^3 shield. The values of the mesh tally were combined with the ^{60}Co photon emission spectrum (two lines at 1.17 and 1.33 MeV) to form the source for the photon transport step with a total strength of 5.95×10^{13} photon/s. This step also used previously computed variance reduction parameters and a 60 minute MC calculation to compute a photon dose rate of 106.167 ± 0.026 mrem/hr. Note that this uncertainty only reflects the uncertainty associated with the photon transport. A development version of the SCALE package [3] was used for these calculations. MAVRIC [4] was used to compute the variance reduction parameters and the multi-group Monaco code was used for the MC calculations.

The brute force technique was used to compute the uncertainty contribution to the final dose rate due to the source uncertainties. Sixty-four clones of the problem (both steps) were made with different starting random number seeds. The average dose rate was 103.4 mrem/hr with an observed standard deviation of 3.05 mrem/hr, or 2.95%. This represents both the uncertainty of the photon transport sampling and the uncertainties in the source distribution determined by the neutron transport MC. Because the uncertainty due to the photon transport averaged 0.029 mrem/hr (0.028%) among the 64 clones, the uncertainty due to the noisy source, σ_S, constituted nearly all of the observed standard deviation of 3.05 mrem/hr.

Estimate of Uncertainty Due to Source

An adjoint calculation using the dose rate response function at the detector location was performed using the discrete-ordinates code Denovo [5]. This calculation used a 2×5×5 cm^3 voxel size in the shield close to the detector and a 2×10×10 cm^3 voxel size far from the detector. An S_4 angular quadrature and a P_1 expansion of the scattering cross section were used. The adjoint fluxes were combined with the uncertainties of the mesh-based cobalt source to estimate both the photon dose rate (to judge the accuracy of the adjoint fluxes) as 145.7 mrem/hr and the uncertainty in the dose rate due to the source as 1.82 mrem/hr (or 1.25%). This estimate of the uncertainty is lower than the uncertainty observed in the brute force technique. Note that the adjoint-based estimate of the response was 40% higher than the Monte Carlo value, indicating that the adjoint calculation could be refined for more accuracy.

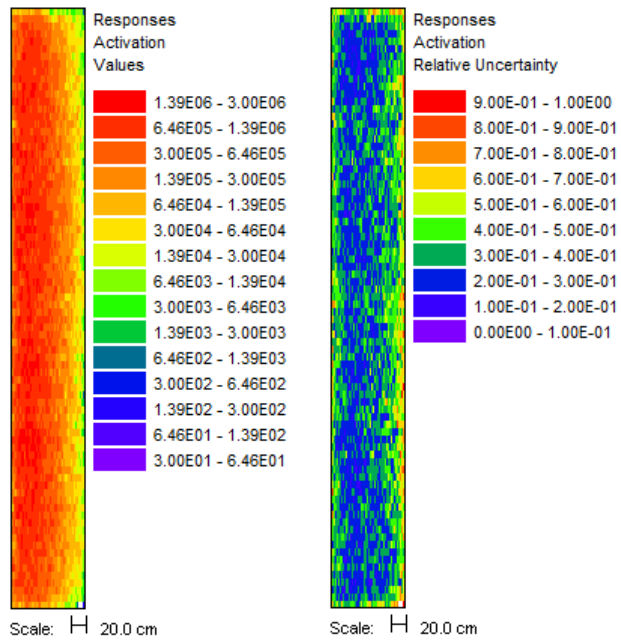

Fig. 2. The computed activation rate (left) and its relative uncertainty (right).

Adjoint Calculation Refinement

The impact of refinements in the deterministic calculation of the adjoint was investigated. Results for the adjoint-based estimate of R and σ_S are shown in Table I for different mesh parameters, quadratures, and scattering orders. As more refinement is made, especially in the mesh size close to the surface of the shield near the detector, the estimate of R approaches the Monte Carlo average of 103.4 mrem/hr from the brute force technique. Using the adjoints with more accurate estimates of R shows that the estimate of σ_S approaches about half of the observed value of 3.05 mrem/hr.

Different Amounts of Source Uncertainty

A short study was done to explore how the estimate of the uncertainty due to the source changed with the amount of noise in the activation source. The above results refer to a 15 minute MC calculation of the activation source and a 60 minute MC calculation of the dose rate. By changing the run time, T, of the activation source calculation, the uncertainty in the dose rate due to

the source should behave as $1/\sqrt{T}$. This was tested by increasing the activation calculation time to 30, 60, and 120 minutes while keeping the dose rate calculation fixed at 60 minutes. For each activation calculation, 64 clones were used to compute the actual uncertainty in the dose rate due to the source. The predicted uncertainty used the 47 group/S_8/P_3/0.5 cm mesh adjoint solution. The results listed in Table II and shown in Fig. 3 show that the predicted value of the uncertainty does behave as $1/\sqrt{T}$, and is consistently about one-half of the value from the brute force calculations.

SUMMARY

The lower bound of the uncertainty of a Monte Carlo derived source used in a subsequent transport calculation can be found using a single adjoint calculation. This new method can give the practitioner some measure of the source uncertainty in the final response calculation without a series of brute force calculations. The accuracy of the adjoint uncertainty estimate is dependent on the accuracy of the adjoint flux solution and on the correlation between source voxels. For a simple neutron activation/photon dose rate calculation, the adjoint estimate was a factor of two lower than the observed uncertainty.

Table I. Impact of Adjoint Refinement

Adjoint Parameters				Response	
energy groups	S_n/P_l	Mesh (cm)	Time (min)	Value mrem/hr	Unc.
19	4/1	2.0	6.4	153	1.89
		1.0	7.2	125	1.71
		0.5	8.1	118	1.66
	8/3	2.0	30.6	149	1.92
		1.0	33.4	116	1.68
		0.5	37.5	107	1.61
47	4/1	2.0	15.3	146	1.82
		1.0	17.5	116	1.62
		0.5	19.4	109	1.57
	8/3	2.0	72.3	140	1.83
		1.0	80.7	107	1.59
		0.5	90.8	99	1.52

Table II. Dose Rate (mrem/hr) Trends with Time

Step 1 (min)	Observed Value	Observed Unc.	Predicted Value	Predicted Unc.
15	103.4	3.053	108.0	1.654
30	103.6	2.416	104.9	1.183
60	103.6	1.563	105.5	0.886
120	103.7	1.224	106.1	0.609

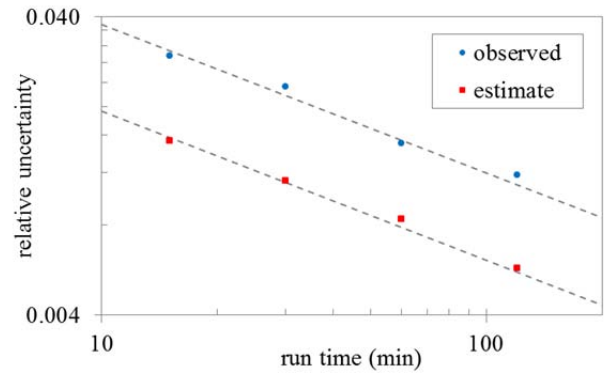

Fig. 3. Relative uncertainty in the dose rate due to the activation source as a function of activation source calculation time. Dotted lines are fits to $1/\sqrt{T}$.

ACKNOWLEDGMENTS

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