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An S_n Approach to Predicting Monte Carlo Cost with Weight Dependent Variance Reduction

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INTRODUCTION

The use of deterministic particle transport calculations to accelerate the convergence of Monte Carlo particle transport calculations is an active research field. These methods are referred to as "hybrid" methods, but existing methods do not use moments of the history score distribution higher than the first (the first moment is the same as the adjoint/importance) or the additional computer time resulting from the need to track more particles introduced by the biasing function.

This work presents a method to deterministically calculate the cost of the Monte Carlo calculation $\sigma^2\tau$, where σ^2 is the population variance of the history score distribution and τ is the expected Monte Carlo computer time per history. This cost function is inversely proportional to the figure of merit computed by Monte Carlo codes, which is defined to be $1/(\bar{\sigma}^2 T)$, where $\bar{\sigma}^2 = \sigma^2/N$ is the variance of the mean, N is the number of histories, and $T = N\tau$ is the computational time for all N histories. This work is similar to that of the DSA method of [1] in that both techniques attempt to minimize the cost of the Monte Carlo calculations. However, the DSA method relies on stochastic techniques while here deterministic methods are employed.

The calculation of the cost function is performed by solving the history score moment equations [2] (or just the moment equations) with an S_n calculation. Similar work was performed by [3], but all calculations there were limited to weight-independent variance reduction, e.g. importance splitting. In this paper, a method is developed to account for *weight-dependent* games, e.g. weight windows.

BACKGROUND

The moment equations derived by [2] begin by developing an integral expression for the score probability distribution function $\psi(\mathbf{P}, s)$ in terms of the standard transport and collision kernels, as well as, kernels that describe the transition of Monte Carlo particle weight w. Here, the phase-space variable in general is $\mathbf{P} = (\mathbf{r}, \hat{\mathbf{\Omega}}, E, t, w)$ and s is the score from a Monte Carlo history. $\psi(\mathbf{P}, s)ds$ is the probability that a Monte Carlo particle at $\mathbf{P}$ will contribute a score in ds about s. An integral equation for the rth moment $M_r(\mathbf{P})$ is then developed by evaluating

$$M_r(\mathbf{P}) = \int_{-\infty}^{\infty} ds\, s^r \psi(\mathbf{P}, s) \quad . \tag{1}$$

The moment equations are adjoint to the Boltzmann transport equation [4]. Therefore, the source for the moment equations is the score resulting from a specific Monte Carlo tally. The moment functions resulting from that specific tally can then be used to compute the population variance, dependent on the physical source, of the history score distribution by

$$\sigma^2 = \langle S(\mathbf{P}), M_2(\mathbf{P})\rangle_{\mathbf{P}} - \langle S(\mathbf{P}), M_1(\mathbf{P})\rangle^2_{\mathbf{P}}\,, \tag{2}$$

where $S(\mathbf{P})$ is the physical source distribution for the Monte Carlo calculation, including weight, and the operator $\langle\cdot\rangle_{\mathbf{P}}$ indicates an integral inner product over $\mathbf{P}$.

For weight-independent games, the weight dependence of the moments is separable. Moreover, the weight is always separable for the first moment because the expected score contribution alway scales with the particle's weight. This however is not the case for higher moments. It was under the assumption of weight separability that the work of [3] was performed. In this work, the weight dependence is not assumed to be separable. Algorithms have been developed and implemented to compute the explicit weight changes and their effect on the cost function with a locally developed S_n code.

METHOD

A one-dimensional, S_n, diamond-differencing code was written to explicitly solve for the population variance of the history score distribution σ^2 by solving the first and second moment equations. The code also calculates the expected computer time for the Monte Carlo code to process a single history τ. This expected time per history computation is performed by allowing the source for the moment equations to be a global source of the individual times required for the Monte Carlo code to process major history events, e.g. collisions, surface crossings, weight windows, etc. MCNP [5] is used for the comparison, and the times required to process the individual events were obtained by profiling the code. Having computed both σ^2 and τ, the cost of Monte Carlo calculation can be estimated by their product.

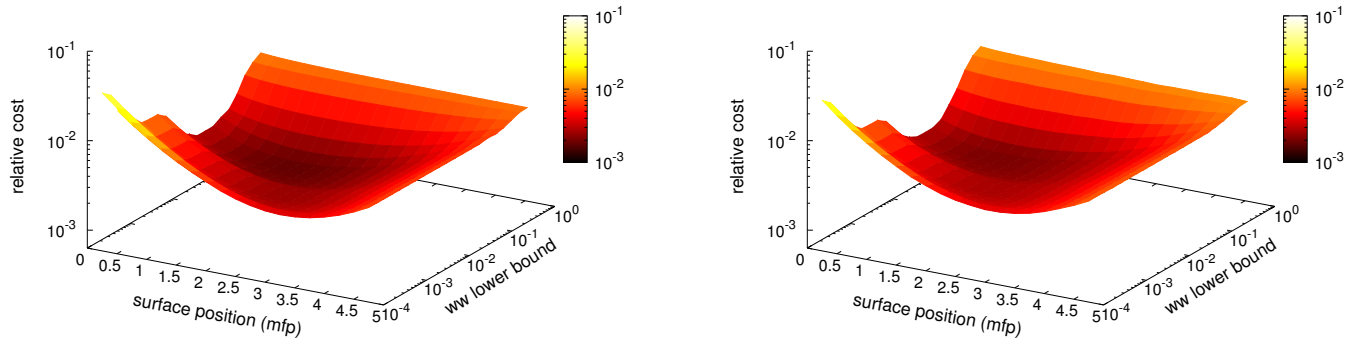

Fig. 1. Monte Carlo calculation cost as a function of surface location and weight-window lower bound in second cell as determined by (a) an S_n calculation and (b) a scaled MCNP calculation

RESULTS

Here two problems are investigated with the goal to determine parameters that minimize the cost of a Monte Carlo simulation of the problem with MCNP5 (RSICC version 1.51). In these problems, the weight window technique is used, and weight-windows are specified in the same manner as with MCNP. In all problems, isotropic scattering is assumed.

Investigating Weight-Window Boundary Location and Lower Bound

The method was used to evaluate the cost of an MCNP calculation with varying problem parameters. The problem geometry is a two-cell slab in which the two cells of the slab are separated by a single surface. The source is assumed to be isotropically incident on the left side of the slab, and the tally is a surface current tally on the right surface of the slab 5 mean-free-paths (mfp) from the source. The position of the surface separating the two cells is varied from 0.25 to 4.75 mfp in increments of 0.25 mfp. The weight-window lower bound of the left cell (nearest the source) is fixed at 0.5, while the weight-window lower bound of the right cell (nearest the tally) is logarithmically varied from 10^{-4} to 0.5.

A comparison of the cost functions calculated with the S_n method and MCNP is presented in Fig. 1 for a one-group problem with $\Sigma_s/\Sigma = 0.25$. Similar results have been obtained for scattering ratios up to 0.85. The cost calculated is proportional to the inverse of the figure of merit, and therefore Fig. 1(b) is normalized to our S_n cost function.

It is clear from a comparison of Fig. 1(a) and Fig. 1(b) that all the major features of the surface are present in the S_n calculation. Differences in these values are due to the estimation of τ not σ^2, as our studies have shown that the code precisely calculates σ^2. The minimum cost occurs when the separating surface is at 1.75 mfp and the right cell's weight-window lower bound is approximately 0.025. The optimum surface location differs from that presented by [3] where it was found that the optimum is at 3 mfp for a factor of 2 splitting. The difference between importance splitting/rouletting and weight windows as well as the splitting magnitude were eliminated as potential reasons for the difference. Because this method requires accurate reflection of the Monte Carlo code's variance reduction routines in the S_n code, the discrepancy is most likely a result of using different Monte Carlo codes for comparison. Here MCNP is used, whereas in [3] MCSI, a special purpose code, was used.

Optimizing an Iron-Window-Like Problem

A second two-group slab problem was also investigated. This problem is designed to represent transport in a material with a substantial antiresonance region where a specific energy group has a cross section orders of magnitude lower than those around it, similar to the iron antiresonance. Because particles within the antiresonance region are likely to stream much farther than particles outside the antiresonance, they can, in general, contribute higher scores and thus have a larger importance. If a particle enters the antiresonance region an importance-based split will produce many particles which a Monte Carlo code now has to track. The split particles require more time to process, but do not typically reduce the variance commensurately. Table 1 gives the cross sections for this problem.

The 5 cm slab was divided into four cells, each having its own weight window for each energy group. Current is tallied on the right plane of the slab, and the source, all within $g = 1$, is isotropically incident on the left plane. Let

Table 1. two-group cross sections representing an antiresonance (all units in cm^{-1})

g	Σ	Σ_c
1	1	0.9
2	1×10^{-5}	7×10^{-6}

$\Sigma_{gg'}$	1'	2'
1	0.05	0.05
2	0	3×10^{-6}

$I_g(x)$ represent the importance/adjoint function for group g. Then, the average importance in cell c is defined as $I_{gc} = \int_{x \in c} dx\ I_g(x) \Big/ \int_{x \in c} dx$. This quantity is then normalized so that the importance in the source cell c_s is unity, and the scaled importances $\overline{I}_{gc}$ are $\overline{I}_{gc} = I_{gc}/I_{gc_s}$. Finally, the weight-window lower bound w_{gc} for a cell is assumed to be inversely proportional to the average importance in the cell, namely $w_{gc} = k/\overline{I}_{gc}$. In this work, $k = 0.5$ to ensure particles are born into the adjoint generated biasing function. The problem is optimized by creating a new set of weight-window lower bounds w'_{gc} such that $w'_{gc} = A_g w_{gc}$, where A_g is a constant scalar multiplier to be determined by minimizing the calculation cost.

When A_1 = A_2 = 1, the calculation is the same as using the importance as the biasing function. A gradient descent algorithm was employed to determine the multipliers that minimize the function, and they are found to be $A_1 = 0.0375$ and $A_2 = 2.78$. With these A values, a predicted cost reduction by a factor of approximately 2.8 is predicted with respect to the adjoint biasing function.

Three MCNP calculations were performed to compare efficiency results for weight-windows obtained using MCNP's weight-window generator, the adjoint function to construct weight windows, and this cost-minimization method. The figures of merit are presented in Table 2, and the weight-window lower bounds used to obtain these FOMs are given in Table 3. The cost-minimization method produces a figure of merit over twice that of the other methods, though not an efficiency increase of 2.8 as predicted. As the variances of the calculations are computed within 5%, the deviation of the predicted gain from the realized gain must be the result of inadequate estimation of the computation time and a better estimate may be needed.

Table 2. efficiency comparison for three different methods of obtaining a weight window set

Method	FOM
MCNP WW Generator	274858
Adjoint	360349
Cost Minimization	732740

CONCLUSIONS

A method has been developed to predict and minimize the cost of a Monte Carlo calculation using a modified S_n method. The S_n calculations determine the cost by solving the moment equations up to the second moment to calculate both the population variance of the history score distribution and an estimate of the computer time required by the Monte Carlo code to obtain that variance. This implementation surpasses similar previous works by including Monte Carlo particle weight as a parameter of the moments and, thereby, allows its use in weight-dependent variance reduction analysis. The results presented show the applicability of this method to optimizing weight-window lower bounds and surface locations between weight-window regions to minimize calculation cost. Differences between the predicted and realized cost gains are a result of the estimates of the Monte Carlo calculation time. No difficulties are expected in extending this method to higher spatial dimensions, and higher dimension problems problems currently under investigation.

Table 3. weight-window lower bounds obtained from different generation methods (g represents the energy group number and c represents the cell number from left to right in the slab)

g \ c	1	2	3	4
MCNP weight-window generator[a]				
1	5.00000E-01	1.87180E-01	9.01845E-02	2.71272E-02
2	8.09417E-03	7.48382E-03	6.87346E-03	6.76491E-03
adjoint-generated weight windows				
1	5.00000E-01	3.70176E-01	2.19845E-01	5.83799E-02
2	2.29280E-02	2.29267E-02	2.29255E-02	2.29243E-02
cost-minimized weight windows				
1	1.87517E-02	1.38828E-02	8.24491E-03	2.18944E-03
2	6.38584E-02	6.38548E-02	6.38514E-02	6.38481E-02

[a]MCNP weight windows were renormalized so particles were in the window when born

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