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Title: **An Enhanced Geometry-Independent Mesh Weight Window Generator for MCNP**

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Abstract

A new, enhanced, weight window generator suite has been developed for MCNP^{TM}. The new generator correctly estimates importances in either an user-specified, geometry-independent orthogonal grid or in MCNP geometric cells. The geometry-independent option alleviates the need to subdivide the MCNP cell geometry for variance reduction purposes. In addition, the new suite corrects several pathologies in the existing MCNP weight window generator. To verify the correctness of the new implementation, comparisons are performed with the analytical solution for the cell importance. Using the new generator, differences between Monte Carlo generated and analytical importances are less than 0.1%. Also, assumptions implicit in the original MCNP generator are shown to be poor in problems with high scattering media. The new generator is fully compatible with MCNP's AVATAR^{TM} automatic variance reduction method. The new generator applications, together with AVATAR, gives MCNP an enhanced suite of variance reduction methods. The flexibility and efficacy of this suite is demonstrated in a neutron porosity tool well-logging problem.

1 INTRODUCTION

The efficiency of variance reduction schemes in Monte Carlo codes is highly dependent on user insight and experience. The process may be simplified by incorporating deterministic adjoint solutions as importance functions for preferential sampling along specific transport paths. This type of automatic variance reduction is available in several codes.[1-4] The automatic variance reduction scheme in MCNP, AVATAR, uses an adjoint deterministic solution from THREEDANT^{TM}[5] to generate weight windows on a geometry-independent grid.[6,7] We have enhanced AVATAR by developing a weight window generator that estimates the importances on an user-defined, geometry-independent grid[8] utilizing the forward-adjoint method.[9] The new generator may be used to iterate the adjoint map from THREEDANT, or it may be used independently of any deterministic calculation. Also, as opposed to the existing MCNP generator, the new generator is completely automated allowing for easy batch runs of iterated problems.

In addition to providing the geometry-independent functionality, the new generator also correctly implements the forward-adjoint algorithm as originally postulated by Booth and Hendricks.[9] The present version of the MCNP cell-based generator contains implicit assumptions that were necessary for memory management issues. In many cases these assumptions are robust; however, in problems with multiple particles, high secondary particle yields, and highly scattering media the estimated weight windows will not be optimal. The new generator fixes these assumptions and provides correct estimations of the importance.

In this paper we will demonstrate the accuracy, efficiency, and functionality of the new generator. First we will derive the analytical solution for the forward importance in slab geometry. These analytical solutions will be compared to the old and new generator estimates of the importance. After validating the correctness of the new generator, we will demonstrate its effectiveness and flexibility in a neutron porosity tool well-logging problem. These calculations will illustrate the capabilities of the new variance reduction suite in MCNP.

2 VERIFICATION OF THE FORWARD-ADJOINT METHOD

2.1 CALCULATION OF THE IMPORTANCE FUNCTION

Booth[10] has prescribed the analytical importance functions in slab geometry. Consider an 1-D slab with dimensions $0 \leq x < T$. The importance function is cast as a set of coupled differential equations featuring the importance of particles moving in the positive x direction and the negative x direction. We define these importances as the forward importance, $N(x)$, and the backward importance, $L(x)$.

Accordingly, the equations governing these terms are

$$\frac{dN}{dx} = (\sigma - \sigma_s f)N(x) - \sigma_s r L(x), \tag{1}$$

$$\frac{dL}{dx} = -(\sigma - \sigma_s f)L(x) + \sigma_s r N(x), \tag{2}$$

where f is the forward scattering probability and r is the backwards scattering probability. The total cross section, σ, has an absorption and scattering component,

$$\sigma = \sigma_a + \sigma_s. \tag{3}$$

Defining $\gamma = \sigma - \sigma_s f$ and taking the Laplace transform of Eqs. (1) and (2) gives the following general solutions for the forward and backwards importances,

$$N(x) = Ae^{-gx} + Be^{gx}, \tag{4}$$

$$L(x) = Ce^{-gx} + De^{gx}, \tag{5}$$

where $g = \sqrt{\gamma^2 - (\sigma_s r)^2}$. The importance functions satisfy the boundary conditions

$$N(T) = 1, \tag{6}$$

$$L(0) = 0. \tag{7}$$

Substituting the solutions for $N(x)$ and $L(x)$ into Eqs. (1) and (2) and applying the boundary conditions, one solves for the constants A, B, C, and D,

$$A = \frac{-(-g+\gamma)}{-(-g+\gamma)e^{-gT} + (g+\gamma)e^{gT}}, \tag{8}$$

$$B = \frac{(g+\gamma)}{-(-g+\gamma)e^{-gT} + (g+\gamma)e^{gT}}, \tag{9}$$

$$C = \frac{(\gamma+g)A}{\sigma_s r}, \tag{10}$$

$$D = \frac{(\gamma-g)B}{\sigma_s r}. \tag{11}$$

The weight window generator estimates the forward importance that is expressed analytically be Eqs. (4), (8), and (9).

The forward-adjoint importance is estimated by the weight window generator[9] using

$$I_i = \frac{S_i}{W_i}, \tag{12}$$

where I_i is the estimated importance in phase space cell i, S_i is the total scored weight of particles entering i, and W_i is the total weight of particles entering i. The importance in each cell is a function of the dependent variables of the phase space,

$$I_i \equiv I(p_i, \mathbf{r}_i, E_i, t_i, \hat{\Omega}_i). \tag{13}$$

In the above p is particle type, $\mathbf{r}$ is position, E is energy, t is time, and $\hat{\Omega}$ is angle. The phase space may be broken down into as many dependent variables as desired. However, the new generator only considers particle type, position, and energy.

From these definitions one can think of I_i as an estimate of the expected score from particles entering cell i. Thus, each track can only contribute to a phase space cell once upon entering that cell. When a track reenters a region of phase space it is not contributing to the expected score. Likewise, particles only contribute to the accumulation of S_i by entering a cell before scoring. Particles that enter a cell after tallying through a region will not contribute a score to the importance estimator.

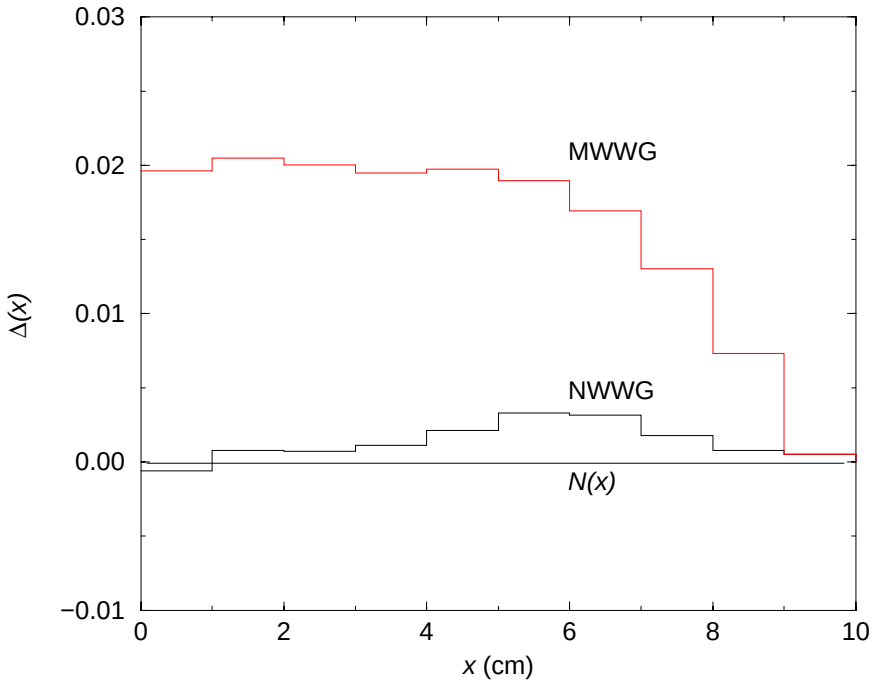

Fig 1. Fractional difference between the estimated importance, Eq. (12), and the analytical importance, Eq. (4), for $c = 0.1$ and $\sigma = 0.2$ /cm. NWWG and MWWG refer to the new and existing MCNP weight window generators.

2.2 COMPARISON WITH ANALYTICAL SOLUTIONS

Equation (12) is evaluated by tallying all particles entering a phase space cell. The subtle point is that each particle may only contribute to a cell once per history. The present geometry-dependent weight window generator in MCNP and the geometry-independent mesh generator developed by Liu and Gardner[11] rely on the assumption that particles reentering a phase space cell do not significantly bias the estimated importance. The new AVATAR weight window generator properly scores particles that reenter phase space cells; no weight is contributed to the importance tally.

The effect of the different scoring algorithms is illustrated by the 1-D slab problem. Consider a slab with dimensions $0 \leq x < 10$. Source particles are born on the $x = 0$ surface in the $(1, 0, 0)$ direction. The importances are optimized for a current tally crossing the $x = 10$ surface. The slab is divided into 10 MCNP cells that are coincident with 10 phase space cells defined by the geometry-independent mesh. The parameter c determines the collision survival probability,

$$c = \frac{\sigma_s}{\sigma}. \tag{14}$$

To insure that a significant number of particles score, the mean free path is set at 5 cm corresponding to $\sigma = 0.2$ /cm. Also, the forwards and backwards scattering ratios are equal, $f = r = 0.5$.

Figure 1 shows the fractional differences between the estimated importances and the analytical importance for $c = 0.1$. The fractional differences for $c = 0.9$ are illustrated in Figure 2. The comparisons show that the assumptions in the MCNP weight window generator cause deviations from the predicted value of up to 20% for highly scattering media. The reason the importance estimates are poorer near the source is backscattering. Cells far away from the source will experience few events from reentering backscattered particles. In real problems this effect will be particularly severe in thick shields with high

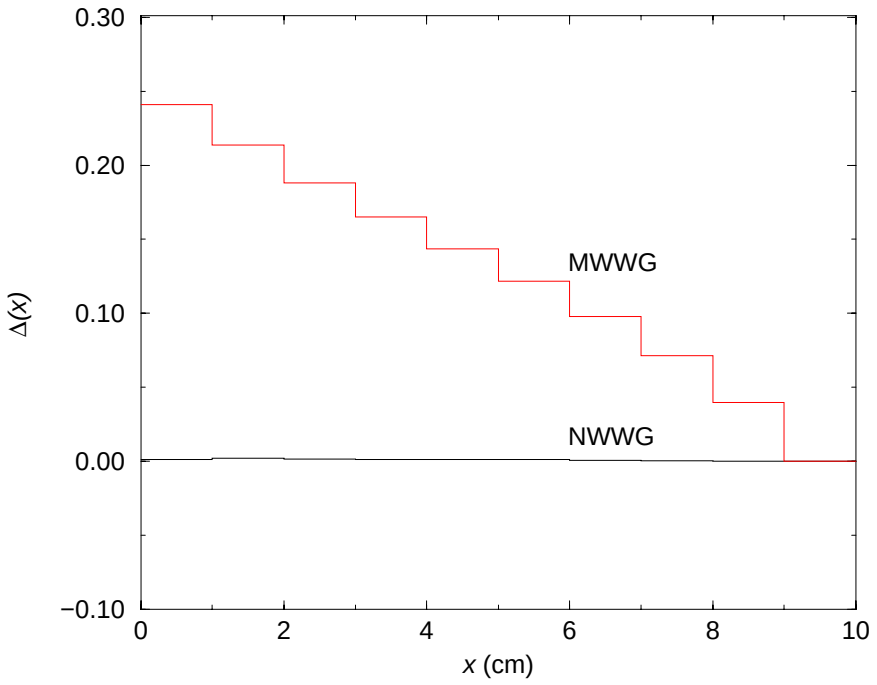

Fig 2. Fractional difference between the estimated importance, Eq. (12), and the analytical importance, Eq. (4), for $c = 0.9$ and $\sigma = 0.2$ /cm. NWWG and MWWG refer to the new and existing MCNP weight window generators.

Table 1. Different permutations of the neutron porosity tool problem. All variance reduction options use five neutron energy groups.

Problem	Description
ANA	The problem is run analog without variance reduction.
MWWG	The problem is divided into 231 MCNP geometric cells. Weight windows are calculated in each cell using the existing MCNP generator without the corrections described in Section 2.
GDWWG	The problem is divided into 231 MCNP geometric cells. Weight windows are calculated in each cell. This option uses the new implementation of the weight window generator with the corrections described in Section 2.
GIWWG	The problem is divided into 8 MCNP cells. A geometry-independent grid with dimensions $27 \times 26 \times 25$ is used to calculate weight windows.
AVATAR	The problem is divided into 8 MCNP cells. A $24 \times 28 \times 28$ cell importance map generated by THREEDANT is used by AVATAR for weight windows.
AVRWWG	The AVATAR map produced above is iterated using the geometry-independent weight window generator on a $27 \times 26 \times 25$ dimension grid.

Table 2. Results of the neutron porosity tool well logging problem. Number of iterations refers to the number of runs required to converge the importance map. The FOMs are for problems utilizing a converged set of weight windows.

Problem	Iterations	FOM
ANA	n/a	1.0
MWWG	3	108
GDWWG	3	119
GIWWG	3	105
AVATAR	n/a	79
AVRWWG	1	108

scattering cross sections. In summary, the pathologies in the existing MCNP weight window generator yield erroneous estimates of the cell importance. The effect is particularly severe in regions with high scattering ratios. The new implementation of the forward-adjoint method corrects these shortcomings and yields results that are in excellent agreement with theory.

3 WELL-LOGGING PROBLEM

The efficacy of the improved weight window applications is demonstrated using the neutron porosity tool problem, MCNP4B test set problem 12. To illustrate the robustness and functionality of the new variance reduction suite the problem is run in six permutations as described in Table 1. The results of the calculations are presented in Table 2. The efficiency of each method is analyzed using the Figure of Merit (FOM),

$$FOM = \frac{1}{\sigma^2 T}, \tag{15}$$

Table 3. Timing study of the various weight window routines for the neutron porosity problem. External refers to deterministic code (THREEDANT) runtimes. All iterations are run with 500,000 histories. All problems are run on an IBM-AIX cluster.

	External	Iteration 1	Iteration 2	Iteration 3	Total time
Problem	(min)		(seconds/particle)		(min)
MWWG	0	9.56×10^{-3}	1.27×10^{-2}	8.83×10^{-3}	259.08
GDWWG	0	1.01×10^{-2}	9.96×10^{-3}	8.66×10^{-3}	239.33
GIWWG	0	1.05×10^{-2}	2.18×10^{-2}	1.27×10^{-2}	375.05
AVATAR	5.32	0	0	0	5.32
AVRWWG	5.32	1.59×10^{-2}	0	0	137.68

where σ is the standard deviation and T is the computer time required to get the solution. The results in Table 2 show that each method considerably improves the problem efficiency.

To determine the most effective method we must consider the problem preparation and runtimes. In particular, AVATAR requires setup of the deterministic problem in addition to the MCNP input, and the forward-adjoint methods methods require iterations to converge the importance map. Table 3 looks at the computer time required to generate a converged importance map. This data shows that the weight window generator methods require considerable time to prepare an optimized importance map. Also, the cell tracking routines required by the geometry-independent generator results in an overhead of 40–50%. The problems that utilize AVATAR are the most efficient choices.

On the other hand, the geometry-independent option has the easiest user interface and the quickest problem setup. The geometry-dependent generator and AVATAR may require considerable problem preparation time. To effectively use a geometry-dependent weight window the problem cells must be small enough to avoid large fluctuations of the importance across the cell. To achieve this condition the user must subdivide the MCNP geometry into many cells. The geometry-independent generator avoids this difficulty. AVATAR also involves additional problem preparation because of the deterministic problem setup. The forward-adjoint methods have an advantage because they are fully available in a single code. In summary, a balance must be maintained between problem execution and problem setup. The advantage of the new suite of weight window applications is that the user has tremendous flexibility in achieving this balance based on the problem specifications.

4 CONCLUSIONS

We have developed a new, enhanced suite of variance reduction applications for MCNP. These methods all utilize the MCNP forward-adjoint and weight window methods. The pathologies in the original MCNP weight window generator have been corrected. The new implementation has been verified by comparisons with the analytical solution for the cell importance. These comparison calculations show that the new forward-adjoint implementation effectively estimates the importance function.

Because of the inherent robustness of weight window methods, the applications described in this paper require little user adjustments. In addition, this suite provides tremendous flexibility and functionality for approaching a wide variety of problems. The combination of AVATAR with the geometry-independent weight window generator allows one to perform very efficient variance reduction with a minimum of user overhead or experience. While not as efficient, the forward-adjoint methods have the advantage that they are available in a single code. Furthermore, the new implementation of the weight window generator is easily automated for iteration runs and requires little user-preparation time. In summary, this suite of applications is designed to provide the user with expanded options for challenging transport problems.

5 ACKNOWLEDGMENTS

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