Monte Carlo Variance Reduction Using Finite Element Adjoint Weight Windows

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Abstract

The use of Monte Carlo variance reduction techniques is unavoidable on present day computers in obtaining numerical solutions in complex shielding, deep penetration or other radiation transport problems such as nuclear well logging and ex-core reactor core modeling etc. A deterministic variance reduction technique based on the finite element adjoint weight window (FEAWW) scheme is developed and applied in the well-known and widely used Monte Carlo radiation transport code MCNP. The scheme involves generating importance maps from the adjoint deterministic EVENT transport calculations which are then extracted and used as 'weight window lower bounds' suitable for acceleration of the forward Monte Carlo radiation transport calculations. The 'holy grail' of an automatic variance reduction technique is to provide a single method which provides systematic or nearly systematic ways to eliminate much of the user's intervention. The proposed method employs the adjoint solutions to the problem of interest which has been folded into the MCNP weight window scheme. The FEAWW method is tested on a number of complex deep penetration and neutron streaming problems and compared against the standard Monte Carlo generated variance reduction techniques with encouraging results.

KEYWORDS: Variance Reduction, MCNP4C, Finite Element Adjoint Deterministic Solutions, EVENT

1. Introduction

Although Monte Carlo (MC) method is capable of solving neutron transport problems almost in any geometry in three-dimensional complex shielding problems [1], [2] it requires reasonably accurate and robust variance reduction (VR) techniques to be employed. The use of VR is very important to obtain solutions in acceptable time (CPU) particularly in deep penetration and streaming problems. In theory (or ideally), one has to solve the adjoint form of the transport equation to obtain the corresponding adjoint flux distribution for a given problem. But numerical solutions of the adjoint transport equation are equally lengthy and time consuming using MC methods. The users of MC codes have to then wait until a solution of the adjoint equation is obtained to be able to solve the

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actual (or forward) problem. For this reason, various approximate techniques have been developed in industry and academia to find the answers to this problem.

One such VR method has been developed in this work using the finite element transport code EVENT [3] and linked to the MC code MCNP4C [4]. The method is referred to Finite Element Adjoint Weight Windows (FEAWW). The basic underlying theory behind the new scheme was also developed [5]. In this scheme the parameters used to accelerate MC simulations are produced deterministically without to much demand on the computational CPU time. These parameters are adjoint fluxes or 'importances' which are related to neutron weights [6] and therefore can be used for biasing purposes. The MC methods can be also used to generate importances in MCNP via its weight window generator [7]. Historically, statistical fluctuations are often appeared with the weights which can suppress performance of the MC techniques. A second series of runs maybe needed to be performed in order to optimize these weights. In this respect it maybe necessary for the user to manually adjust the weights so that the number of iterations is minimized. However, this is not straight forward for the complex multi-dimensional shielding problems. In practice, at least two and/or more iterations are always required in order to smooth out the set of importances before they can be used as optimum weights to accelerate the forward MC calculation. This process can become very expensive when all the iterations times (CPU time plus user expertise) are taken into account. Consequently the performance of the technique is dramatically reduced if the MC method is used as a stand alone technique. In this paper a new technique is proposed which combines the advantages of both the deterministic and MC methods in solving shielding problems in complex geometries. Various test problems involving deep penetration and streaming of neutrons were solved to show that the method is efficient and robust.

2. The Finite Element Adjoint Weight Window (FEAWW)

The acceleration of MC solution obtained from MCNP is achieved by solving the neutron adjoint problem using the finite element neutron transport code EVENT. The latter code is based on the solution of second order even parity transport equation using the finite elements in space and spherical harmonics in angle to represent the directional flux [3]. The energy dependence was treated in one-group to test the technique. The first step in FEAWW is to solve the adjoint transport equation using a suitable mesh with the EVENT code. Secondly, the importances (inverse of the adjoint solution) are converted to the weight windows scheme in MCNP. The finite element mesh is also converted into cell-based splitting mesh in MCNP so that the importance data can be generated automatically. The importances generated are intended of course to increase efficiency of simulated particles, which is judged by the FOM (Figure of Merit is defined as $\sigma^{-2}\ t^{-1}$ here 'σ' is the relative error for the sample mean and 't' is the total time spend to track 'n' particles').

The efficiency of the newly developed FEAWW scheme is tested on a series of test problems, which is compared against pure MC generated adjoint function referred as PMCWW (see Table 1) available in MCNP. In this paper, the performance of FEAWW was checked on a homogeneous and a neutron streaming 'dogleg duct' problem in rectangular geometry (X-Y geometry).

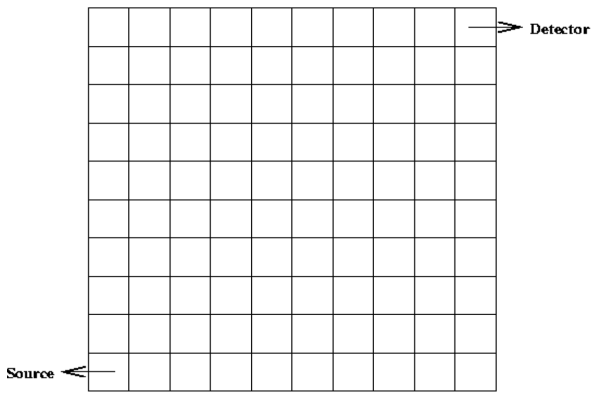
3. Test Problems

The test cases chosen to demonstrate the FEAWW scheme are based on two-dimensional homogeneous and heterogeneous problems. In the latter a dogleg duct streaming problem was solved.

3.1 Homogeneous Problem

The geometrical arrangement of this problem represents a two-dimensional (X-Y) rectangular geometry having a total area of 20 x 20 cm^2, which is uniformly divided into (10 x 10) MC cells. Each cell has a length and width of 2 cm which corresponds to 2 mean free path (mfp) (the total cross-section is modeled as 1.0 cm^{-1}). The number of regions was exactly the same for the deterministic calculations to obtain the region averaged adjoint scalar fluxes. The scattering cross section varied in the range 0.1 to 0.9 cm^{-1} to define a number of cases with different material properties. For example, the lower (0.1) and the higher (0.9) scattering ratio (Σ_s/Σ_t) represent a low and highly scattering mediums respectively. The neutron source is isotropic uniformly distributed and located in a square of area (2 x 2) cm^2 at the bottom left hand corner of the model (see Figure 1). The track length estimate of neutron flux detector was placed in a cell/region at the top right hand corner of the geometry. A 2-D configuration of the problem including source, detector positions and splitting cells for the MC model is shown in Figure 1. Bare surface (void) boundary conditions were applied outside the physical (modeled) geometry.

The transport calculations were carried out using the finite element deterministic code EVENT [3]. The code can provide spherical harmonics P_N neutron transport solutions to the problem for N=1, the P_1 (diffusion approximation) and for N>1 the higher order P_N approximations such as P_3, P_5, P_7 and P_9. EVENT can also provide simplified spherical harmonics approximation (SP_N) solutions which provide more accurate solutions than the diffusion approximation with less computational resource requirements. EVENT adjoint solutions were used to construct the weight windows to accelerate the forward MC calculations. Both the higher order spherical harmonics P_9 solution of EVENT and simplified P_N (SP_N) solutions are performed and the MCNP weight windows were constructed based on these adjoint solutions. In order to carry out 1- and 2-mfp calculations two different but uniform cell divisions were constructed in both MC and deterministic calculations. Cell divisions of (1 x 1) and (2 x 2) were used which resulted in a total of (20 x 20) and (10 x 10) cells for the problem domain. It is important to note that the variation of weight window parameters must not be too large between any two adjacent cells. Large variation of weights may occur when the distance to collision (mfp) sampling results in an unusually long particle path. Such sampling may lead to scoring by particles of abnormally large weight results an increase in the variation. To alleviate this problem, the weight window bounds are applied in MCNP at every mean free path along the particle's path.



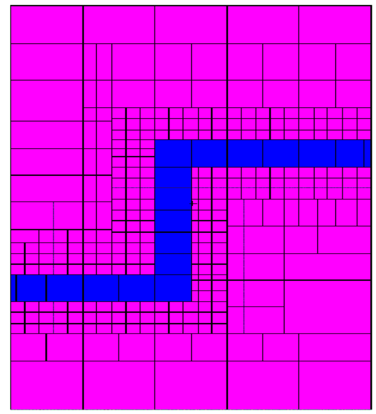


Figure 1: Schematic of a homogeneous problem showing the position of the source and the detector in rectangular geometry.

Figure 2: 2-D dogleg duct problem showing the splitting planes and/or regions of weight window generator used in MCNP.

The weight window parameter ‘wwp’ in MCNP forces the weights of the particles to remain within an upper and lower bounds of the weight window. If the weight associated with the particle becomes below the lower bound value the particle is then rouletted. If the weight exceeds the upper bound the particle is then split [4]. In MCNP, the extent of the window is constant i.e. the ratio of the upper weight bound and the survival weight (the weight which is increased after Russian roulette) to the lower weight bound are constant in all energy intervals and in all physical cells. The default values of these ratios are 5 and 3 respectively. The default weight control parameter (wwp 5 3 5) has been used in all calculations presented in this work. The wwp parameter has also been varied to look at the subsequent variation of the FOM. A further two parameters define the kind of weight window game played in MCNP: the input data defined in MXSPLN restricts the amount of splitting or Russian roulette allowed (no more than MXSPLN-to-1 splitting or no less than 1-in-MXSPLN RR, the weight value being 5); MWHERE defines where the weight window game is played – at collisions only, at surfaces only or at both collisions and surfaces. The default is at surface and upon exiting collisions.
In all MCNP calculations 10^6 particle histories are simulated using variance reduction techniques based on weight window generator and FEAWW scheme.

3.2 Heterogeneous Problem

This problem is a 2-D ‘dogleg duct’ modeled in rectangular geometry having a total area of (100 x 150) cm^2 and an air duct of two bends which runs through the bulk medium. This problem was studied with different material properties by varying the macroscopic scattering and absorption cross sections, Σ_s and Σ_a in a series of MCNP and EVENT calculations. The legs of the duct have equal length of 50 cm and a width of 10 cm. Figure 2 shows the geometrical arrangement and the cell divisions used in MCNP to model this problem. In Figure 6, the adjoint scalar flux distribution in the whole geometry is presented, when the source and the detector is located at the entrance and the end of the air duct.

The material properties used were also varied as in the homogenized problem; considering a range of scattering cross sections 0.1, 0.3, 0.5, 0.7 and 0.9 with the total macroscopic cross section being 1.0 cm^{-1} outside the duct. In the duct material total macroscopic cross section is assumed to be 0.01 cm^{-1} with the scattering cross section varying from 0.001 to 0.009. An isotropic source distributed over an area of length 2 cm and width 10 cm was placed at the duct opening. A total neutron current tally was placed at the other end of the duct. Void boundary conditions are applied outside the geometry. The deterministic and MC models used the same geometric regions/cells. Cells are uniformly divided on both side of the duct in order to follow the streaming particles along the duct. The cells 50 cm away from the duct surface are considered to be non-contributing and are coarsely divided so that particles heading into this direction can be rouletted. This problem represents a difficult neutron streaming/penetration problem and therefore high order transport (P_9) approximation was used to generate the importances using the EVENT code. All MC calculations were carried out using 5 million particle histories except for the scattering ratio (Σ_s/Σ_t) 0.1. For this 8 million particle histories were required in order to reduce the overall error for FEAWW scheme to 5%. But using the PMCWW generator scheme required 15 million particles in order to achieve the same overall error.

Table 1: Results from different variance reduction schemes comparing FOMs from FEAWW and PMCWW techniques for the homogenous problem.

Σ_s/Σ_t	Acceleration Scheme Used	EVENT CPU time (sec)	MCNP CPU time (sec)	Error %	FOM (default)	FOM (optimum)
0.1	FEAWW (P9)	15.81	138.0	3.2	383	404
	FEAWW (SP9)	0.21	122.5	3.5	355	399
	PMCWW	-	284.4	3.8	145	-
0.3	FEAWW (P9)	16.25	166.0	2.0	792	879
	FEAWW (SP9)	0.23	212.0	1.9	775	809
	PMCWW	-	212.0	2.0	688	-
0.5	FEAWW (P9)	15.97	248.0	1.1	1763	1818
	FEAWW (SP9)	0.23	337.0	1.0	1773	1786
	PMCWW	-	248.0	1.2	1695	-
0.7	FEAWW (P9)	15.72	529	0.61	3042	3079
	FEAWW (SP9)	0.24	599	0.63	3017	3018
	PMCWW	-	600	0.61	2678	-
0.9	FEAWW (P9)	15.92	759	0.44	3698	4028
	FEAWW (SP9)	0.25	797	0.44	3974	3974
	PMCWW	-	981	0.41	3599	-

4. Results

The FOMs obtained from applying the FEAWW to the homogeneous and dogleg duct problems are presented in Tables 1 to 4 and in Figures 3 to 5. The FOM obtained for the optimum set of weights in both schemes are presented in Table 1. The first column of the table shows the scattering ratio, the second column indicates the particular VR scheme used. The third and fourth column present the CPU time in seconds required to perform the EVENT and MCNP calculations. The relative errors achieved in the MC calculations are converted into percentages, shown in the fifth column (all these results lay within one standard deviation of the Monte Carlo statistics). In the same table sixth and seventh column indicate the FOM obtained with a default set of parameters (wwp 5 3 5) and with varying the weight window parameter 'wwp'. In Table 2, the 'corrected' FOMs are presented taking the relative error at the final run and combining all iteration times. This correction is important since at least two calculational steps are involved in both the schemes. Specifically in the PMCWW technique the weights are updated iteratively in order to produce an optimum FOM. This would enable us to make a fair comparison of performance of the techniques.

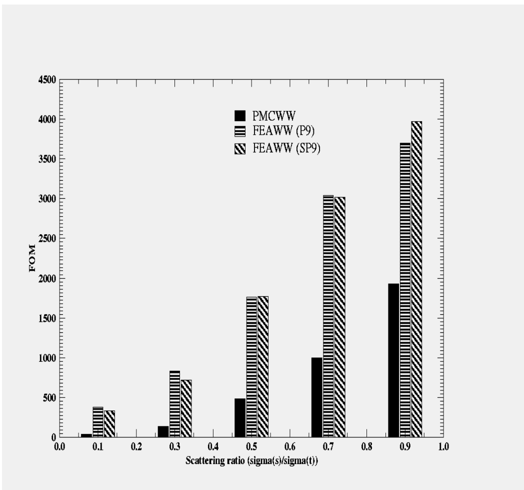


Figure 3: Comparison of FOM obtained from PMCWW and FEAWW VR schemes

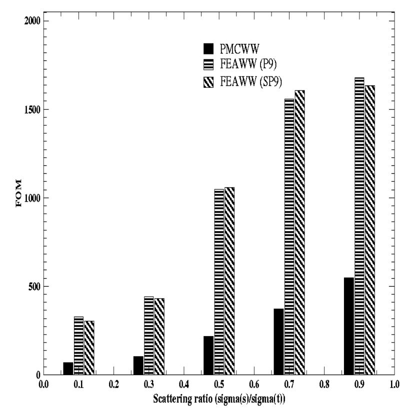


Figure 4: Comparison of FOM obtained from PMCWW and FEAWW VR schemes

Figure 3 shows the results of the FOM obtained for the 1mfp calculations. The scheme FEAWW performs well in all scattering scenarios against the PMCWW. The performance of the new scheme gradually increased toward the lower scattering (high absorption) medium where the MC method suffers mostly from losing efficiency. This is because particle attenuation occurs or the flux changes significantly as the particles travel through the high absorption medium and results in variations in the particle weights. In this situation automatic variance reduction techniques can help by reducing the variation in the particle weights (for example by increasing the number of particles). In other words more biasing is needed to push particles through the medium to score at the detector. This is demonstrated by the results for the FEAWW scheme presented in the tables. Conversely for highly scattering media the variation of particle weights is not as much as in the case of highly absorption media. The reason for this is that each collision reduces particle weight only slightly leading to a smooth variation in particle weights.

These results of the FEAWW scheme indicate the improved performance (in terms of efficiency) of the FEAWW scheme compared to the PMCWW scheme for the 2-D homogeneous problem investigated here. The overall benefit (in terms of the ratio of the FOMs) means that the FEAWW scheme is 2 to 9 times more efficient than the PMCWW scheme (these results are presented in Table 2 and Figure 3) for this problem. The higher FOM for the FEAWW scheme indicates the improved performance of the scheme over the PMCWW scheme. For example, increasing the FOM by a factor of 2 means that the same statistical accuracy is achieved in one-half the CPU time, or the statistical errors reduced by the square root of 2 in the same amount of CPU time.

Table 2: Results from the variance reduction schemes studied comparing FOMs from FEAWW and MCWW techniques for 1mfp calculations for the homogeneous problem.

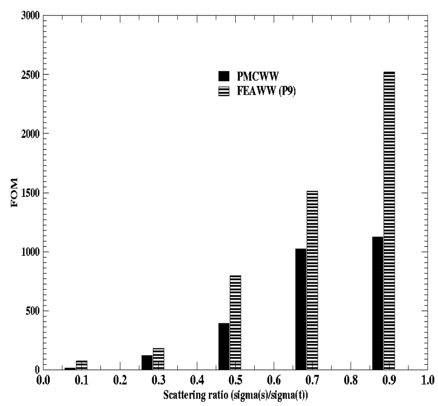
Σ_s / Σ_t	Acceleration Scheme Used	EVENT CPU time (sec)	MCNP CPU time (sec)	Total CPU time (sec)	Error %	FOM
0.1	FEAWW (P9)	15.81	138.0	153.81	3.2	380
	FEAWW (SP9)	0.21	122.5	122.71	3.5	398
	PMCWW	-	1000.0	1000.0	3.8	41
0.3	FEAWW (P9)	16.25	166.0	182.25	2.0	832
	FEAWW (SP9)	0.23	212.0	212.23	1.9	718
	PMCWW	-	1095.0	1095.0	2.0	133
0.5	FEAWW (P9)	15.97	248.0	263.97	1.1	1763
	FEAWW (SP9)	0.23	337.0	337.23	1.0	1773
	PMCWW	-	878.0	878.0	1.2	482
0.7	FEAWW (P9)	15.72	529.0	544.72	0.61	3042
	FEAWW (SP9)	0.24	599.0	599.24	0.63	3017
	PMCWW	-	1615.0	1615.0	0.61	998
0.9	FEAWW (P9)	15.92	759.0	774.92	0.44	3698
	FEAWW (SP9)	0.25	797.0	797.25	0.44	3974
	PMCWW	-	1852.0	1852.0	0.41	1927

Table 3: Results from the variance reduction schemes studied comparing FOMs from FEAWW and PMCWW techniques for 2mfp calculations for the homogenous problem.

Σ_s / Σ_t	Acceleration Scheme Used	EVENT CPU time (sec)	MCNP CPU time (sec)	Error %	FOM
0.1	FEAWW (P9)	15.24	111.6	3.9	327
	FEAWW (SP9)	0.19	120.6	4.0	305
	PMCWW	-	368.0	4.9	68
0.3	FEAWW (P9)	15.75	281.4	2.16	442
	FEAWW (SP9)	0.25	340.2	2.02	430
	PMCWW	-	505.8	3.37	104
0.5	FEAWW (P9)	16.17	541.2	1.02	1047
	FEAWW (SP9)	0.23	654.0	0.93	1058
	PMCWW	-	778.8	1.88	218
0.7	FEAWW (P9)	16.29	1097.4	0.59	1557
	FEAWW (SP9)	0.24	1111.8	0.58	1604
	PMCWW	-	2213.8	1.15	373
0.9	FEAWW (P9)	15.93	2117.4	0.41	1678
	FEAWW (SP9)	0.25	2184.0	0.41	1633
	PMCWW	-	4107.2	0.72	549

Note that the analyst time to produce the full input data in both EVENT and MCNP codes are not included in all results presented in this manuscript.

In Figure 4, 2mfp calculations are performed to check the sensitivity of the new scheme against the PMCWW. The FOM of both the techniques are reduced as it was expected but the new scheme performs consistently better compared to the PMCWW which is promising. The results are also shown in Table 3.



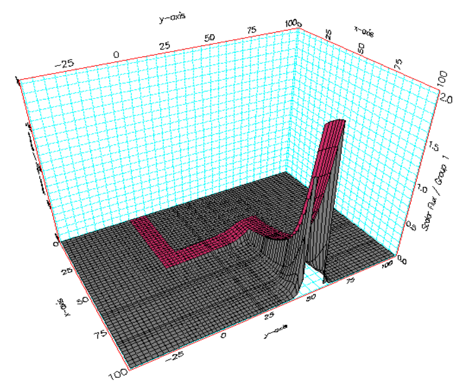


Figure 5: Comparison of FOMs obtained From PMCWW and FEAWW schemes

Figure 6: The adjoint function generated using FEAWW for the dogleg duct problem

In Table 4 the results of FOM are presented for the dogleg duct problem in which both neutron streaming and scattering take place. The results are also shown in Figure 5. The FOM obtained from the FEAWW are very encouraging in this problem. High performance is achieved at the low scattering medium which was similar to the homogeneous problem. It can be seen that FOMs have been improved compared to the PMCWW scheme.

Table 4: Results from the variance reduction schemes studied comparing FOMs from FEAWW and PMCWW techniques for the dogleg duct (heterogeneous) problem.

Σ_s / Σ_t	Acceleration Scheme Used	EVENT CPU time (sec)	MCNP CPU time (sec)	Total CPU time (sec)	Error %	FOM
0.1	FEAWW (P9) PMCWW	139.2 -	163.8 918.0	303.0 918.0	5.13 6.50	75 15
0.3	FEAWW (P9) PMCWW	135.0 -	91.2 339.6	226.2 339.6	3.84 3.83	180 120
0.5	FEAWW (P9) PMCWW	135.6 -	171.0 878.0	306.0 878.0	1.57 1.91	794 393
0.7	FEAWW (P9) PMCWW	139.2 -	214.2 531.0	353.4 531.0	1.06 1.05	1511 1024
0.9	FEAWW (P9) PMCWW	145.8 -	325.8 1027.8	471.6 1027.8	0.71 0.72	2523 1126

5. Discussion and Conclusions

A new VR scheme, FEAWW, has been developed to accelerate MCNP which is based on high order finite element/spherical harmonics transport solutions using the EVENT code. The scheme was tested in two-dimensional one-group benchmark problems. The effectiveness of the FEAWW is compared against the PMCWW technique with satisfactory results. A good performance has been achieved especially for low scattering media (high absorption) for which most MC based acceleration techniques suffer [8]. The performance of the FEAWW scheme was demonstrated for 1mfp and 2mfp homogeneous geometry calculations the latter scheme showing an improved performance compared to the former which is promising. The performance of the scheme was also tested on a 2-D dogleg streaming heterogeneous geometry problem and the FOMs achieved using the FEAWW technique were higher than those obtained using the PMCWW technique. This demonstrates the potential advantages of the deterministic based weight window over the MC based techniques. More information of the finite element method used can be found in [9] and some industrial applications of modeling streaming problems studied previously is given in reference [10].

It is important to point out the fact that 'data preparation' was necessary in order to format the results from the deterministic adjoint EVENT solutions to be used as an input in the MCNP calculations which is of course problem dependent. This can be viewed as a potential disadvantage which requires additional analyst's time. But the benefits of using this two-step approach cannot be disregarded. The VR scheme outlined here uses deterministic high order transport theory solutions in the general purpose MC transport theory code and is therefore applicable to wide range of radiation transport problems.

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