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SIMULATING SMALL CHANGES IN SYSTEM RESPONSE BY MCNP

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ABSTRACT

Correlated sampling and perturbation are two developed techniques that enable MCNP to simulate small changes in system response with an acceptable uncertainty at reasonable number of particle histories. In this work the performance of correlated sampling is investigated. It is found that under certain conditions using the default output format of MCNP5 and the original practice of batch statistics developed for correlated sampling may overestimate the uncertainty of the change in system response. The cause of the overestimation is analyzed; correspondingly two improved procedures are proposed for correlated sampling to ensure correct estimation of the uncertainty. In addition, the performance of improved correlated sampling method is also compared with that of the perturbation technique of MCNP5. In terms of precision of the change in system response, the perturbation technique is found to be capable of producing smaller uncertainty than correlated sampling when response change is small; as response change becomes larger, the uncertainty predicted by correlated sampling is comparable with or even better than that predicted by the perturbation technique. In terms of accuracy of the change in system response, however, it is found that the perturbation technique may produce less accurate results than correlated sampling for certain problems that involve intermediate or even small changes in system response. Overall, correlated sampling seems to be a more robust technique than the current perturbation technique of MCNP5 for simulating small changes in system response.

Key Words: Small change; System response; MCNP; Correlated sampling; Perturbation

1. INTRODUCTION

Problems often arise that require the use of MCNP to simulate a small change in a system response due to a variation in system parameters. The direct way to determine such small change in system response is to perform two calculations, one with the original data and another with the perturbed data, and then subtract between the two system responses. However, this direct computation approach often leads to a too large statistical uncertainty (or standard deviation) for the change in system response to be acceptable when the response difference is small. One can certainly reduce the uncertainty to an acceptable level by increasing the number of particle histories (NPS) in the MCNP simulations, which, however, is often computationally too expensive because the standard deviation reduces with NPS by $\sqrt{1/\mathrm{NPS}}$.

Over the last few decades, two improved techniques have been particularly developed for MCNP to estimate small changes in system response with an acceptable uncertainty at reasonable NPS. The first technique is called correlated sampling which allows tally difference to be estimated between two different runs by correlating their random number sequences, so it can enable the evaluation of small quantities that would otherwise be masked by the statistical errors in uncorrelated calculations. This method was originally suggested by Matthes [1] in 1960’s and was first implemented in MCNP for fixed source problems by Pregg [2] in late 1970’s. Though not being presented in MCNP Manual [3], T.E. Booth showed in 1980’s that the uncertainty of the difference between two correlated runs can be estimated by batch statistics [4]. However, very limited work has been published on the performance and applications of correlated sampling since then.

The other developed method applied in MCNP is the differential operator perturbation technique, by which the response change is defined as the first and second order terms of the Taylor series expansion around the initial, unperturbed problem parameters of interest. This formalism was first introduced by Olhoeft in the early 1960’s [5] and has been gradually evolved into a standard MCNP feature after constant enhancements in user interface and corrections for cross-section dependent tallies [6-8]. However, the perturbation operator used in the current version MCNP5 has certain limitations [3,9-10], thus it may not always predict accurate results for certain problems. Though there are some papers and technical reports that discussed applications of the MCNP perturbation technique, there are almost no publications in the open literature that ever compared this technique with the correlated sampling method.

In this paper the original procedure of doing batch statistics [4] to calculate the uncertainty for correlated sampling is investigated by using the current version of the code, MCNP5. It is found that the original practice may overestimate the uncertainty under certain circumstances. The cause of the overestimation is discussed and correspondingly two improved procedures are proposed for correlated sampling to ensure correct estimation of uncertainty. In addition, the perturbation technique is also compared to the improved correlated sampling method in terms of accuracy and precision of response change.

2. THE CORRELATED SAMPLING METHOD

The correlated sampling method is based upon the following theory. Assume that the response of the i^{th} sample for the original, unperturbed problem of interest is f_i (i = 1, 2, ..., n), the response mean of the problem is I_1, the variance of I_1 is σ_1^2, and the corresponding quantities for the perturbed problem are g_i, I_2, and σ_2^2, respectively, then the change in system response between the original and perturbed problems is

$$\Delta I = I_1 - I_2 = \frac{1}{n}\sum_{i=1}^{n}(f_i - g_i). \quad (1)$$

The variance of ΔI is given by

$$\sigma_{\Delta I}^2 = \frac{1}{n(n-1)}\sum_{i=1}^{n}[(f_i - g_i) - (I_1 - I_2)]^2 = \sigma_1^2 + \sigma_2^2 - 2\,\mathrm{cov}(I_1, I_2) \quad (2)$$

where $\text{cov}(I_1, I_2)$ is the covariance between the two processes, defined by

$$\text{cov}(I_1, I_2) = \frac{1}{n(n-1)} \sum_{i=1}^{n} (f_i - I_1)(g_i - I_2). \tag{3}$$

Note that when f_i and g_i are statistically independent, their covariance is zero and thus the variance of ΔI is reduced to

$$\sigma_{\Delta I}^2 = \sigma_1^2 + \sigma_2^2. \tag{4}$$

By default MCNP always insures positive correlation between I_1 and I_2 by providing the i^{th} particle history for both the original and perturbed problems with same pseudorandom number sequence; thus $\text{cov}(I_1, I_2)$ is positive and correspondingly $\sigma_{\Delta I}$ is reduced.

2.1. The Original Procedure of Error Estimate – Batch Statistics

To calculate the covariance by Eq. (3), one needs to know tally score of every particle history (or average tally score for a batch of particle histories) for both problems (i.e., f_i and g_i); however, such information is not given in the MCNP output files. The original approach of estimating the uncertainty for the difference between two correlated runs was provided by Booth [4], in which the tally fluctuation chart is used to do batch statistics by the following procedure: (a) Total particle histories are evenly divided into m batches and MCNP is controlled to output tally means at particle history numbers $N_i = i \cdot (NPS/m)$, with $i = 1, 2, \cdots, m$ and NPS/m being the batch size, i.e., the number of particle histories in a batch; (b) The output tally means are used to compute the average scores for each batch by

$$s_i = \frac{M_i \times N_i - M_{i-1} \times N_{i-1}}{N_i - N_{i-1}} \tag{5}$$

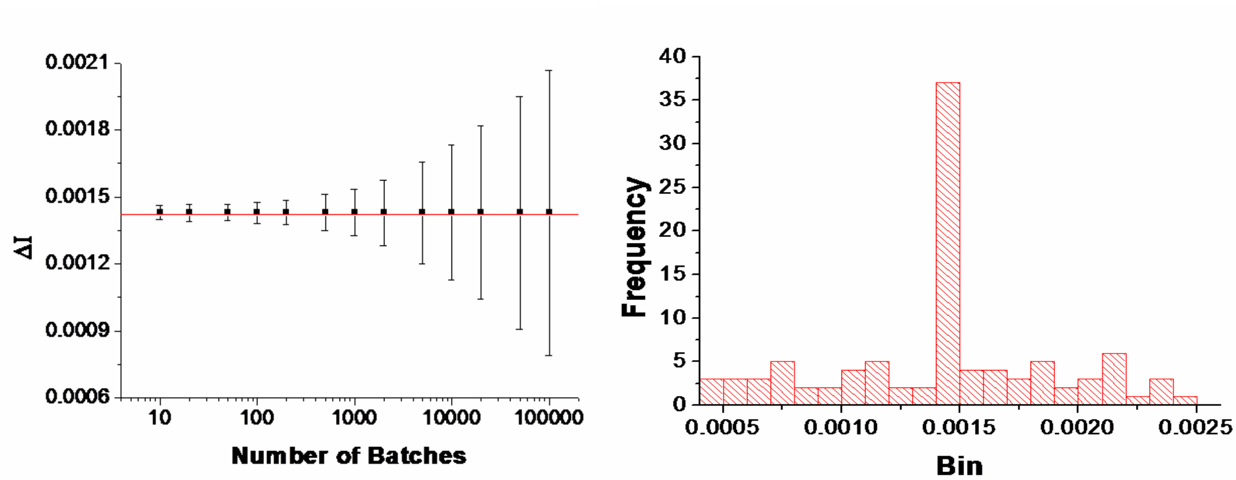
where M_i is the tally mean of a problem at number of history N_i and s_i is the average score for the batch containing number of histories from N_{i-1} to N_i; (c) After average batch scores for both the original and perturbed problems, f_i and g_i, are obtained by Eq. (5), the change in system response for each batch is then computed by

$$\Delta I_i = f_i - g_i. \tag{6}$$

These $\Delta I_i'$s are finally used to compute ΔI and $\sigma_{\Delta I}$ by the statistical formulae.

Tests have been conducted to examine the performance of correlated sampling, using the foregoing outlined procedure. For all the tests, the original model consists of a homogeneous coal sphere of 30 cm radius, with an isotropic point source located at the center of the sphere that emits neutrons having a uniform energy distribution from 1 to 14.1 MeV. The initial density of coal is 0.67552 g/cm^3. For one perturbed case to be presented in this section, the density of the coal ball is increased by 1% and the change in neutron current across the sphere surface is simulated at different NPS. For a given NPS, different batch numbers are used to conduct the batch statistics.

Numerical calculations show that the original procedure of batch statistics for correlated sampling works fine and can produce valid results most of time. However, under certain circumstances the computed standard deviation of ΔI is found to vary significantly with the batch number used in the uncertainty analysis, especially at large NPS and small batch size. This unphysical phenomenon is shown in Fig. 1(a), where presented are the results of ΔI and its error bar (defined as $\pm\sigma_{\Delta I}$) computed by using different batch numbers for the case of NPS = 10^6. The (red) solid horizontal line given in Fig. 1(a) represents the result of ΔI computed at NPS = 10^8, which can be regarded as a reference or "benchmark" result for the problem. For finding the cause of the strange behavior shown in Fig. 1(a), the distribution of computed ΔI_i is also analyzed to see if they follow a normal distribution, as should. Figure 1(b) shows the histogram of ΔI_i for the test case, computed by using one hundred batches, with each batch containing 10,000 particle histories. This figure clearly demonstrates that these computed ΔI_i are not generated accurately thus they do not follow a normal distribution.



(a) Error Bar vs. Batch Number (b) Histogram of ΔI_i

Figure 1. Results Obtained by the Original Procedure for NPS = 10^6

We believe the inaccurate estimation of ΔI_i is caused by: (a) the significant figures of tally means given in the MCNP5 output files by default are limited to four digits after the decimal point, thus round-off error exists in tally means at the fourth digit after the decimal point; and (b) the round-off error in tally means is passed to ΔI_i through the two operations given by Eqs. (5) and (6); in fact each operation amplifies the effect of that error dramatically.

To quantify the effect of round-off error in tally means on the calculation of ΔI_i, we denote the tally mean given in the MCNP output file at particle history number N_i as

$$M_i' = M_i(1+\delta_i), \qquad (7)$$

where M_i is the true tally mean and δ_i is the relative round-off error, which is generally in the order of 10^{-5}. Using Eq. (7) in Eq. (5), we find that the computed averaged score of a batch for a problem is then given by

$$\begin{aligned} s_i' &= \frac{M_i' \times N_i - M_{i-1}' \times N_{i-1}}{N_i - N_{i-1}} = \frac{M_i \times N_i - M_{i-1} \times N_{i-1}}{N_i - N_{i-1}} + \frac{M_i \times \delta_i \times N_i - M_{i-1}\delta_{i-1} \times N_{i-1}}{N_i - N_{i-1}} \\ &= s_i + \frac{M_i \times \delta_i \times N_i - M_{i-1}\delta_{i-1} \times N_{i-1}}{N_i - N_{i-1}} = s_i \left[1 + \frac{M_i \times \delta_i \times N_i - M_{i-1}\delta_{i-1} \times N_{i-1}}{s_i \times \left(N_i - N_{i-1}\right)} \right] \end{aligned} \tag{8}$$

where s_i is the true average batch score, computed by the true tally means. The second term inside the square bracket in the above equation, to be denoted by $\delta(s_i)$ in the following, represents the relative error of the computed batch score for a problem. When number of particle histories N_i is large, we have $M_i \approx M_{i-1} \approx s_i$ so they can be cancelled out in the expression of $\delta(s_i)$. If we further assume that δ_i and δ_{i-1} are close in quantity but may have different signs, i.e., $|\delta_{i-1}| \approx |\delta_i|$, then the absolute value of $\delta(s_i)$ is reduced to $|\delta_i|$ when δ_i and δ_{i-1} have the same signs; however, when δ_i and δ_{i-1} have the different signs, $|\delta(s_i)|$ is reduced to

$$|\delta(s_i)| \approx |\delta_i| \times \frac{N_i + N_{i-1}}{N_i - N_{i-1}} < |\delta_i| \times \frac{2 \cdot NPS}{N_i - N_{i-1}} = 2m \cdot |\delta_i|, \tag{9}$$

where ($N_i - N_{i-1}$) is the batch size and m is the batch number. This result shows that the use of Eq. (5) leads the computed batch scores to having a relative error up to 2m times of the relative round-off error existed in tally means.

In applications, batch number cannot be too small in order for the statistics formulas to be valid; it usually changes from tens to hundreds. Thus each computed batch score could have a relative error in the range of $10^{-3} - 10^{-2}$, which doesn't sounds too bad for one individual batch score. However, this kind of error exists in computed batch scores for both the original and perturbed problems, i.e., in both f_i and g_i. Then when f_i and g_i are used to calculate the response change for a batch by Eq. (6), the relative error for ΔI_i can be much worse. A similar analysis as Eq. (8) yields that the maximum relative error for ΔI_i is given by

$$|\delta(\Delta I_i)| \approx |\delta(s_i)| \cdot \frac{f_i + g_i}{\Delta I_i} \tag{10}$$

which occurs when relative errors of f_i and g_i have almost the same value, i.e.,$|\delta(f_i)| \approx |\delta(g_i)| \equiv |\delta(s_i)|$, but different signs. Clearly, when the change in system response ΔI_i is small, say only of one percent of the unperturbed score f_i, $|\delta(\Delta I_i)|$ can be few hundred times of $|\delta(s_i)|$. Thus the maximum relative error of ΔI_i is in the order of $10^{-1} - 10^{0}$.

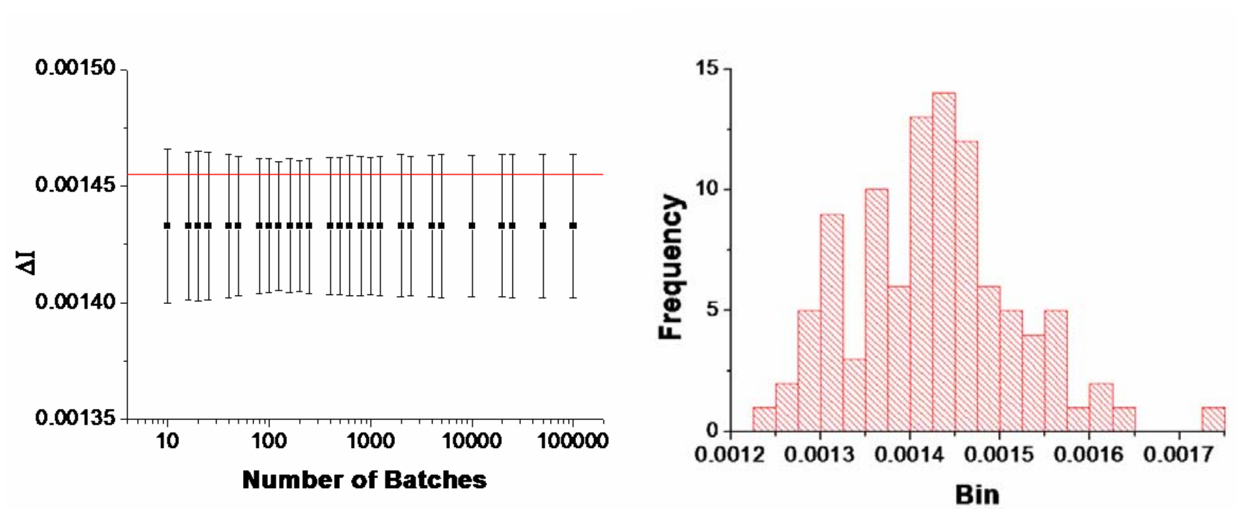
The foregoing analysis reveals that the round-off errors in the tally means may make the original practice of batch statistics yield inaccurate estimation of ΔI_i, thus overestimate the uncertainty

$\sigma_{\Delta I}$, especially for those problems that involve small changes in system response and thus require the use of a large NPS.

2.2. Two Suggestions for Correct Estimation of the Uncertainty

The weakness associated with the inaccurate estimation of ΔI_i can be corrected by at least two measures. The first one is to increase the number of significant figures for tally means in the MCNP5 output file (a similar recommendation was suggested years ago [11] on the output of variances), thus the effect of round-off error will be eliminated or at least reduced significantly. This task can be accomplished by changing and recompiling MCNP source code, which is not a difficult exercise for experienced MCNP users.

To verify the analysis given in Section 2.1 and the above suggestion, we increase the significant figures of tally means to eight digits after the decimal point in the MCNP output file, which reduces the relative round-off error to less than 10^{-8} in tally means, and then re-run the problem shown in Fig. 1, using the same procedure and parameters. The results are presented in Fig. 2, which this time shows that ΔI and $\sigma_{\Delta I}$ almost do not vary with the selection of batch number, as expected, even when very large batch number (m = 10^5) is used. In addition, the histogram of computed ΔI_i given in Fig. 2(b) is significantly improved from that given in Fig. 1(b), showing that the 100 computed ΔI_i roughly follow a normal distribution. Thus we conclude that after increasing the significant figures of tally means the procedure suggested by Booth [4] for batch statistics works well.



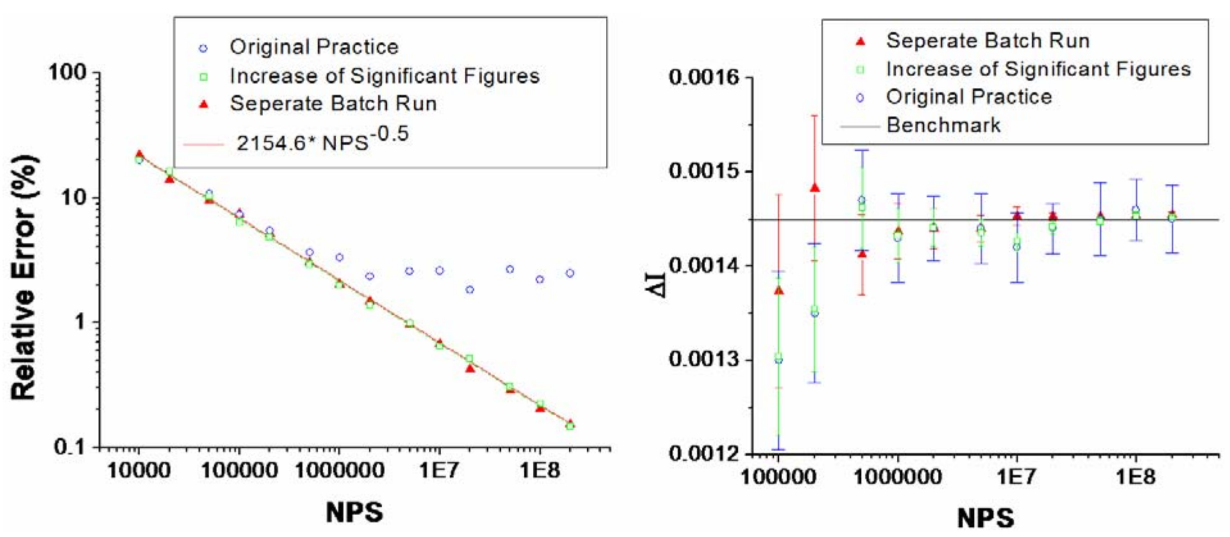
(a) Error Bar vs. Batch Number (b) Histogram of ΔI_i

Figure 2. Results Obtained after Increase of Significant Figures for NPS = 10^6

The second suggestion that we propose doesn't involve changing the significant figures of tally means so it is suitable for those who don't want to recompile the MCNP source code. In this new procedure, each batch of MCNP calculation is run separately using a different random number sequence (RNS), either by starting with a new random number or by changing the random number stride or multiplier on the RAND card of MCNP5. Thus the batch scores are obtained directly without using the tally fluctuation chart and Eq. (5). That is, instead of running one million NPS together for a problem, one just runs one hundred batches of MCNP calculations separately, each for ten thousand NPS and using a different random number sequence, to get one hundred batch scores directly. Note that performing a series of MCNP5 runs with varying RNS can be conveniently accomplished by a tool called MCNP_pstudy [12] that uses only one input card for all the batch calculations. It should be also reminded that the same RNS must be used for the same batch calculations of both the original and perturbed problems to ensure correlated sampling.

Since this proposed procedure produces batch scores directly for both the original and perturbated problems, it can generate accurate enough ΔI_i for each batch. In fact it has been confirmed by numerical tests that the ΔI_i generated by this procedure follow a similar distribution as shown in Fig. 2(b).

For further validating the two proposed procedures, more MCNP calculations are done to compute ΔI and $\sigma_{\Delta I}$ for the same problem by using one hundred batches and different NPS. Figure 3 presents the relative error (defined as the ratio of $\sigma_{\Delta I}$ to ΔI) and the error bar of ΔI (defined as $\Delta I \pm \sigma_{\Delta I}$) computed at different NPS by the original procedure and by the two improved procedures, which clearly shows that the two new procedures always predict proper and almost identical $\sigma_{\Delta I}$ that follow the $\sqrt{1/NPS}$ rule while the results obtained by the original approach don't follow the rule at large NPS.



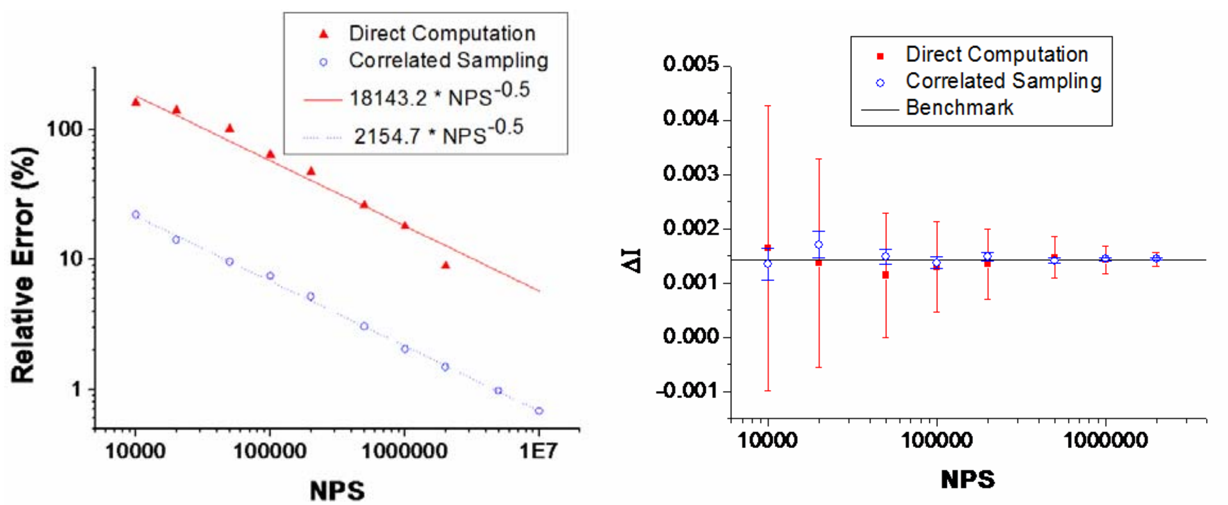
(a) Relative Error of ΔI vs. NPS (b) Error Bar of ΔI vs. NPS

Figure 3. Comparisons of Different Approaches of Correlated Sampling

2.3. Effect of Correlated Sampling

The effectiveness of correlated sampling is demonstrated by comparing its performance with that of un-correlated sampling. Since the two new proposed procedures for correlated sampling yield very similar results when NPS is large enough, only the correlated sampling results obtained by the new approach of separate batch run are presented in the following parts of the paper.

Presented in Fig. 4 are the results of the same test problem, obtained at different NPS by the direct, un-correlated computation [whose standard deviation is defined by Eq. (4)] and by correlated sampling that uses 100 batches. Since standard deviation is proportional to $\sqrt{1/NPS}$, appropriate expressions are obtained by curve fitting to show how the relative error changes with NPS for both types of calculations. The obtained expressions are given and also plotted in Fig. 4(a). Figure 4(a) shows that relative errors of ΔI produced by un-correlated sampling and correlated sampling both follow the $\sqrt{1/NPS}$ rule. Comparing the coefficients of the expressions shows that overall the relative error of ΔI estimated by correlated sampling is roughly about 1/9 of that estimated by the direct uncorrelated calculation at the same NPS for this case. That is, correlated sampling is about 81 times faster than un-correlated sampling to reach to a required uncertainty for this test case. The figure also shows that both calculations predict roughly the same results for ΔI. Thus it can be concluded that the relatively large uncertainty for small response change can be effectively reduced by the correlated sampling method.



(a) Relative Error of ΔI vs. NPS (b) Error Bar of ΔI vs. NPS

Figure 4. Comparisons between Correlated Sampling and Un-correlated Computation

3. COMPARISON BETWEEN CORRELATED SAMPLING AND PERTURBATION TECHNIQUE

MCNP5 has a PERT card that allows perturbation calculations in material density, composition or cross-section data to be performed. For such problems, perturbation technique can provide a quick and precise estimate for a small change in tally responses even when the uncertainty of the unperturbed tally is large. However, MCNP5 perturbation calculations may be inaccurate for some problems primarily due to two reasons: (1) MCNP5 only includes the first and second order terms in the Taylor series expansion; which is inadequate for some problems; and (2) it ignores the second order cross-differential term that represents the interaction between perturbations if relative concentrations of two or more nuclides are changed; this ignorance may yield large false second order perturbation terms for some problems [9-10]. Because of such weaknesses, application of perturbation technique in MCNP is recommended [3] to obey the following rules of thumb: (1) the first order perturbation estimator may offer efficient accuracy if response changes are less than 5%; (2) the first plus second order estimator can provide acceptable accuracy if response changes are less than 20–30%; and (3) If the magnitude of the second-order estimator exceeds 30% of the first-order estimator, higher-order terms are always necessary for an accurate prediction.

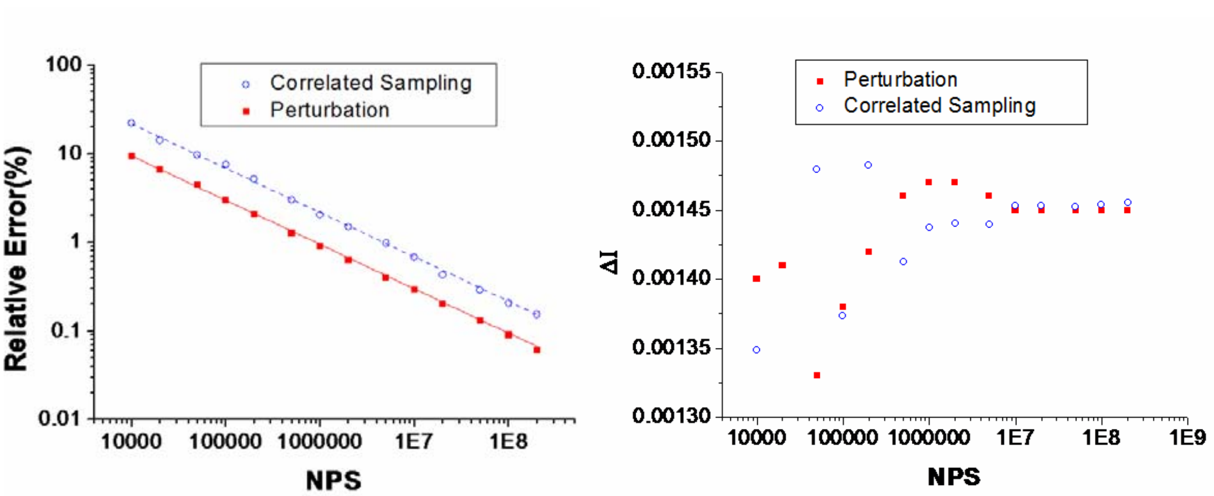
Performances of the MCNP5 perturbation technique and correlated sampling are compared on their capabilities to estimate small changes in system response. Since any one of the improved correlated sampling procedures doesn't introduce bias in calculations, the results of response change obtained by correlated sampling at very large NPS are considered as "benchmarks" in the comparison; thus the accuracy of MCNP5 perturbation is evaluated by comparing the perturbation results with those obtained by correlated sampling at large NPS.

Three types of tests are conducted. The first one is the same test problem described in Section2.1: a coal sphere that suffers perturbation in material density while the relative material composition remains unchanged. Figure 5 presents the comparison for the test problem that involves the change of neutron current across the sphere surface due to the increase of material density by 1% and 10%, respectively. As this figure shows, when the perturbation is small (the case of 1% perturbation in density leading to ~0.2% change in neutron current), the perturbation technique (with the 1st and 2nd order terms) and the correlated sampling predict very close results for the response change ΔI at large NPS; and the relative errors predicted by perturbation are smaller than those predicted by correlated sampling, but not significantly so. For this case the second order perturbation terms almost have no contribution to the total perturbation results. However, as the perturbation in density becomes larger (the case of 10% perturbation in density leading to ~2% change in neutron current), the perturbation technique performs worse than the correlated sampling: it not only predicts a less accurate result for ΔI (about 4% less than that of correlated sampling at large NPS) but also yields a slightly larger uncertainty for ΔI than the correlated sampling method. Also shown in Fig. 5(b) is that the second order perturbation terms contribute about only 2% of the total perturbation results for this case.

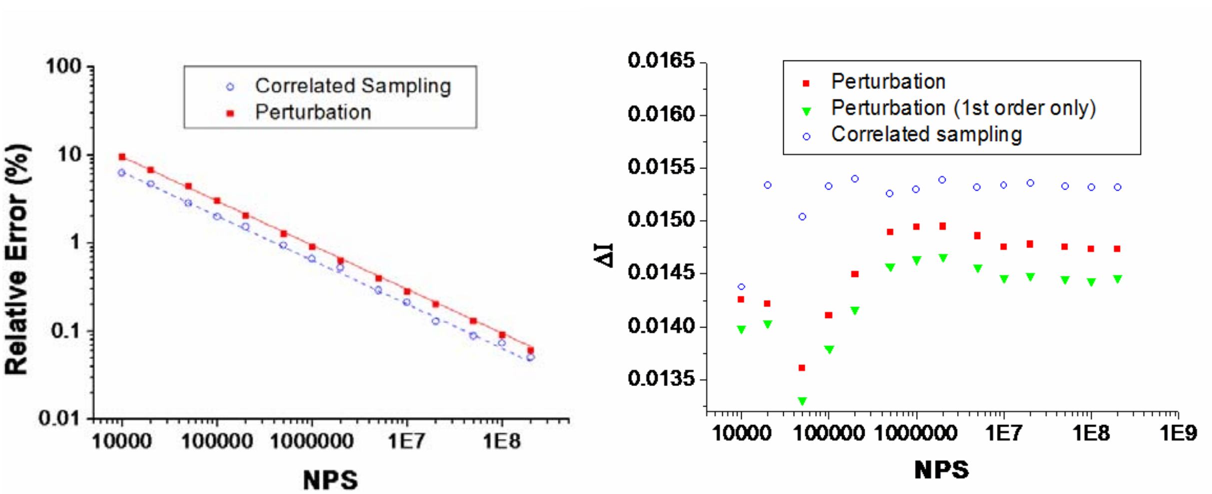
The second test uses the same unperturbed model as in Test 1. But for the perturbed model, a void of different sizes is introduced inside the sphere. Results show that performances of the two methods for this problem are very similar to those shown in Fig. 5 and thus they are presented here.

The third test problem, again, uses the same unperturbed model as in Test 1. However, in the perturbed model, uneven variation in material composition is introduced. Specifically, the atom number density of carbon is increased by 4.62% (with the relative atom number changed from

0.693 to 0.725), the atom number density of oxygen is reduced by 11.76% (from 0.17 to 0.15), while the atom number densities of all the other elements of coal remain unchanged. Such variation in material composition causes the total atom number density of coal to be increased by 1.2% and leads to a less than 0.03% of variation in system response – the neutron current across the sphere surface.



(a) 1% Perturbation in Density



(b) 10% Perturbation in Density

Figure 5. Comparisons between Perturbation and Correlated Sampling for Test 1

Figure 6 presents the comparison between perturbation and correlated sampling for the third test problem. It shows that the MCNP5 perturbation technique (with the 1st and 2nd order terms) and correlated sampling predict almost the same and small enough relative errors for the variation in system response at large NPS. However, the current MCNP5 perturbation technique fails to predict an accurate result for this problem, as more than 20% difference always exists at any NPS between the ΔI predicted by the perturbation technique and that predicted by correlated sampling (which can be regarded as a "benchmark" result at very large NPS). The inaccuracy of perturbation is due to the large, maybe false, second order perturbation estimator, partially caused by the negligence of the cross-differential term in the second order perturbation terms [3]. Besides, Figure 6 shows that the magnitude of the second-order estimator exceeds 30% of the first-order estimator; thus per the third rule of thumb higher-order perturbation terms are necessary for an accurate prediction for this test problem. This example demonstrates that even when the change in system response is extremely small, the current version of MCNP5 perturbation may still perform poorly and produce a precise but inaccurate result under certain circumstances.

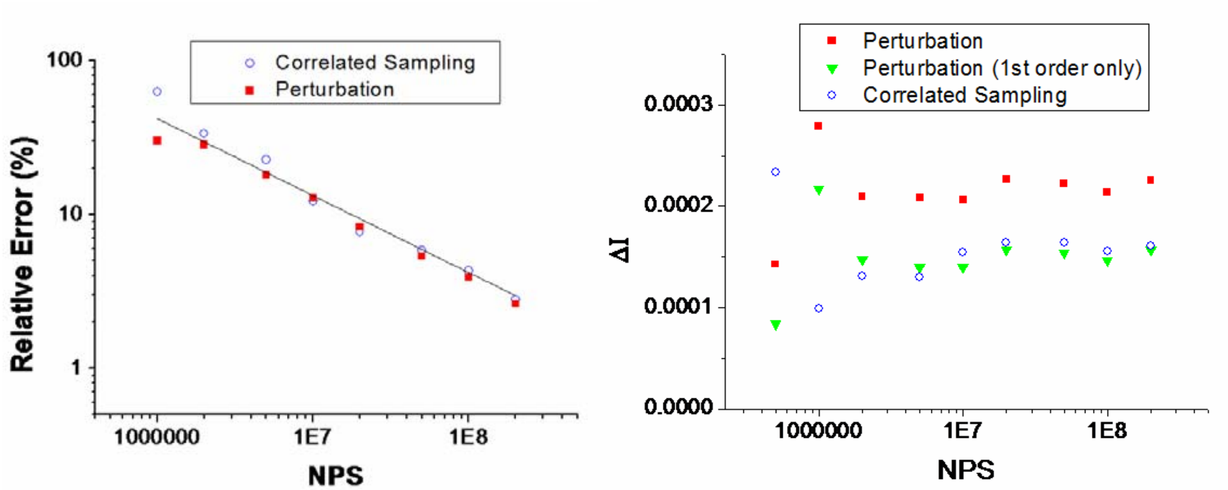


Figure 6. Comparisons between Perturbation and Correlated Sampling for Test 3

Based on the foregoing comparisons, the current MCNP perturbation technique doesn't seem to have many advantages over correlated sampling. In addition, since the current perturbation technique only allows perturbation calculations in material density, composition or cross-section data, it is not applicable to certain problems such as those that involve a small variation in source particles' spatial and/or energy distribution. Therefore, correlated sampling seems to be a more robust technique than the current perturbation technique of MCNP5 for simulating small changes in system response.

4. CONCLUSIONS

Several conclusions can be drawn from this work. First of all, using the default MCNP output and the original practice of doing batch statistics for correlated sampling may overestimate the uncertainty for small changes in system response. Two improved procedures are proposed to correct this weakness and are in fact tested to be effective. Secondly, the correlated sampling method is suitable to simulate small changes in system response with acceptable uncertainty. It has wide applications and can produce unbiased results for various problems; and it may yield a standard deviation that is only one-tenth of that predicted the direct, uncorrelated simulation. Lastly, the comparison between MCNP perturbation technique and correlated sampling shows that perturbation technique doesn't provide too many advantages over correlated sampling. Generally the current version perturbation technique predicts smaller uncertainty than correlated sampling only for problems with very small *ΔI*. However, the perturbation technique may produce less accurate results than correlated sampling for certain problems that involve intermediate or even small changes in system response. MCNP users must follow all the rules of thumb (especially the last one) in any perturbation applications to avoid inaccurate results.

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