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CONFIDENCE INTERVALS IN MCNP

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ESTIMATION AND INTERPRETATION OF k_{eff} CONFIDENCE INTERVALS IN MCNP

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ABSTRACT

MCNPTM has three different, but correlated, estimators for calculating k_{eff} in nuclear criticality calculations: collision, absorption, and track length estimators. The combination of these three estimators, the three-combined k_{eff} estimator, is shown to be the best k_{eff} estimator available in MCNP for estimating k_{eff} confidence intervals. Theoretically, the Gauss-Markov Theorem provides a solid foundation for MCNP's three-combined estimator. Analytically, a statistical study, where the estimates are drawn using a known covariance matrix, shows that the three-combined estimator is superior to the individual estimator with the smallest variance. The importance of MCNP's batch statistics is demonstrated by an investigation of the effects of individual estimator variance bias on the combination of estimators, both heuristically with the analytical study and empirically with MCNP.

INTRODUCTION

In criticality calculations, MCNPTM ³ has three types of individual k_{eff} estimators: collision, \bar{k}_c ; absorption, \bar{k}_a ; and track length, \bar{k}_t [1]. At each cycle, or computational fission generation, MCNP produces a k_{eff} estimate of each type. The final k_{eff} estimator of each type is the average of several cycle k_{eff} estimates. MCNP's best estimator is a combination [2,3], in least squares fashion, of all three estimators, that takes into account variances and covariances between the individual estimators. This work examines the theory of the three-combined estimator and its behavior and performance in both an analytical study and in an MCNP study. It is emphasized that the final result from an MCNP criticality calculation is not a point estimate of k_{eff} , but rather a confidence interval.

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THREE-COMBINED k_{eff} ESTIMATOR

The three-combined k_{eff} estimator is appealing because it uses all the available information. It is essentially the least squares solution of a multivariate linear regression of the cycle k_{eff} estimates of one estimator type on those of the other two types and is based mainly on a paper by M. Halperin [4]. The three individual k_{eff} estimators (collision, absorption, and track length) have a population covariance matrix, Σ ,

$$\Sigma = \begin{bmatrix} \sigma_c^2 & \sigma_{ca}^2 & \sigma_{ct}^2 \\ \sigma_{ac}^2 & \sigma_a^2 & \sigma_{at}^2 \\ \sigma_{tc}^2 & \sigma_{ta}^2 & \sigma_t^2 \end{bmatrix}. \quad (1)$$

The three-combined k_{eff} estimator, \hat{k} , in matrix and reduced form [2,3] is as follows:

$$\hat{k} = \bar{k}_c - \Sigma_{z12} \Sigma_{z22}^{-1} \bar{\mathbf{d}} = \frac{\sum_{t=1}^3 f_t \bar{k}_t}{\sum_{t=1}^3 f_t}, \quad (2)$$

where $\bar{\mathbf{d}} = (\bar{k}_a - \bar{k}_c, \bar{k}_t - \bar{k}_c)'$;

$$\Sigma_z = \begin{bmatrix} \Sigma_{z11} & \Sigma_{z12} \\ \Sigma_{z21} & \Sigma_{z22} \end{bmatrix}, \quad (3)$$

where

$$\Sigma_{z11} = \sigma_c^2 \quad (4)$$

$$\Sigma_{z12} = \begin{bmatrix} \sigma_c^2 - \sigma_{ca}^2 & \sigma_c^2 - \sigma_{ct}^2 \end{bmatrix}, \quad (5)$$

$$\Sigma_{z21} = \begin{bmatrix} \sigma_c^2 - \sigma_{ca}^2 \\ \sigma_c^2 - \sigma_{ct}^2 \end{bmatrix}, \quad (6)$$

$$\Sigma_{z22} = \begin{bmatrix} \sigma_c^2 + \sigma_a^2 - 2\sigma_{ca}^2 \\ \sigma_c^2 + \sigma_{at}^2 - \sigma_{ca}^2 - \sigma_{ct}^2 \end{bmatrix} \quad (7)$$

$$\begin{bmatrix} \sigma_c^2 + \sigma_{at}^2 - \sigma_{ca}^2 - \sigma_{ct}^2 \\ \sigma_c^2 + \sigma_t^2 - 2\sigma_{ct}^2 \end{bmatrix}; \quad (8)$$

and

$$f_\ell = \sigma_{jj}^2 (\sigma_{kk}^2 - \sigma_{ik}^2) - \sigma_{kk}^2 \sigma_{ij}^2 \quad (9)$$

$$+ \sigma_{jk}^2 (\sigma_{ij}^2 + \sigma_{ik}^2 - \sigma_{jk}^2), \quad (10)$$

where ℓ indicates a particular partial permutation of i , j , and k , with 1 \equiv collision, 2 \equiv absorption, and 3 \equiv track length.

The three-combined estimator variance, σ_k^2 in matrix and reduced form [2,3] is as follows:

$$\sigma_k^2 = \left(\Sigma_{z11} - \Sigma_{z12} \Sigma_{z22}^{-1} \Sigma_{z21} \right) \cdot \left(\frac{1}{n} + \frac{\mathbf{d}' \Sigma_{z22}^{-1} \mathbf{d}}{n-1} \right) \quad (11)$$

$$= \frac{S_1}{gn(n-3)} \left(1 + n \left(\frac{S_2 - 2S_3}{(n-1)g} \right) \right), \quad (12)$$

where n is the number of k_{eff} cycles used; $(n-3)$ is the correct number of degrees of freedom; g is the sum of all three f_ℓ 's; and

$$S_1 = (n-1) \sum_{\ell=1}^3 f_\ell \sigma_{\ell\ell}^2, \quad (13)$$

$$S_2 = \sum_{\ell=1}^3 \left(\sigma_{jj}^2 + \sigma_{kk}^2 - 2\sigma_{jk}^2 \right) k_\ell^2, \quad (14)$$

$$S_3 = \sum_{i=1}^3 \left(\sigma_{kk}^2 + \sigma_{ij}^2 - \sigma_{jk}^2 - \sigma_{ik}^2 \right) k_\ell k_j. \quad (15)$$

The Gauss-Markov Theorem states that, when the variance-covariance matrix is known, the least squares solution of the linear regression parameters is unbiased and has minimum variance; it is the best possible. Here, the variance-covariance matrix is not known and must be estimated from the data. The three-combined k_{eff} estimator uses the estimated variance-covariance matrix and is therefore almost optimal. Statistical studies show that this almost optimal estimator is very good [2,3].

CONFIDENCE INTERVALS

A confidence interval is a range of values that is expected to contain the precise value with some specified confidence. The precise value is the expected value, that obtained from an infinite number of histories. Confidence intervals are constructed by including some multiple of the estimated standard deviation (square root of the variance) above and below the average value. This multiplier is the Student's t -percentile and depends on the desired confidence level and the degrees of freedom available in the estimation of the standard deviation [3]. To increase the probability that a k_{eff} confidence interval contains the precise k_{eff} , the interval must be made larger; to decrease the size of a given confidence interval, more histories need to be run.

Understanding confidence intervals is especially important in criticality safety. To present a 68% confidence interval implies that there is a 32% chance that the interval does not include the precise value. The 68% confidence intervals for the three-combined estimator are shown in Figure 1 for each of one hundred independent MCNP runs [2,3] for a U-233/light water system. The horizontal lines demark the 68% confidence interval for the average over all 100 runs, which is the best estimate of the precise value. Of the one-hundred 68% confidence intervals, 70 cross the mean and 30 do not. The 99% confidence intervals (not shown) all cross the mean. Since the confidence intervals include the precise mean the expected number of times, the coverage rates in this example are good.

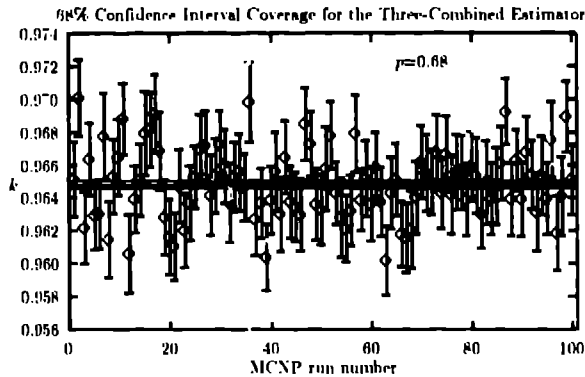


Figure 1: The 68% confidence intervals from 100 independent runs (vertical lines) shown with the 68% confidence interval of the overall mean (horizontal lines).

AN EXAMPLE OF THE BEHAVIOR OF THE THREE-COMBINED ESTIMATOR

One property of the three-combined estimator is that, for highly positively correlated estimators, it may lie outside the range of the three individual estimators. This is correct, as shown in a statistical study, where the expected value of each of three highly correlated estimators is unity. The estimators are drawn from the following *population covariance matrix*:

$$\Sigma = (0.02)^2 \begin{pmatrix} 1 & 2 & 2 \\ 2 & 5 & 8 \\ 2 & 8 & 21 \end{pmatrix}. \quad (16)$$

The first estimator has the smallest population standard deviation (0.02), and the third estimator has the largest population standard deviation (~ 0.09). The correlation coefficients are

$$\begin{aligned} \rho_{12} &= 0.89 \\ \rho_{13} &= 0.44 \\ \rho_{23} &= 0.78. \end{aligned} \quad (17)$$

All these estimators are highly positively correlated.

This behavior study simulated 100 independent MCNP runs, each with 100 active cycles. The three-combined estimator is calculated using not the known covariances, but the covariances estimated from the data, just like

MCNP does. Figure 2 shows that, of 100 samples, 64 have estimator ranges that do not include unity. Of those, 55 have three-combined estimators that lie outside the individual estimator range and closer to the expected value. The three-combined k_{eff} estimator performs better than the simple average and the individual estimator with the smallest variance [3]. The latter is evident in that it is clustered closer to unity than the inside edge of the range bars in Figure 2.

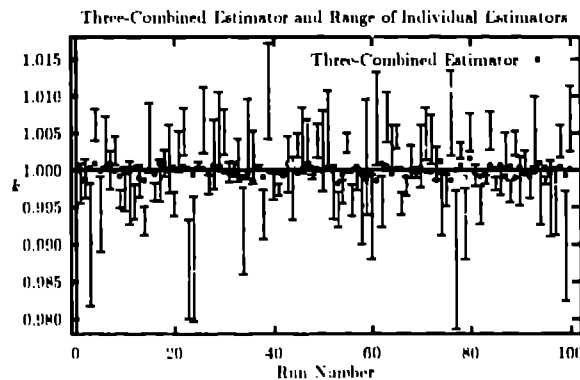


Figure 2: The range of three individual estimators, connected by vertical lines, and the three-combined estimator for 100 samples.

EFFECT OF VARIANCE BIAS

A good quality of the three-combined estimator is that it uses all the available information. If the individual estimator variances are underestimated due to a bias, their coverage rates may be inadequate. Moreover, this bias may propagate to the estimated standard deviation of the three-combined estimator. We investigate this effect by introducing various artificial biases to the individual estimator variances in the previous section's analytic study.

Table 1 shows how introducing different artificial, individual estimator variance biases affects the estimated standard deviation of the three-combined k_{eff} estimator. For a single run, or sample, containing 100 cycles, there is a reported variance of the mean for each of the three individual estimators. Normally, these variances are converted to population variances, then plugged into Equations 2 and 12 to estimate the three-combined estimator

and its variance. In this bias study, we convert the individual variances to population variances, and then add biases *before* plugging them into Equations 2 and 12. Therefore the combination perceives the biased variances as the actual variances. So, if there is a negative bias on a variance, the combination will think it is smaller than it actually is. Note that if a negative bias on the individual estimator variance was real, its coverage rates would be less than expected. This study examines how these biases would propagate to the three-combined estimator variance and affect its coverage rates.

In general, the standard deviation of the mean from one run is the population standard deviation one could expect if several runs, or replicas, were made. Therefore, to check the validity of the calculated standard deviation from one run, we make 100 independent runs. The spread of the 100 values of the three-combined estimator is represented as σ_{actual} . A value of σ_k/σ_{actual} less than one indicates an underestimation, or negative bias. The bias typically seen in criticality calculations is negative.

Row 1 is the control run, where no artificial biases are introduced. The three-combined estimated standard deviation shows no underestimation. If the biases on the individual variances and covariances are equal (rows 2 and 3), σ_{actual} is unaffected, since the biases explicitly cancel out in the expression for \hat{k} . In Row 2, the standard deviation, and hence the confidence interval, on the first estimator is overestimated by a factor of

$$\sqrt{(.0001 + .0002)/.0001} = 1.22 .$$

The estimated standard deviation of the three-combined estimator, with its 2.45 overestimation, conservatively overestimates the positive bias in the individual estimator variance bias

The results in Row 3 are especially noteworthy. All the variances and covariances are underestimated by the same additive amount. Again, the variance/covariance biases explicitly cancel out in the expression of \hat{k} . Here, though, the estimated standard deviation σ_k overestimates the actual standard deviation because the deviations between the individual estimators themselves are significant and

accounted for in the expression for σ_k . Equations 12, 14 and 15.

Row 4 is an attempt to fool the combination into thinking that the first estimator is better than it actually is. After 100 cycles, or samples, the combination thinks that

$$\sigma_{11}/\sqrt{100} = \sqrt{.0004 - .0002}/10 = 0.0014$$

instead of its actual nominal value of

$$\sqrt{0.0004}/10 = 0.002 .$$

The population covariances σ_{12}^2 and σ_{13}^2 are also halved. Halving a variance translates into a

$$1 - \sqrt{.5} = .29$$

reduction in the standard deviation. Row 4 shows a 19% underestimation propagating to the three-combined standard deviation. The actual variance of the three-combined estimator doesn't show the gains as in the unbiased case because the correlation between the first estimator and the other two was artificially weakened. In fact, the three-combined variance tends to look like the actual variance of the first estimator.

Row 5 shows the result when the second-best individual variance and its associated covariance are underestimated. Again, the correlation between the first and second estimators is weakened, and the three-combined variance tends to emulate that of the first (still the best) estimator.

Row 6 shows that an underestimation in the variance of the individual estimator with the highest variance has a smaller effect on the three-combined variance. The gain is a little less, but there is no underestimation.

Typically, the cause of the variance in one individual estimator will cause a similar bias in the other estimators. Therefore, we reduce all individual estimator variances and covariances by 50% in Row 7. This bias directly propagates through to give a 50% underestimation in the three-combined variance, which corresponds to a 29% underestimation in the standard deviation. The value of the three-combined standard deviation is small enough so that 29% does not amount to much.

We have shown a range of effects on the three-combined estimator variance due to a bias in the individual estimator variances. An

| row | absolute artificial bias in | | | | | | \hat{k} | $\sigma_{\hat{k}}$ | σ_{actual} | $\frac{\sigma_{\hat{k}}}{\sigma_{actual}}$ |
|-----|-----------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------|--------------------|-------------------|--|
| | σ_{11}^2 | σ_{12}^2 | σ_{22}^2 | σ_{13}^2 | σ_{23}^2 | σ_{33}^2 | | | | |
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1.0001 | .0006 | .0006 | 1.00 |
| 2 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | 1.0001 | .0016 | .0006 | 2.45 |
| 3 | -.0002 | -.0002 | -.0002 | -.0002 | -.0002 | -.0002 | 1.0001 | .0013 | .0006 | 2.00 |
| 4 | -.0002 | -.0004 | 0 | -.0004 | 0 | 0 | 1.0019 | .0015 | .0018 | 0.81 |
| 5 | 0 | -.0004 | -.001 | 0 | -.0016 | 0 | 1.0019 | .0022 | .0024 | 0.91 |
| 6 | 0 | 0 | 0 | -.0004 | -.0016 | -.0042 | 1.0010 | .0013 | .0012 | 1.07 |
| 7 | -.0002 | -.0004 | -.001 | -.0004 | -.0016 | -.0042 | 1.0001 | .0005 | .0007 | 0.71 |

Table 1: Bias effects on the estimated standard deviation of the three-combined estimator.

equal negative absolute bias across the board (Row 3) results in an overestimation of the three-combined variance. An equal negative multiplicative bias across the board (Row 7) demonstrates a direct propagation of the bias. We now look at realistic situations where variance bias rears its ugly head and a way to detect and squelch it.

MCNP EXAMPLE

As we did in the analytic study, performing several independent replicas of a run is the best way to verify any standard deviation of a mean. For a Monte Carlo criticality calculation, the replication examination should have the number of replicas statistically similar to the number of active cycles in each run [3]. Then the quantities compared will be similarly distributed.

The coverage rates of the three-combined k_{eff} confidence intervals in MCNP were verified for several systems [2,3]. We present an interesting case involving a Godiva sphere and Jezebel sphere, separated 80 cm center-to-center. Systems like this, with weak neutron communication between distant regions, have high dominance ratios (ratio of the second eigenvalue to the dominant eigenvalue) and tend to have underestimated individual k_{eff} variances. The cause of this underestimation is the serial, or cycle-to-cycle, correlation of the fission source. Running 100 independent MCNP runs demonstrated that the individual estimator variances were slightly underestimated and, therefore, so, too, was the three-combined k_{eff} estimator variance. This underestimation causes inadequate coverage rates at the 68% and 95% confidence levels,

as shown in Table 2. Note that the variance underestimations for each individual estimator are multiplicatively similar, so this real situation is like the situation in Row 7 of Table 1. Fortunately, the batching statistics in MCNP can help detect a variance underestimation. Batching groups of cycles together diminishes some of the cycle-to-cycle correlation and reduces any existing variance underestimation. Figure 3 shows how batching can detect an underestimation in the estimated standard deviation. Using the variance from 40 batches of 20 cycles each, Table 3 shows much improved coverage rates.

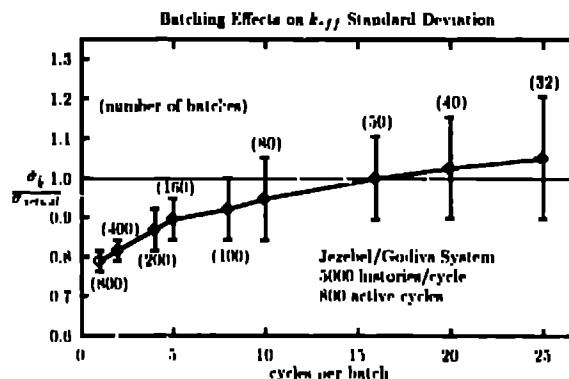


Figure 3: For 800 active cycles and 100 independent runs, MCNP's batch data show an underestimation in the calculated standard deviation for too few cycles per batch. The error bars represent the observed variation in $\hat{\sigma}_k$ at the 68% confidence level.

| k_{eff} estimator | \bar{k}_{eff} | $\sigma_{observed}$ | $\bar{\sigma}_{calculated} (\sigma_{\bar{\sigma}})$ | coverage rates | | |
|---------------------|-----------------|---------------------|---|----------------|-----|-----|
| | | | | 68% | 95% | 99% |
| collision | 1.01249 | 0.00055 | 0.00040 (0.00002) | 52 | 86 | 94 |
| absorption | 1.01249 | 0.00055 | 0.00041 (0.00002) | 51 | 86 | 94 |
| track length | 1.01252 | 0.00037 | 0.00030 (0.00000) | 57 | 90 | 98 |
| col/abs/trkl | 1.01252 | 0.00038 | 0.00030 (0.00001) | 54 | 88 | 98 |

Table 2: k_{eff} estimates for the two-component system, Godiva and Jezebel reactor mock-up and their associated standard deviations and coverage rates for 100 independent runs.

| k_{eff} estimator | \bar{k}_{eff} | $\sigma_{observed}$ | $\bar{\sigma}_{calculated} (\sigma_{\bar{\sigma}})$ | coverage rates | | |
|---------------------|-----------------|---------------------|---|----------------|-----|-----|
| | | | | 68% | 95% | 99% |
| collision | 1.01249 | 0.00055 | 0.00050 (0.00007) | 63 | 93 | 97 |
| absorption | 1.01249 | 0.00055 | 0.00050 (0.00007) | 62 | 94 | 97 |
| track length | 1.01252 | 0.00037 | 0.00039 (0.00005) | 71 | 97 | 100 |
| col/abs/trkl | 1.01252 | 0.00039 | 0.00040 (0.00005) | 70 | 95 | 99 |

Table 3: k_{eff} estimates for the two-component system, Godiva and Jezebel reactor mock-up and their associated standard deviations and coverage rates for 100 independent runs, where the 800 active cycles have been batched into 40 batches of 20 cycles each.

CONCLUSION

The three-combined k_{eff} estimator has been derived and verified, both theoretically and empirically (for the cases studied), to be the best available estimator in MCNP. It has been shown to be superior to other estimators such as the simple average and the individual estimator with the smallest variance. Analytic studies have verified its behavior and properties.

For high dominance ratio systems, the individual estimators may have underestimated variances, which may propagate to the variance of the three-combined estimator. The aforementioned analytic study was heuristically used to examine the effects of individual variance bias on the combination. An equal additive bias on all individual variances and covariances conservatively overestimates the three-combined variance, whereas an equal multiplicative bias on all individual variances and covariances propagates the same multiplicative bias to the three-combined variance. In MCNP, batch statistics provide an assessment and alleviation of any existing variance bias.

The three-combined k_{eff} estimator, like any Monte Carlo estimator, should be presented as a confidence interval. The three-combined k_{eff} confidence intervals in MCNP

have been shown to have the correct coverage rates for several realistic problems.

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