LA-12658-MS C.3

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Estimation and Interpretation of k_{eff} Confidence Intervals in MCNP

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Edited by Patricia W. Mendius, Group CIC-1
Prepared by M. Ann Nagy, Group XTM

LA-12658

UC-910
Issued: November 1995

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by

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ABSTRACT

MCNP's criticality methodology and some basic statistics are reviewed. Confidence intervals are discussed, as well as how to build them and their importance in the presentation of a Monte Carlo result. The combination of MCNP's three k_{eff} estimators is shown, theoretically and empirically, by statistical studies and examples, to be the best k_{eff} estimator. The method of combining estimators is based on a solid theoretical foundation, namely, the Gauss-Markov Theorem in regard to the least squares method. The confidence intervals of the combined estimator are also shown to have correct coverage rates for the examples considered.

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Reading This Report

We anticipate that the readers of this report will possess a broad spectrum of desires and technical backgrounds. Therefore, we outline our perceived levels for reading this report.

Level 1. You desire only a briefing on how MCNP performs a criticality calculation and which estimator you should use. Read the Introduction, Section 2: Monte Carlo Calculation of k_{eff} for Confidence Intervals, Section 4: MCNP's k_{eff} Estimators, and the Conclusion.

Level 2. You want a briefing on how MCNP performs a criticality calculation, the basic statistics behind the calculation, which estimator to use, and how to build a confidence interval. Read the Introduction, Section 2: Monte Carlo Calculation of k_{eff} for Confidence Intervals, Section 3: Basic Statistical Concepts in Statistical Inference, Section 4: MCNP's k_{eff} Estimators, the part of Section 5 entitled Statistical Studies for the Three-Combined Estimator, and the Summary and Conclusions.

Level 3. You are familiar with Monte Carlo criticality calculations and want to know about the combined estimator in detail. Read from the Introduction to the Summary and Conclusions, skipping Section 2, if desired. Additionally, you may want to take a good look at the Appendices to gain some background on common distributions arising in statistics, to gain insight on linear regression solved by both the least squares and maximum likelihood methods, and to look at the propagation of variance bias in the combined estimator.

I. INTRODUCTION

Throughout this report, we emphasize that MCNP does not produce a point estimate of the system k_{eff}. It provides a range of values that, with some specified confidence, will include the true k_{eff}. In this report, a true value from a stochastic calculation is the precise value for an infinite number of histories. To increase the probability that the range includes the true k_{eff}, either more histories need to be run, or the range must be increased. This range is called a *confidence interval* and goes hand-in-hand with any Monte Carlo result. We will describe how to construct confidence intervals from the estimate of k_{eff} and its standard deviation or, in general, any mean and standard deviation.

MCNP has three separate k_{eff} estimators: the collision, absorption, and track length estimators. Each one has its own characteristic qualities that allow it to perform better for different physical and computational situations. The best k_{eff} estimator is the least squares combination of them, or, more appropriately, the maximum likelihood combination with the additional constraint of an underlying multivariate normal distribution. The Gauss-Markov Theorem states that, for a known covariance matrix, the least squares combination has the minimum variance among all estimators.[1, chapter VI; 2, page 14; 3, page 198] MCNP combines its three estimators using least squares, or maximum likelihood, but it uses a covariance matrix estimated from the data. This results in an almost-optimum estimator that approaches the optimum estimator with increasing cycles and is the best available estimator. We derive the detailed method of combining the three estimators; the derivation is based heavily on a paper by Max Halperin.[4]

We examine the behavior of the combined estimator, both theoretically and empirically. The most striking behavior of the combined estimator is that it sometimes lies outside the range of highly and positively correlated individual estimators. This behavior is absolutely correct and should cause no concern. The issue was taken up by the nuclear data community in the form of "Peelle's Pertinent Puzzle" and has brought about better understanding of the application and behavior of the least squares method of combining data. The results of a statistical simulation demonstrate the efficacy of combining three estimators that are relatively highly correlated. We also perform statistical studies on MCNP results for a homogeneous U-233/water mixture in both finite and infinite mediums, the Godiva reactor, a simplified Jezebel reactor, and a two-component system. All the examples supply further evidence of the superiority of the three-combined estimator.

II. MONTE CARLO CALCULATION OF k_{eff} FOR CONFIDENCE INTERVALS

MCNP™ is a general Monte Carlo code for neutron and radiation transport with a specific option applicable to nuclear criticality: estimating the k_{eff} of a multiplying system. Once k_{eff} is estimated, it is used with its estimated standard deviation to build a k_{eff} confidence interval, as discussed in Section B.

A. k_{eff} Defined

k_{eff} is generally thought of as the ratio of the number of neutrons in one generation to the number in the previous generation in a system containing fissionable material. It is the dominant eigenvalue of the neutron transport equation and is used to describe the state of criticality of a fissionable system. Therefore, k_{eff} may also be thought of as the number by which $\bar{\nu}$ must be divided to make the system exactly critical, where $\bar{\nu}$ is the average number of neutrons produced per fission. It can also be thought of as the ratio of neutron production to neutron loss. If production equals loss, then $k_{eff} = 1$ and the system is said to be critical. If the production is less than the loss, $k_{eff} < 1$, the system is subcritical, and, in the absence of neutron sources, the number of neutrons decreases with each subsequent generation. If the production is greater than the loss, $k_{eff} > 1$, the system is supercritical, and the number of neutrons increases with each generation.

B. Monte Carlo Criticality Methodology

A Monte Carlo criticality calculation literally approximates the neutron generations by discrete cycles, where each cycle is made up of simulated neutrons. The term "cycle" refers to a computational approximation of a generation. Instead of simulating the actual number of neutrons in a generation, say 10^8 to 10^{16}, only computationally practical numbers are simulated, on the order of hundreds or thousands. The simulated neutrons, one by one, are transported through their lifetime, from birth to death. The simulated neutron lifetime is termed a "history." Both the number of cycles and histories per cycle are specified by the user. Appropriate physical probability density functions are sampled to determine the energy of the newly born neutron, what direction and how far it travels before its next collision, with which isotope it collides, whether it scatters or is absorbed, the number of fission neutrons produced, if any, and so on. A key to the Monte Carlo criticality calculation is the production of new fission neutrons. If, at a collision, a fission neutron is produced, it is stored and becomes one of the starting fission neutrons for the *next* cycle. The fission production is normalized so that the original number of starting fission neutrons is approximately maintained for each cycle.

At every collision with a fissionable isotope, an appropriate contribution is made to the collision and absorption estimators. For every distance traversed in a fissionable material, a contribution is made to the track length estimator. At the end of a cycle, when all of the fission neutron histories have been completed, the values of the estimators are three separate, but correlated, estimates of k_{eff} for that cycle.

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Before accumulating any k_{eff} or other tally data, enough cycles must be performed so that the fission neutrons are distributed according to the fundamental eigenmode of the system. These cycles are called the inactive, or settling, cycles. Unlike a deterministic calculation, a Monte Carlo criticality calculation does not produce meaningful k_{eff} and tally results until the spatial fission source distribution converges. Given that the dominance ratio is the ratio of the second eigenvalue to the dominant eigenvalue, it is seen that for systems with large dominance ratios, usually large systems, the higher order eigenmodes will persist, and the calculation will require a large number of settling cycles. Good spatial sampling is paramount to reaching, and maintaining, the fundamental eigenmode. Maintaining the fundamental eigenmode may become difficult when you consider that the spatial distribution of fission neutrons is correlated between cycles. If, at some cycle, there are statistically too many neutrons in a region of the system, the large number will probably still remain at the next cycle. The same argument applies to an undersampled region of the system. The effects of the cycle-to-cycle correlation are even more pronounced for systems with high dominance ratios, because there is effectively less neutron communication between different regions of the system.

Once the active cycles begin, the cycle k_{eff} estimates are accumulated. For each of the three estimators, the cycle k_{eff} estimates are averaged over all active cycles to give the best estimate for that particular estimator. At any given active cycle, the average and standard deviation for each individual estimator are presented as confidence intervals, a range that should contain the true value of k_{eff} with some given probability. MCNP presents the 68%, 95%, and 99% confidence intervals. The three individual estimates (collision, absorption, and track length) are then optimally combined to give the best estimate of k_{eff}, which is also presented as three confidence intervals. Users may also build their own confidence intervals by using MCNP's estimate and standard deviation and looking up Student's t-percentile for the desired confidence level and the number of degrees of freedom. The Student's distribution and the process of building a confidence interval are presented in Section III.B.

MCNP checks to see that the cycle estimates for each estimator appear to be normally distributed. If the estimates do not appear normally distributed, it may indicate that the source has not converged. MCNP also produces estimates for batches of various numbers of cycles. For example, a run with 100 active cycles could be batched into 50 batches of 2 cycles each or 25 batches of 4 cycles each, although, for statistical purposes, any batch data considered should contain at least 30 batches. The purpose of the batching is to see that the unbatched results do not differ significantly from the batched results. If they do differ, the cycle-to-cycle correlation may be contributing to an underestimation of the variance.

To find the optimum number of inactive and active cycles, MCNP presents the estimates with different number of skipped cycles. At some number of inactive cycles, the variance of the combined estimate is a minimum, due to the competition between source convergence and having a statistically significant number of active cycles. These checks in MCNP are part of the new statistical package in version 4A.

When determining the number of neutron histories per cycle and the number of cycles to run, there are some considerations to keep in mind. Assuming a certain limit on computer resources, there will be a trade-off between these two values. A large number of histories per cycle may give a cycle estimate with small inherent variance, but the effectively reduced number of cycles will not allow for convergence of the source. Conversely, a large number of cycles with a small number of histories per cycle, may allow the source to converge faster, but the variance of the estimators will be higher.[5] Poor spatial sampling is also a consideration with few neutrons per cycle. Bias is another pitfall. Given that the entire phase space is adequately sampled, the remaining bias in k_{eff} is that which is inversely proportional to the number of histories per cycle. Also, Gelbard and Gu show[6] that

$$\frac{|\delta k|}{\sigma} < \frac{N}{2}\left(\frac{\sigma}{k}\right) \quad , \tag{1}$$

where σ is the true standard deviation of k at the end of the problem, k is the true k_{eff}, N is the number of cycles, and δk is the bias. For example, if the relative error was 0.0025 and N is less than 800, then the bias will be less than a standard deviation, and therefore negligible. Note that the bias itself is independent of N since σ^2 goes as $1/N$. Therefore, one desires an adequate number of histories per cycle and a number of cycles that is statistically large enough, but not too large such that the bias in the k_{eff} estimate becomes a significant fraction of the final estimated standard deviation.

III. BASIC STATISTICAL CONCEPTS IN STATISTICAL INFERENCE

The Monte Carlo method is computational experimentation. Data are collected and statistically analyzed in an attempt to estimate true values associated with an underlying, generally unknown, distribution. Using finite samples to acquire knowledge of a distribution is called *statistical inference*,[7] a practice that, for the Monte Carlo method, translates the accumulated data into results. The data collected are called observables and, in Monte Carlo, are samples of random variables because they originate from independent stochastic processes. From the data, then, are estimated the sample mean and sample variance. For Monte Carlo, the culmination of statistical inference is the determination of a confidence interval, that is, a range that includes the true value with some specified confidence.

A. Random Variables and Probability Distributions

A random variable is associated with a probability distribution that describes the relative frequency of all possible values of the random variable.[7] A common distribution is the normal distribution, which is a distribution that many observations in nature seem to follow. The persons responsible for identifying the Normal distribution and developing its proper application are DeMoivre, Laplace, and Gauss (which is why it is also called the Gaussian distribution).[8] It takes the form[9]

$$P_n(x, \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \quad . \tag{2}$$

P_n is the probability that a random sample would take the value x, where the sampling is from a parent distribution with true mean μ and true standard deviation σ. The normal distribution is positive, bell-shaped, and symmetric about zero.

1. Expected Value

The expected value[10,*page* 43] of x, denoted as $E(x)$, is an informative and convenient quantity of a random variable. For the case where the random variable x is discrete, and the probability that $x = a$ is $p(a)$ for all discrete a, the expected value of x is

$$E(x) = \sum_{\text{all } a} a p(a) \quad . \tag{3}$$

When x is a continuous random variable with probability density distribution $f(y)$, the expected value of x is

$$E(x) = \int_{y=-\infty}^{\infty} y f(y) dy \quad . \tag{4}$$

2. Sample Mean, Population Variance, and Variance of the Mean

The sample mean of n samples, x_i, from a probability density distribution $f(x)$,

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \tag{5}$$

and the sample population variance,

$$s^2(x) = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2 \tag{6}$$

estimate the true mean and population variance of the underlying distribution and are calculated with no conditions on the distribution, except that it has a finite variance. Thus,

$$E(\bar{x}) = \mu \tag{7}$$

$$E(s^2(x)) = \sigma^2(x) \quad . \tag{8}$$

The square root of the population variance is the population standard deviation and is a measure of the spread of individual x_i's sampled from the probability density distribution $f(x)$. The relation of the true variance of the mean to the true population variance,[11,5]

$$\sigma^2(\bar{x}) = \frac{\sigma^2(x)}{n} \quad , \tag{9}$$

gives us the expression for the sample standard deviation of the mean,

$$s(\bar{x}) = \frac{s(x)}{\sqrt{n}} \quad . \tag{10}$$

The sample standard deviation of the mean is a measure of the spread of many means, if several were calculated independently with n samples each.[5]

3. The Central Limit Theorem

Since we are dealing with finite samples, our task of statistical inference is not complete. We need to build a confidence interval around the sample mean to give us an idea of how well it estimates the true mean. To do this, we rely upon the distribution of the mean being normal. For Monte Carlo applications, this reliance is justified by the Central Limit Theorem, which states that the mean of a set of n independent random variables from identical distributions with finite variance will be approximately normally distributed for large n, *regardless* of the underlying distribution of the random variables.[7] The Central Limit Theorem is the foundation for statistical inference from Monte Carlo calculations.

B. Building a Confidence Interval

Whenever the estimated mean, $\bar{x}$, of n samples of a random variable is presented along with its standard deviation, s, one must be careful not to build a confidence interval casually by saying that the true answer is in the range $\bar{x} \pm s$. According to the Central Limit Theorem, the distribution of the estimated mean approaches a normal distribution as n approaches ∞. For a finite number of non-normal samples, the distribution is not exactly normal. This non-normal distribution is approximated by Student's t distribution. Student's t distribution, like the normal distribution, is positive, somewhat bell-shaped, symmetric about zero, and approaches the normal distribution as $n \to \infty$. It is used to describe the random variable t,[7] where

$$t = \frac{\bar{x} - \mu}{s(\bar{x})} = \frac{\bar{x} - \mu}{s(x)/\sqrt{n}} \quad . \tag{11}$$

If the x's are normally distributed, the random variable t is distributed exactly as a Student's t distribution. Although the random variable t involves the unknown true value μ, the distribution of t does not rely upon knowledge of μ.[12] Note that, if t contained the true standard deviation, $\sigma(x)$, instead of the sample standard deviation, and the x's were sampled from a normal distribution, t would be normally distributed with mean zero and unit variance.[1,page 131]

The Student's t distribution has a different distribution for each n, written as t_{n-1}, where $n-1$ is the number of degrees of freedom, as depicted in Fig. 1. The degrees of freedom are the number of available independent measurements. Here, we lose one degree of freedom by using all the data to estimate the mean. Additionally, points on the abscissa of a graph of the Student's t distribution are called the *percentiles of the distribution* and are written as $t_{n-1,1-\frac{\alpha}{2}}$, where the second subscript is the confidence level. See Fig. 2. Here, we are considering both sides of the symmetric distribution, so, for a given confidence level $(1-\alpha)$, we have the following equivalent statements:

- with probability $\alpha/2$, t is greater than $t_{n-1,1-\frac{\alpha}{2}}$,
- with probability $\alpha/2$, t is less than $-t_{n-1,1-\frac{\alpha}{2}}$,
- with probability $1-\alpha$, $|\, t \,|$ is less than $t_{n-1,1-\frac{\alpha}{2}}$.

These probabilities are simply the area under the distribution curve. The distributions are tabulated as the percentiles of the t distribution, $t_{n-1,1-\frac{\alpha}{2}}$, as a function of the degrees of freedom and $\frac{\alpha}{2}$, or α, or $1-\alpha$.

The percentile of the Student's t distribution, $t_{n-1,1-\frac{\alpha}{2}}$, serves as a multiplier of the estimated standard deviation of the mean to produce a $(1-\alpha)100\%$ confidence interval:

$$\bar{x} - t_{n-1,1-\frac{\alpha}{2}} s(\bar{x}) \le \mu \le \bar{x} + t_{n-1,1-\frac{\alpha}{2}} s(\bar{x}) \quad . \tag{12}$$

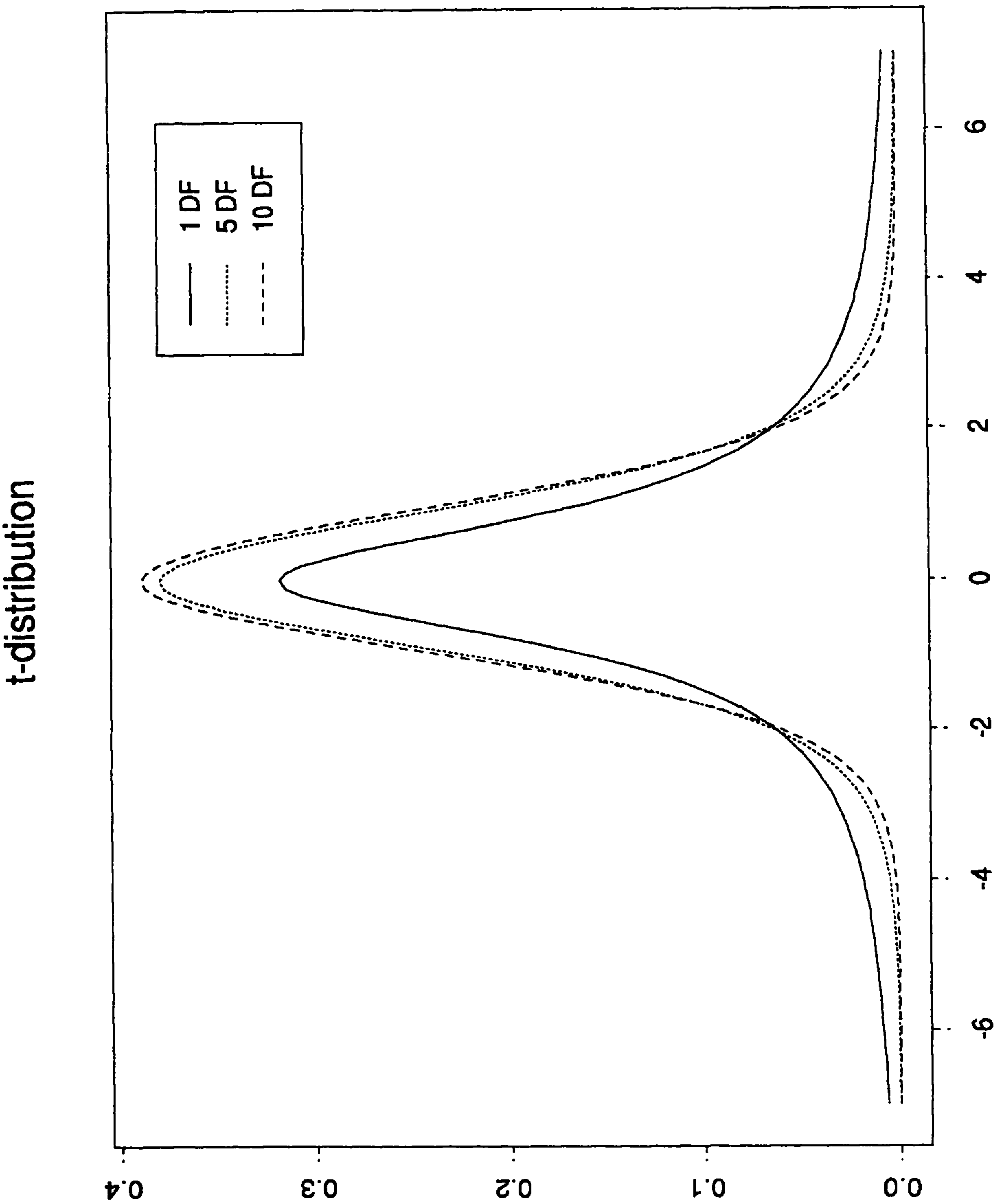

Fig. 1. The Student's t distribution for various degrees of freedom (DF).

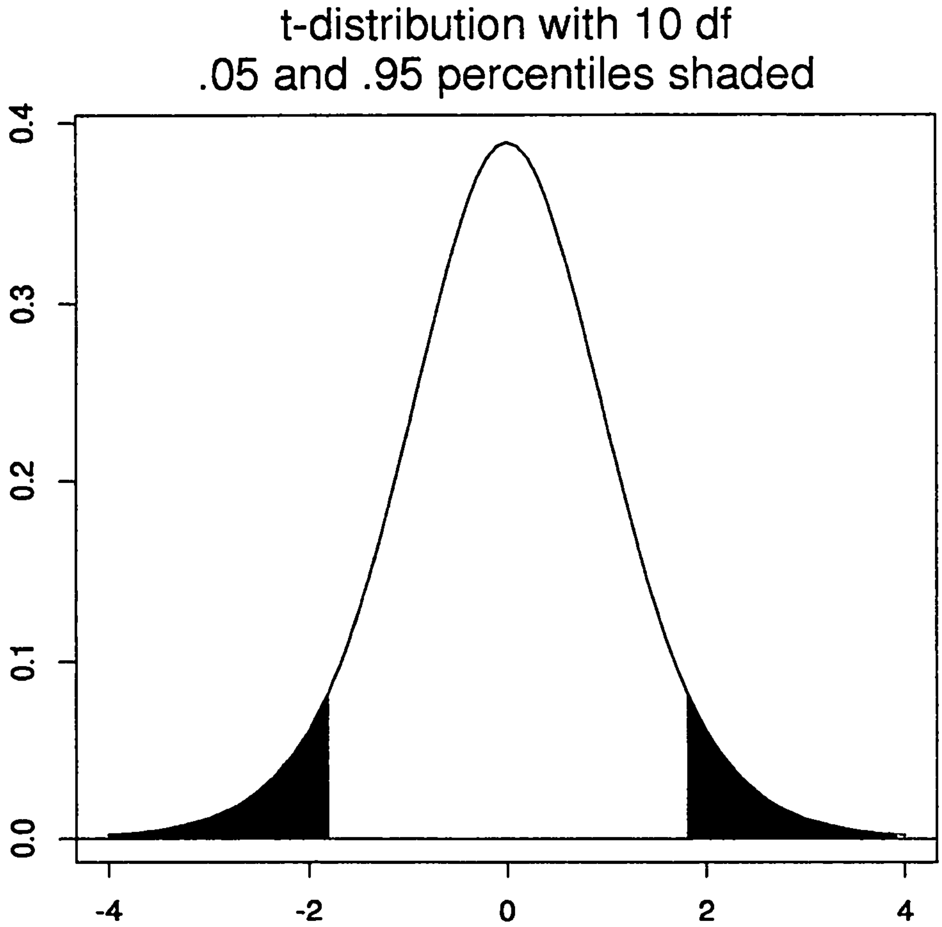

Fig. 2. The Student's t-percentile for a $1-\alpha$ confidence level on a the Student's t-distribution with $n-1$ degrees of freedom (df).

We say that, with $(1-\alpha)100\%$ confidence, this interval includes the true mean, or, alternatively, if the n samples were repeated several times, this interval would *not* include the true mean α 100% of the time.

D. L. Barr[13] cautions us regarding the interpretation of the confidence interval. Actually, a confidence interval is just one observation on a true random interval–just like an estimate is one observation on an estimator.

C. Correlation Between Estimators

The preceding discussions have dealt with the characteristics of one variable. Now consider two random variables, x and y, that are distributed according to a joint probability distribution $f(x, y)$. The linear correlation coefficient, ρ_{xy}, is defined as

$$\rho_{xy} = \frac{\sigma_{xy}^2}{\sqrt{\sigma_x^2 \sigma_y^2}} \quad , \tag{13}$$

where σ_{xy}^2 is the covariance between x and y. The correlation coefficient is approximated by $\hat{\rho}_{xy}$,

$$\hat{\rho}_{xy} = \frac{\hat{\sigma}_{xy}^2}{\sqrt{\hat{\sigma}_x^2 \hat{\sigma}_y^2}} \tag{14}$$

$$= \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum(x_i - \bar{x})^2 \sum(y_i - \bar{y})^2}} \quad , \tag{15}$$

where the sums are from 1 to n. Both the numerator and denominator in Eq. 15 have a divisor equal to $(n-1)$, the degrees of freedom, that cancels out.

The correlation coefficient may be as low as -1, meaning x and y are fully anticorrelated, or as large as $+1$, meaning x and y are fully correlated. If x and y are independent, they are not correlated and $\rho_{xy} = 0$. However, the converse is not necessarily true.[1,page 87] The degree of correlation tells only about the linear dependency of one variable on the other; it gives an indication of the linear association between the variables. High correlation indicates the ability to predict one variable's *variation* with the *variation* of another. Aitken[1,page 148] has an illustrative example depicting the fact that correlation does not imply dependence or independence:

$$u = a\cos x + b\sin x$$

$$v = a\sin x - b\cos x \quad .$$

We see that u and v are uncorrelated, but (nonlinearly) dependent, since

$$u^2 = -v^2 + a^2 + b^2 \quad .$$

Whereas we use the correlation coefficient to determine variable association, we use regression analysis to examine any causal relation (dependence of one variable on other variables).[11,page 224]

IV. MCNP'S k_{eff} ESTIMATORS

A. Estimators and Their Qualities

Consider a random variable, x, with an associated distribution with unknown mean, μ. Suppose n independent random samples, $\{x_1, x_2, \ldots, x_n\}$, are selected from the probability density distribution of x. An **estimator**, $X(x_1, x_2, \ldots, x_n)$, is a specific function of the random samples that statistically represents the true unknown mean. The particular value of the estimator X is called an **estimate**. Often, the two terms are used interchangeably, even though they are strictly different. In Monte Carlo, the estimator is the average of the random samples. Desirable qualities of an estimator are that it is

- unbiased,
- consistent, and
- efficient.

An estimator, X, is unbiased,[10] if its expected value equals the true value, μ,

$$E(X) = \mu$$

for all μ. If a nonzero bias, b, exists, then

$$E(X) = \mu + b.$$

The concept of unbiasedness has its foundation in repeated experiments, each containing multiple samples.

Consistency, on the other hand, applies to a single experiment where the sample size, n, becomes large.[10] An estimator, X, is consistent if it approaches, in the probabilistic sense, the true value, μ, as n gets large.

If, in a group of unbiased estimators, there exists one estimator with minimum variance, it is called the efficient estimator among the group.[10]

In MCNP, we assume the k_{eff} estimators are unbiased. They are consistent since the variance of the estimates decreases as $1/n$, where n is the number of cycles.[14] The three-combined estimator is efficient since, by the Gauss-Markov Theorem, it has the smallest variance among linear estimators.[1,chapter VI;2,page 14;3,page 198]

B. k_{eff} Estimators in MCNP and Their Presentation

MCNP has three different estimators that it uses to estimate k_{eff}, the criticality of a multiplying system. They are the collision, absorption, and track length estimators. The absorption estimator takes two forms: analog absorption, or implicit absorption when implicit capture, a common variance reduction technique, is employed.

Let us look at the mathematical expression of each estimator in MCNP. These equations are taken directly from the MCNP manual[15] and each is the estimate of k_{eff} at a particular cycle. Averaging over all cycles gives the final estimate of k_{eff} for each of the three estimators. The superscripts C, AA, IA, and TL indicate collision, analog absorption, implicit absorption, and track length, respectively.

For collision,

$$k_{eff}^{C} = \frac{1}{N}\sum_{i} W_i\left\{\frac{\sum_k f_k\overline{\nu}_k\sigma_{F_k}}{\sum_k f_k\sigma_{T_k}}\right\} \qquad (16)$$

where
i = collisions where fission is possible,
k = isotopes involved in the i^{th} collision,
σ_{T_k} = total microscopic cross section for nuclide k,
σ_{F_k} = microscopic fission cross section for nuclide k,
$\overline{\nu}_k$ = average number of prompt or total neutrons produced per fission by the collision isotope at the incident energy,
f_k = atomic fraction for nuclide k,
N = nominal source size for cycle, and
W_i = weight of particle entering the collision.

For analog absorption,

$$k_{eff}^{AA} = \frac{1}{N}\sum_{i} W_i\frac{\overline{\nu}_k\sigma_{F_k}}{\sigma_{A_k}+\sigma_{F_k}} \qquad (17)$$

where i is summed over each analog capture event in the k^{th} isotope, and

σ_{A_k} = microscopic absorption cross section, **not** including fission (traditional nomenclature has absorption including fission).

For implicit absorption,

$$k_{eff}^{IA} = \frac{1}{N}\sum_{i} W_i\left(\frac{\sigma_{A_k}+\sigma_{F_k}}{\sigma_{T_k}}\right)\frac{\overline{\nu}_k\sigma_{F_k}}{\sigma_{A_k}+\sigma_{F_k}} \qquad (18)$$

where i is summed over all collisions where fission is possible, and

$$\frac{\sigma_{A_k}+\sigma_{F_k}}{\sigma_{T_k}}$$

is the frequency of analog capture at each collision, the quantity by which the weight is adjusted at each collision.

For track length,

$$k_{eff}^{TL} = \frac{1}{N}\sum_{i} W_i \rho d \sum_{k} f_k \overline{\nu}_k \sigma_{F_k} \tag{19}$$

where d = distance traversed by the neutron since the last event,
i = all neutron trajectories, and
ρ = atomic density in the cell.

Each of the three estimators provides an estimate of k_{eff} for each cycle. Averaging over all cycles gives a mean and a standard deviation of the mean which allow for the building of confidence intervals, as discussed in Section B of Chapter III.

C. Behavior of MCNP's k_{eff} Estimators

There are certain cases where one estimator may be expected to outperform another, as evidenced by its smaller sample variance (relative efficiency). The determining factors include the kind of material in the system, the number of materials in the system, size of the regions, neutron energy, and the use of variance reduction. These factors also affect the correlation between the three estimators.

Estimator superiority due to material effects is evident in the case of systems with a dominant fissionable isotope that is a $1/v$-absorber. In this case, both the numerator and denominator of the analog absorption estimator, Eq. 17, will exhibit a $1/v$ behavior and tend to cancel, thus producing a smaller overall variance than the other estimators.

For optically thin regions with few collisions, the track length estimator should allow a better sampling of the region and, hence, a smaller variance.

For larger regions, we expect the collision estimator to have a lower variance than the track length estimator since the collision estimator is a point-wise value and, depending on the particle weight, may exhibit less variation than the track length estimator. As the total cross section gets increasingly large, the collision estimator approaches the track length estimator,[16] since the length between collisions becomes vanishingly small.

Note that for only one fissionable isotope and implicit capture, the collision and absorption estimators are exactly the same and it follows that they are perfectly positively correlated. In this case, the information acquired from one estimator is not increased by considering the other estimator.

Given that the correlation coefficient is the degree with which one can predict the *variation* in one variable due to the *variation* in another, it is dangerous and incorrect to infer any sort of dependency between the variables from a correlation coefficient. But, it is difficult to resist hypothesizing the cause of the magnitude and sign of the correlation coefficient, at least for simple problems. We consider an infinite medium made up of a homogeneous mixture of U-233 and water. In particular, we look at the effects of using either analog or implicit capture on the correlation coefficients. For a specific MCNP run, we obtained the correlation coefficients as found in Table I.

TABLE I. Estimator Correlation for Implicit and Analog Capture

pairwise estimators	correlation coefficient analog	correlation coefficient implicit
collision/absorption	-0.0404	-0.8545
absorption/track length	-0.0412	-0.8459
collision/track length	0.9958	0.9876

Table I shows that the collision and track length estimators are highly correlated for both analog and implicit capture. However, the correlation between these two and the absorption estimator is highly dependent upon the type of capture. For analog capture, the scattering is such that the absorptions appear nearly independent of the collisions and track lengths. For implicit capture, they are highly anticorrelated. For implicit capture, the collision and absorption estimators compete for the weight. When a large contribution is made to the absorption estimator, the subsequent weight reduction leaves less contribution to both the track length and collision estimators. Resonance regions would produce an even more pronounced effect. This trade-off at the event level causes the anticorrelation. Typically, the drastic behavior shown in Table I is not seen in realistic systems.

D. The Best Estimate of k_{eff}

In an attempt to get the best estimate of k_{eff}—to produce the smallest valid confidence interval, the variances of the three individual estimates and their statistical relationships to each other are utilized to the fullest. This superiority is found in the three-combined estimator, which we discuss in the next section. It outperforms the individual estimators in the sense that it almost always has the smallest interval, while using all the available information.

V. MCNP'S COMBINED k_{eff} ESTIMATOR

MCNP presents confidence intervals for the three separate k_{eff} estimators. MCNP also calculates the simple pairwise average of the three individual estimates and the simple average of all three estimates. In addition, the two-combined averages are calculated. The big winner though is the three-combined estimator in that it almost always produces intervals with the shortest length. The two- and three-combined estimator are specific applications of linear regression.

Regression analysis is a statistical study where the relationship between one dependent variable, y, and one or more independent variables is estimated.[7] For one independent variable, we have $y = f(x)$, which is called the regression of y on x.[1] The coefficients that constitute f are called the regression parameters, which would be the slope and intercept of a line. There are many ways to estimate the regression parameters, such as the least squares method, the principle of maximum likelihood, and the method of moments. It is interesting to note that the maximum likelihood principle with the assumption of normality produces the same parameter estimation as the least squares method. Appendix B contains a detailed derivation of the least squares parameter estimation, as well as a brief look at the maximum likelihood principle to show that, indeed, both result in the same parameter estimation.

The authoritative reference on the combination of unbiased correlated estimates is a paper by Max Halperin, "Almost Linearly-Optimum Combination of Unbiased Estimates."[4] The paper is terse, so we will reproduce the derivation of the combined estimator in more detail and specifically gear it toward application in MCNP. Thus, we will look only at Halperin's Case I, that of correlated estimators with unequal but unknown variances.

A. Derivation of the Combined Estimator (Annotation of Halperin's Paper)

We begin with the multivariate distribution from which we obtain the multivariate samples X: $\{x_{1,1}, \ldots, x_{1,n}; x_{2,1}, \ldots, x_{2,n}; \ldots, x_{k,n}\}$, where n is the number of active k_{eff} cycles and k is the number of estimators, where, in MCNP, $k = 3$. The average over n active cycles yields a vector of estimators of length k, $\bar{\mathbf{X}} = (\bar{x}_1, \ldots, \bar{x}_k)$, where each element may have a different variance and is correlated to the others. The expected value of each $\bar{x}$ is the true value of k_{eff}, u, and the variances and covariances make up a full covariance matrix,[17] $\mathbf{\Sigma}$. Thus, the multivariate sample is, under Halperin's assumption, normally distributed with mean vector $u\mathbf{e}$ and variance $\mathbf{\Sigma}$, $X \sim N(u\mathbf{e}, \mathbf{\Sigma})$, where the vector $\mathbf{e}$ is a vector of ones and $\sim N(u\mathbf{e}, \mathbf{\Sigma})$ means "distributed normally with mean $u\mathbf{e}$ and variance $\mathbf{\Sigma}$." Note that Halperin represents a vector as a row instead of a column.

Halperin first explores the maximum likelihood estimator and its variance, where we see the multivariate extension of the maximum likelihood equations in Appendix B. Using an "H" to indicate an equation in Halperin's paper, note that Eq. H2.1 contains the true expressions for the mean, u, and the covariance matrix. Equations H2.2 are obtained by setting equal to zero the partial derivatives of L with respect to u, σ_{ii}, and σ_{ih}, respectively. The latter two equations give an estimate of the inverse covariance matrix as Halperin does in Eq. H2.3. Equation H2.2a gives an estimate of the mean, but uses the unknown true inverse covariance matrix; substitution of the estimated inverse covariance matrix allows the estimation of u, $\hat{u}$, in Eq. H2.4. The asymptotic variance of u is denoted by σ^2_{opt}:

$$\sigma^2_{opt} = \frac{1}{n\mathbf{e}\Sigma^{-1}\mathbf{e}'}. \quad (20)$$

This is the asymptotic variance because, as Halperin states, the maximum likelihood estimator, $\hat{u}$, is "asymptotically normal and efficient." An efficient estimator is the one, among a set of estimators, that has the smallest variance. So, for small n, σ^2_{opt} will not correctly describe the true variance and an estimate of it cannot be used to build a confidence interval.

Halperin then proposes minimizing Eq. H2.6, the residual sum of squares, which is the first step in the least squares method (see Appendix B), and would produce the same normal equations as the maximum likelihood principle, where the normal equations are obtained by maximizing the likelihood function. He additionally introduces a transformation to $\bar{\mathbf{X}} = (\bar{x}_1, \ldots, \bar{x}_k)$

$$\mathbf{z}' = \mathbf{A}\bar{\mathbf{x}}', \quad (21)$$

where

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & \cdot & \cdot & \cdot & 0 \\ 1 & -1 & & & & \\ \cdot & & \cdot & & 0 & \\ \cdot & & & \cdot & & \\ \cdot & & 0 & & \cdot & \\ 1 & & & & & -1 \end{pmatrix}. \quad (22)$$

The transformed vector, $\mathbf{z}$, is

$$\mathbf{z}' = \begin{pmatrix} \bar{x}_1 \\ \bar{x}_1 - \bar{x}_2 \\ \bar{x}_1 - \bar{x}_3 \\ \vdots \\ \bar{x}_1 - \bar{x}_k \end{pmatrix}. \quad (23)$$

Observe that $E(z_1) = u$ and $E(z_2) = \cdots = E(z_k) = 0$, since all k estimators are unbiased. Halperin uses this transformation because it allows the building of confidence intervals with Student's t-percentiles. The covariance matrix becomes, under the transformation,[2,page 8]

$$\Sigma_z = \mathbf{A}\Sigma\mathbf{A}' \quad (24)$$

$$\Sigma_z^{-1} = \mathbf{A}'\Sigma^{-1}\mathbf{A}. \quad (25)$$

In accordance with the transformation, Halperin partitions the transformed covariance matrix as shown in Eq. H2.10, where Σ_{z11} is a (1×1) matrix and Σ_{z22} is a $(k-1)\times(k-1)$ matrix. He then looks at the difference between the logarithm of the density of $\{z_1, z_2, \ldots, z_k\}$ and the logarithm of the density of $\{z_2, \ldots, z_k\}$. The partial derivative of this quantity with respect to u yields an estimate of u—Eq. H2.13 and, subsequently, Eq. H2.14, where Σ is replaced by S,

$$\hat{u} \;=\; z_1 - \mathbf{S}_{z12}\,\mathbf{S}_{z22}^{-1}\bar{\mathbf{d}}', \tag{26}$$

where $\bar{\mathbf{d}}' = (z_2,\ \ldots,\ z_k)'$

At this point, Halperin observes that the estimate of u, $\hat{u}$, looks like an intercept in a regression analysis, and considers the conditional distribution of z_{1j} given $z_{2j}, z_{3j}, \ldots, z_{kj}$, concluding that the z_{1j} are independent and normally distributed with mean z_1 as given by Eq. H2.13 and variance [3,page 69,also]

$$\begin{aligned}\boldsymbol{\Sigma}_{z11} - \boldsymbol{\Sigma}_{z12}\boldsymbol{\Sigma}_{z22}^{-1}\boldsymbol{\Sigma}_{z21} &= \frac{1}{\mathbf{e}\boldsymbol{\Sigma}^{-1}\mathbf{e}'} \\ &= n\sigma_{opt}^2. \end{aligned} \tag{27}$$

The variance of $\hat{u}$ (given in Eq. H2.14) is given at the bottom of page 39 of Halperin's paper as

$$\sigma_{\hat{u}}^2 \;=\; n\sigma_{opt}^2\left(\frac{1}{n} + \bar{\mathbf{d}}\;\mathbf{S}_d^{-1}\;\bar{\mathbf{d}}'\right). \tag{28}$$

It is easily seen as a generalization of the variance of the estimated intercept in the simple least squares case of one dependent variable and one independent variable (see Appendix B). The generalization includes heteroscedasticity (unequal variances) and correlation, all in matrix form.

B. MCNP's Combination of Two Estimates

The transformation of $\bar{\mathbf{x}}$ to $\mathbf{z}$ for two different estimates is given by (writing vectors as columns)

$$\mathbf{z} = \mathbf{A}\bar{\mathbf{x}} \;=\; \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \bar{x}_1 \\ \bar{x}_2 \end{pmatrix} = \begin{pmatrix} \bar{x}_1 \\ \bar{x}_1 - \bar{x}_2 \end{pmatrix}. \tag{29}$$

In this case, the regression is for z_1 on z_2, which has an expected value of zero.

For the case of two different estimates, Eq. 24 gives

$$\begin{aligned}\boldsymbol{\Sigma}_z &= \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \sigma_{11}^2 & \sigma_{12}^2 \\ \sigma_{12}^2 & \sigma_{22}^2 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} \sigma_{11}^2 & \sigma_{11}^2 - \sigma_{12}^2 \\ \sigma_{11}^2 - \sigma_{12}^2 & \sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2, \end{pmatrix}. \end{aligned} \tag{30}$$

where the true variances, σ_{ij}, are estimated by $\hat{\sigma}_{ij}$:

$$\begin{aligned}
\hat{\sigma}^2_{ij} &= \frac{s^2_{ij}}{n-1} \\
\hat{\sigma}^2_{ij} &= \frac{1}{n-1}\sum_{\ell=1}^{n}(x_{i\ell}-\bar{x}_i)(x_{j\ell}-\bar{x}_j) \\
&= \frac{1}{n-1}\left[\sum_{\ell=1}^{n}x_{i\ell}x_{j\ell}-\sum_{\ell=1}^{n}x_{i\ell}\sum_{\ell=1}^{n}x_{j\ell}/n\right]. \qquad (31)
\end{aligned}$$

The $\hat{\sigma}_{ij}$'s are the sample population covariances between the n values of $x_{i\ell}$ and the n values of $x_{j\ell}$. When $i=j$, $\hat{\sigma}^2_{ii}$ is the estimated population variance of the n values of $x_{i\ell}$. The term s^2_{ij} is called the sum of squares of deviations about the mean, and when divided by the degrees of freedom, here $n-1$, gives the unbiased estimate of σ^2_{ij}. So, $\mathbf{\Sigma}$ contains the elements σ^2_{ij} and $\hat{\mathbf{\Sigma}}$ contains the elements $\hat{\sigma}^2_{ij}$. The matrix $\mathbf{S}$ contains the elements s^2_{ij}, the sums of squares, thus giving the relation $\hat{\mathbf{\Sigma}} = \mathbf{S}/(n-1)$.

The combined estimated mean $\hat{u}$ is given by Eq. 26. For two estimates, the matrix partitions are scalars, thus

$$\mathbf{S}_{z12} = s^2_{11} - s^2_{12}, \qquad (32)$$

and

$$\begin{aligned}
\mathbf{S}^{-1}_{z22} &= \left(s^2_{11}+s^2_{22}-2s^2_{12}\right)^{-1} \\
&= \frac{1}{(s^2_{11}+s^2_{22}-2s^2_{12})}. \qquad (33)
\end{aligned}$$

For two estimates, using Eqs. 29, 32, and 33, Eq. 26 becomes

$$\begin{aligned}
\hat{u} &= \bar{x}_1 - \frac{(s^2_{11}-s^2_{12})(\bar{x}_1-\bar{x}_2)}{s^2_{11}+s^2_{22}-2s^2_{12}} \qquad (34) \\
&= \frac{(\hat{\sigma}^2_{22}-\hat{\sigma}^2_{12})\bar{x}_1 + (\hat{\sigma}^2_{11}-\hat{\sigma}^2_{12})\bar{x}_2}{\hat{\sigma}^2_{11}+\hat{\sigma}^2_{22}-2\hat{\sigma}^2_{12}} \qquad (35) \\
&= \frac{\hat{\sigma}^2_{22}-\hat{\sigma}^2_{12}}{\hat{\sigma}^2_{11}+\hat{\sigma}^2_{22}-2\hat{\sigma}^2_{12}}\bar{x}_1 + \frac{\hat{\sigma}^2_{11}-\hat{\sigma}^2_{12}}{\hat{\sigma}^2_{11}+\hat{\sigma}^2_{22}-2\hat{\sigma}^2_{12}}\bar{x}_2 \\
&= w_1\bar{x}_1 + w_2\bar{x}_2 \qquad (36)
\end{aligned}$$

where Eq. 36 defines the weighting factors w_1 and w_2. Note that $\hat{\sigma}^2$ may be used in Eq. 35 instead of s^2, since the $n-1$ factor cancels. Equation 34 is used to calculate the combined estimator ZH for two different k_{eff} estimates in MCNP's subroutine KCALC.

On the bottom of page 39, Halperin states that under the condition of multivariate normality, $\hat{u}$ is normally distributed and the variance is, substituting Eq. 27 into Eq. 28 (and casting vectors in the usual column form),

$$\sigma_{\hat{u}}^2 = \left(\Sigma_{z11} - \Sigma_{z12}\,\Sigma_{z22}^{-1}\,\Sigma_{z21}\right)\left(\frac{1}{n} + \bar{\mathbf{d}}'\,\mathbf{S}_d^{-1}\,\bar{\mathbf{d}}\right), \tag{37}$$

where Σ and $\mathbf{S}$ are partitioned similarly,

$$\mathbf{S}_d = \mathbf{S}_{z22} \quad ,$$

and, again,

$$\bar{\mathbf{d}} = (\bar{x}_1 - \bar{x}_2, \cdots, \bar{x}_1 - \bar{x}_k)', \tag{38}$$

for k different estimators.

It is appropriate to mention now that the proper way to think about a sample variance, $\hat{\sigma}^2$, is the sums of squares of deviations, s^2, divided by the number of degrees of freedom, df, in the calculation of s^2. The number of degrees of freedom is the number of independent variables available in the calculation. Then the sample variance is an unbiased estimate of the true variance, or, in other words, the expected value of the sample variance is the true variance:[18, *for example*]

$$E(\hat{\sigma}^2) = E\left(\frac{s^2}{df}\right) = \sigma^2 \quad . \tag{39}$$

Having said this, we would estimate the first bracketed term in Eq. 37 by replacing the Σ's by $\mathbf{S}$'s and dividing by the degrees of freedom. For two estimators of n samples each, the degrees of freedom available in the calculation of $\mathbf{S}$ is $n-2$ because the calculation of $\mathbf{S}$ includes two averages. The variance of the two-combined estimator becomes

$$\begin{aligned}\hat{\sigma}_{\hat{u}}^2 &= \frac{1}{n-2}\left(s_{11}^2 - \frac{(s_{11}^2 - s_{12}^2)^2}{s_{11}^2 + s_{22}^2 - 2s_{12}^2}\right)\left(\frac{1}{n} + \frac{(\bar{x}_1 - \bar{x}_2)^2}{s_{11}^2 + s_{22}^2 - 2s_{12}^2}\right) \\ &= \frac{(s_{11}^2 s_{22}^2 - s_{12}^4)}{n(n-2)}\left[\frac{(s_{11}^2 + s_{22}^2 - 2s_{12}^2) + n(\bar{x}_1 - \bar{x}_2)^2}{(s_{11}^2 + s_{22}^2 - 2s_{12}^2)^2}\right].\end{aligned} \tag{40}$$

In the second line of Eq. 40, notice that $(\bar{x}_1 - \bar{x}_2)^2/(n-2)$ is expected to go to zero as $1/n^2$, since the $\bar{x}$'s are both expected to approach the true value as $1/\sqrt{n}$. Therefore, the second bracketed term should asymptotically approach $1/n$, and the variance of the two-combined estimate should asymptotically approach σ_{opt}^2 with a $1/n$ behavior. Equation 40 clearly shows that the variance of the combination is invariant no matter which estimator is selected as x_1.

In MCNP, Eqs. 34 and 40 are used in subroutine KCALC to calculate the pairwise combined estimators and their standard deviations. First, the denominator in Eq. 34 is set to variable T5:

```
t5=cv(i,i)+cv(j,j)-cv(i,j)-cv(i,j)
```

where the CV's are the s_{ij}'s in this report and the pairwise permutations are $i = 1, 2, 3$ and $j = 2, 3, 1$. T5 is checked for relative size compared to the sum of the magnitude of the variances and covariances. If it is too small, it is set to zero, and the combination will not occur:

```
 if(t5.lt.1.e-10*(abs(cv(i,i))+abs(cv(j,j))+
1 abs(cv(i,j))))t5=0.
```

The two-combined estimate and its relative error (which is later converted to a standard deviation by multiplying by the two-combined estimate) are as follows

```
 if(t5.ne.0.)zh(i)=za(i)-(za(i)-za(j))*(cv(i,i)-
1 cv(i,j))/t5
 if(t5.ne.0..and.zh(i).ne.0.)eh(i)=f2*sqrt(abs
1 ((cv(i,i)*cv(j)-cv(i,j)**2)*(t5+f0*(za(i)-za(j))**2)
2 /t5**2))/mc*zh(i)
```

where ZA are the individual estimators: collision, absorption, and track length for $i = 1, 2, 3$; F0 = MC = n; and F2 = $n/(n-2)$.

The estimated correlation coefficient has the usual definition between two estimators of

$$\hat{\rho}_{ij} = \frac{\hat{\sigma}^2_{ij}}{\left(\hat{\sigma}^2_{ii}\hat{\sigma}^2_{jj}\right)^{1/2}} . \tag{41}$$

Equation 41 is used to calculate the correlation coefficient ZC in KCALC:

```
 if(cv(i,i)*cv(j,j).gt.0.)zc(i)=cv(i,j)/sqrt(abs(cv(i,i)
1 *cv(j,j))).
```

Since $\hat{\sigma}^2_{ij}$ may be positive or negative, the values for $\hat{\rho}_{ij}$ range between -1 and 1. For $\hat{\rho}_{ij} = -1$, $\hat{\sigma}^4_{ij} = \hat{\sigma}^2_{ii}\hat{\sigma}^2_{jj}$, thus reducing σ^2_{u} to zero, as seen in Eq. 40. A $\hat{\rho}_{ij}$ value of unity is perfect positive correlation. Perfect positive correlation when $\bar{x}_i$ does not approximately equal $\bar{x}_j$ should be a reason for concern, since it indicates a bias in one or both of the estimators. Independent estimators will result in a $\hat{\rho}_{ij} \approx 0$ (the converse inference is not necessarily true) and $\hat{\rho}_{ij} \approx -1$ indicates nearly perfect negative correlation.

C. The Equations for Three Combined Estimators

The variance matrix for three different estimators using the transformation in Eq. 21 is

$$
\begin{aligned}
\boldsymbol{\Sigma}_z &= \begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \sigma_{13}^2 \\ \sigma_{12}^2 & \sigma_{22}^2 & \sigma_{23}^2 \\ \sigma_{13}^2 & \sigma_{23}^2 & \sigma_{33}^2 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\
&= \begin{pmatrix} \sigma_{11}^2 & \sigma_{11}^2 - \sigma_{12}^2 & \sigma_{11}^2 - \sigma_{13}^2 \\ \sigma_{11}^2 - \sigma_{12}^2 & \sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2 & \sigma_{11}^2 + \sigma_{23}^2 - \sigma_{12}^2 - \sigma_{13}^2 \\ \sigma_{11}^2 - \sigma_{13}^2 & \sigma_{11}^2 + \sigma_{23}^2 - \sigma_{12}^2 - \sigma_{13}^2 & \sigma_{11}^2 + \sigma_{33}^2 - 2\sigma_{13}^2 \end{pmatrix}. \qquad (42)
\end{aligned}
$$

The combined $\hat{u}$ for three different estimators is given by Eq. 26 with Eq. 42 where

$$
\boldsymbol{\Sigma}_{z12} = \begin{pmatrix} \sigma_{11}^2 - \sigma_{12}^2 & \sigma_{11}^2 - \sigma_{13}^2 \end{pmatrix}, \qquad (43)
$$

$$
\begin{aligned}
\boldsymbol{\Sigma}_{z22}^{-1} &= \begin{pmatrix} \sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2 & \sigma_{11}^2 + \sigma_{23}^2 - \sigma_{12}^2 - \sigma_{13}^2 \\ \sigma_{11}^2 + \sigma_{23}^2 - \sigma_{12}^2 - \sigma_{13}^2 & \sigma_{11}^2 + \sigma_{33}^2 - 2\sigma_{13}^2 \end{pmatrix}^{-1} \\
&= \frac{1}{g} \begin{pmatrix} \sigma_{11}^2 + \sigma_{33}^2 - 2\sigma_{13}^2 & -(\sigma_{11}^2 + \sigma_{23}^2 - \sigma_{12}^2 - \sigma_{13}^2) \\ -(\sigma_{11}^2 + \sigma_{23}^2 - \sigma_{12}^2 - \sigma_{13}^2) & \sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2 \end{pmatrix} \qquad (44)
\end{aligned}
$$

and where

$$
g = \left(\sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2\right)\left(\sigma_{11}^2 + \sigma_{33}^2 - 2\sigma_{13}^2\right) - \left(\sigma_{11}^2 + \sigma_{23}^2 - \sigma_{12}^2 - \sigma_{13}^2\right)^2. \qquad (45)
$$

After expansion of Eq. 26 with Eqs. 42, 44, and 45, and replacing the true variances with estimated variances, $\hat{u}$ becomes

$$
\begin{aligned}
\hat{u} = \bar{x}_1 \; &- \frac{(\hat{\sigma}_{11}^2 - \hat{\sigma}_{12}^2)}{g} \Big[\left(\hat{\sigma}_{11}^2 + \hat{\sigma}_{33}^2 - 2\hat{\sigma}_{13}^2\right)(\bar{x}_1 - \bar{x}_2) \\
&- \left(\hat{\sigma}_{11}^2 + \hat{\sigma}_{23}^2 - \hat{\sigma}_{12}^2 - \hat{\sigma}_{13}^2\right)(\bar{x}_1 - \bar{x}_3) \Big] \\
&- \frac{(\hat{\sigma}_{11}^2 - \hat{\sigma}_{13}^2)}{g} \Big[-\left(\hat{\sigma}_{11}^2 + \hat{\sigma}_{23}^2 - \hat{\sigma}_{12}^2 - \hat{\sigma}_{13}^2\right)(\bar{x}_1 - \bar{x}_2) \\
&+ \left(\hat{\sigma}_{11}^2 + \hat{\sigma}_{22}^2 - 2\hat{\sigma}_{12}^2\right)(\bar{x}_1 - \bar{x}_3) \Big]. \qquad (46)
\end{aligned}
$$

Since $\hat{\sigma}_{ij}^2 = \hat{\sigma}_{ji}^2$, Eq. 46 can be rewritten, after lots of algebra, as

$$
\hat{u} = \frac{\sum_{\ell=1}^{3} f_\ell \bar{x}_\ell}{\sum_{\ell=1}^{3} f_\ell}, \qquad (47)
$$

where

$$f_\ell = \hat{\sigma}_{jj}^2\left(\hat{\sigma}_{kk}^2 - \hat{\sigma}_{ik}^2\right) - \hat{\sigma}_{kk}^2\hat{\sigma}_{ij}^2 + \hat{\sigma}_{jk}^2\left(\hat{\sigma}_{ij}^2 + \hat{\sigma}_{ik}^2 - \hat{\sigma}_{jk}^2\right), \tag{48}$$

where ℓ is the partial permutation of i, j, k as listed below,

ℓ	i	j	k
1	1	2	3
2	2	3	1
3	3	1	2

and

$$\sum_{\ell=1}^{3} f_\ell = g \tag{49}$$

$$\begin{aligned} &= \hat{\sigma}_{11}^2\hat{\sigma}_{22}^2 + \hat{\sigma}_{11}^2\hat{\sigma}_{33}^2 + \hat{\sigma}_{22}^2\hat{\sigma}_{33}^2 \\ &\quad +2\left(\hat{\sigma}_{12}^2\hat{\sigma}_{13}^2 + \hat{\sigma}_{13}^2\hat{\sigma}_{23}^2 + \hat{\sigma}_{23}^2\hat{\sigma}_{12}^2\right) \\ &\quad -2\left(\hat{\sigma}_{11}^2\hat{\sigma}_{23}^2 + \hat{\sigma}_{22}^2\hat{\sigma}_{13}^2 + \hat{\sigma}_{33}^2\hat{\sigma}_{12}^2\right) - \left(\hat{\sigma}_{12}^4 + \hat{\sigma}_{13}^4 + \hat{\sigma}_{23}^4\right). \end{aligned} \tag{50}$$

Equations 47 and 48 are used to calculate the three-combined k_{eff} ZQ. The variable AL in Subroutine KCALC is f_ℓ, except using the sums of squares of deviations instead of the sample variances. Therefore, it is beneficial to define a new variable, g_s, that involves s^2 instead of $\hat{\sigma}^2$:

$$g_s = (n-1)^2 g. \tag{51}$$

The estimated variance $\hat{\sigma}_{\bar{u}}^2$ is given by Eqs. 37 and 38 with Eqs. 43, 44, and 45 as

$$\begin{aligned} \hat{\sigma}_{\bar{u}}^2 &= \left(\hat{\sigma}_{11}^2 - \left(\hat{\sigma}_{11}^2 - \hat{\sigma}_{12}^2 \quad \hat{\sigma}_{11}^2 - \hat{\sigma}_{13}^2\right)\Sigma_{z22}^{-1}\begin{pmatrix} \hat{\sigma}_{11}^2 - \hat{\sigma}_{12}^2 \\ \hat{\sigma}_{11}^2 - \hat{\sigma}_{13}^2 \end{pmatrix}\right) \\ &\quad \cdot\left(\frac{1}{n} + (\bar{x}_1 - \bar{x}_2 \quad \bar{x}_1 - \bar{x}_3)\,\mathbf{S}_{z22}^{-1}\begin{pmatrix} \bar{x}_1 - \bar{x}_2 \\ \bar{x}_1 - \bar{x}_3 \end{pmatrix}\right) \\ &= \frac{1}{g}\Bigg(\hat{\sigma}_{11}^2 g - \left(\hat{\sigma}_{11}^2 - \hat{\sigma}_{12}^2\right)\Big[\left(\hat{\sigma}_{11}^2 - \hat{\sigma}_{12}^2\right)\left(\hat{\sigma}_{11}^2 + \hat{\sigma}_{33}^2 - 2\hat{\sigma}_{13}^2\right) \\ &\quad - \left(\hat{\sigma}_{11}^2 - \hat{\sigma}_{13}^2\right)\left(\hat{\sigma}_{11}^2 + \hat{\sigma}_{23}^2 - \hat{\sigma}_{12}^2 - \hat{\sigma}_{13}^2\right)\Big] \\ &\quad - \left(\hat{\sigma}_{11}^2 - \hat{\sigma}_{13}^2\right)\Big[\left(\hat{\sigma}_{12}^2 - \hat{\sigma}_{11}^2\right)\left(\hat{\sigma}_{11}^2 + \hat{\sigma}_{23}^2 - \hat{\sigma}_{12}^2 - \hat{\sigma}_{13}^2\right) \\ &\quad + \left(\hat{\sigma}_{11}^2 - \hat{\sigma}_{13}^2\right)\left(\hat{\sigma}_{11}^2 + \hat{\sigma}_{22}^2 - 2\hat{\sigma}_{12}^2\right)\Big]\Bigg) \end{aligned} \tag{52}$$

$$\times\left(\frac{1}{n}+\frac{(\bar{x}_1-\bar{x}_2)}{g}\left[\left(s_{11}^2+s_{33}^2-2s_{13}^2\right)(\bar{x}_1-\bar{x}_2)\right.\right.$$
$$\left.-\left(s_{11}^2+s_{23}^2-s_{12}^2-s_{13}^2\right)(\bar{x}_1-\bar{x}_3)\right]$$
$$+\frac{(\bar{x}_1-\bar{x}_3)}{g_s}\left[\left(s_{11}^2+s_{23}^2-s_{12}^2-s_{13}^2\right)(\bar{x}_2-\bar{x}_1)\right.$$
$$\left.\left.+\left(s_{11}^2+s_{22}^2-2s_{12}^2\right)(\bar{x}_1-\bar{x}_3)\right]\right). \qquad (53)$$

Equation 53 simplifies to

$$\hat{\sigma}_{\hat{u}}^2 = \frac{S_1}{gn}\left(1+n\left(\frac{S_2-2S_3}{g_s}\right)\right) \qquad (54)$$

where

$$S_1 = \sum_{\ell=1}^{3} f_\ell \hat{\sigma}_{1\ell}^2, \qquad (55)$$
$$S_2 = \sum_{\ell=1}^{3}\left(s_{jj}^2+s_{kk}^2-2s_{jk}^2\right)\bar{x}_\ell^2, \qquad (56)$$
$$S_3 = \sum_{\ell=1}^{3}\left(s_{kk}^2+s_{ij}^2-s_{jk}^2-s_{ik}^2\right)\bar{x}_\ell\bar{x}_j, \qquad (57)$$

and the ℓ's define the i, j, k as in Eq. 48. Equation 54 contains a mixture of $\hat{\sigma}^2$'s and s^2's. In the spirit of properly interpreting a sample variance as a sum of squares of deviations divided by the degrees of freedom, Eq. 54 is converted to contain only sums of squares. Namely, g is converted to g_s by Eq. 51, and S_1 is converted to $S_{s,1}$ by the following conversion:

$$S_{s,1} = S_1(n-1)^3. \qquad (58)$$

Equation 54 becomes

$$\sigma_{\hat{u}}^2 = \frac{S_{s,1}}{n(n-1)}\frac{1}{g_s}\left(1+n\left(\frac{S_2-2S_3}{g_s}\right)\right).$$

But, alas, this is a biased estimate since there are only $n-3$ degrees of freedom instead of $n-1$. Making the replacement yields the correct unbiased estimate,

$$\sigma_{\hat{u}}^2 = \frac{S_{s,1}}{n(n-3)}\frac{1}{g_s}\left(1+n\left(\frac{S_2-2S_3}{g_s}\right)\right). \qquad (59)$$

In MCNP, Eq. 47 is used to calculate the three-combined estimate, ZQ. However, the sums of squares, CV, are used instead of the $\hat{\sigma}$'s in calculating f_ℓ in Eq. 48 (called AL in MCNP), causing no change in the result since the degrees of freedom cancels. Equation 59 is used to estimate the variance of the three-estimator combined estimate. In MCNP, the square root of Eq. 59, the estimated standard deviation, is divided by ZQ and stored in EE as the relative error (later converted to the standard deviation).

```
      do 120 i=1,3
        .
      al=cv(j,j)*cv(k,k)-cv(j,j)*cv(i,k)-cv(k,k)*cv(i,j)+
     1 cv(j,k)*(cv(i,j)+cv(i,k)-cv(j,k))
        .
      a=a+al
        .
      zq=zq+al*za(i)
  120 continue
        .
      zq=zq/a
      ee=sqrt(abs(s1*(1.+f0*(s2-s3-s3)/a)/(a*f0*(f0-3.))))/zq
```

where S1 is $S_{s,1}$, S2 = S_2, S3 = S_3, AL is f_ℓ, A is g_s, and F0 is n.

D. Simple Averages of the Individual Estimators

Merely for reference, the equations for the simple averages of the estimators and the associated variances are also presented. The two- and three-estimator simple averages are stored in ZG and ZP with estimated relative errors stored in EG and EP, respectively. These simple averages do not take estimator variances or covariances into account, which would mean additional weighting for the $\bar{x}_i$'s with higher variances. This inaccuracy is reflected in the estimated variance, which is somewhat enlarged (compared to that of the least squares combination) since it is effectively a weighted average of the individual variances and covariances.

The general formula for the variance of the simple average of k estimates, each obtained from n samples, is

$$\frac{1}{k^2 n} \sum_{i=1}^{k} \sum_{j=1}^{k} \hat{\sigma}_{ij}^2. \tag{60}$$

For the two-estimator case, the simple average is

$$\bar{x}_{ij} = \frac{\bar{x}_i + \bar{x}_j}{2} \tag{61}$$

and its estimated variance is

$$\hat{\sigma}_{\bar{x}_{ij}}^2 = \frac{1}{4n} \left(\hat{\sigma}_{ii}^2 + \hat{\sigma}_{jj}^2 + 2\hat{\sigma}_{ij}^2 \right). \tag{62}$$

For the three-estimator case, the simple average is

$$\bar{\bar{x}} = \frac{\bar{x}_1 + \bar{x}_2 + \bar{x}_3}{3} \tag{63}$$

and its estimated variance is

$$\begin{aligned} \hat{\sigma}^2_{\bar{\bar{x}}} &= \frac{1}{9n} \sum_{i=1}^{3} \sum_{j=1}^{3} \hat{\sigma}^2_{ij} \\ &= \frac{1}{9n} \left(\hat{\sigma}^2_{11} + \hat{\sigma}^2_{22} + \hat{\sigma}^2_{33} + 2\hat{\sigma}^2_{12} + 2\hat{\sigma}^2_{13} + 2\hat{\sigma}^2_{23} \right) . \end{aligned} \tag{64}$$

E. Properties of the Two- and Three-Combined k_{eff} Estimator

In this section, we look at the properties of the combined k_{eff} estimator. First, we look at Peelle's Pertinent Puzzle, which shows that the combined estimates may lie outside the range of the individual estimates. Second, to investigate variance properties, we briefly review Halperin's examination of the variance of the combined estimate and focus on the Gauss-Markov Theorem for theoretical justification of the combined estimator's superiority. Third, we present statistical studies demonstrating the efficacy of the combined estimator and how its confidence intervals demonstrate nominal coverage rates. Lastly, we show how the combination of two estimators will behave in the limits of perfect correlation and equal variances.

1. Peelle's Pertinent Puzzle

Sometimes in MCNP, the three-estimator combined k_{eff} estimate lies outside the range of the three individual estimates. This happens when the individual estimates are highly positively correlated, and it may be, as the MCNP manual puts it,[15] "disconcerting." In the nuclear data community, this phenomenon was studied after the surfacing of what became known as *Peelle's Pertinent Puzzle*, which is recounted and explained in Appendix C. Peelle's Pertinent Puzzle turned out to be an improper application of least squares, but the nuclear data community's response to it has solidified the understanding of a combined estimate falling outside the range of the individual estimates.

To say that the true answer lies between the estimates from two highly correlated estimators is risky. In fact, assuming x_2 and x_1 are observations on two unbiased estimators of the true value, and taking $x_2 > x_1$ (see Appendix D), if

$$\sigma^2_{11} < \sigma^2_{12} < \sigma^2_{22}, \tag{65}$$

then x' lies below the range,[19] or if

$$\sigma^2_{22} < \sigma^2_{12} < \sigma^2_{11}, \tag{66}$$

then x' lies above the range.

As an example, consider two distributions that are fully and positively correlated, such that $\rho = 1$:

$$x_1 = y + d \tag{67}$$
$$x_2 = 2y + 7d \tag{68}$$
$$\sigma_{11}^2 = \sigma_y^2 \tag{69}$$
$$\sigma_{22}^2 = 4\sigma_y^2 \tag{70}$$
$$\sigma_{12}^2 = 2\sigma_y^2, \tag{71}$$

where the expected value of y is zero, and d is a constant.

Suppose for the moment that d *is* zero and we can artificially control y, while maintaining its expectation value of zero. Let us say that y is a cosine function of sample number. Then the graph of the sampled points, x_1 and x_2, is graphed in Fig. 3. Notice that for any sample, both x_1 and x_2 lie on the same side of the true solution, zero. The Least Squares Method will produce, from Eq. 143 or Eq. 36, for each sample, a combined estimate of

$$x' = 2x_1 - x_2 \tag{72}$$

$$= 0. \tag{73}$$

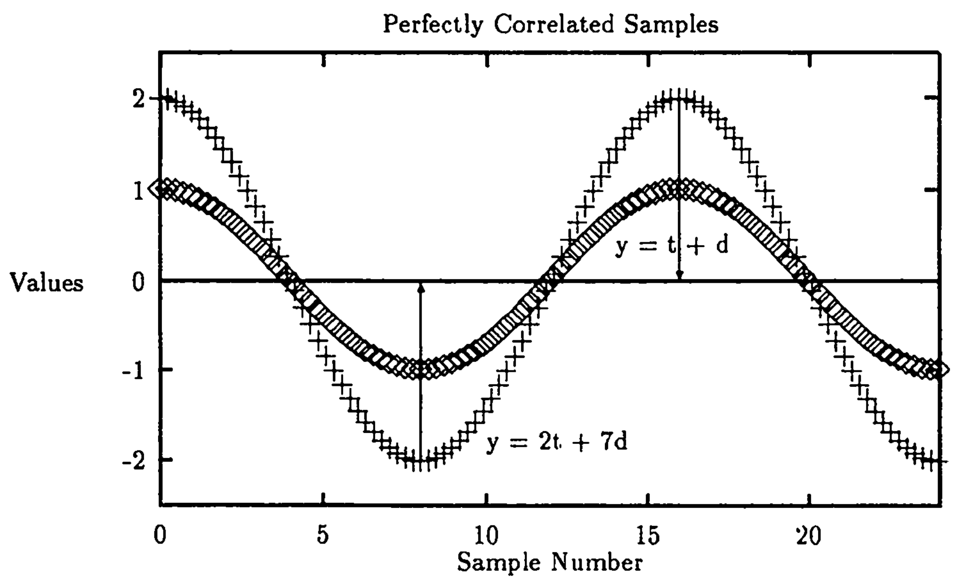

Fig. 3. Perfectly correlated data where the deviations are a cosine function of sample number.

So, every combined estimate gives the correct value of zero!

The previous example, while very illustrative, is hardly realistic. Let us look at an example where two samples are highly and positively, but not fully, correlated. Suppose we have two distributions,

$$\begin{aligned} x_1 &\sim N(0,1) \\ x_2 &\sim N(0,1) \end{aligned}$$

where $\sim N(0,1)$ means that the distribution is normally distributed with mean 0 and variance 1. Now we construct two distributions based on x_1 and x_2:

$$\begin{aligned} y_1 = x_1 + 4x_2 &\quad \sim N(0,17) \\ y_2 = x_2 &\quad \sim N(0,1) \end{aligned}$$

where the variances are calculated as follows:

$$\begin{aligned} \sigma_{y_1}^2 &= 1^2\sigma_{x_1}^2 + 4^2\sigma_{x_2}^2 \\ &= 1 + 16 \\ &= 17, \end{aligned} \tag{74}$$

$$\begin{aligned} \sigma_{y_2}^2 &= 1^2\sigma_{x_2}^2 \\ &= 1 \end{aligned} \tag{75}$$

and the covariance is

$$\begin{aligned} \sigma_{y_1,y_2}^2 &= E((y_1 - E(y_1))(y_2 - E(y_2))) \\ &= E(y_1y_2 - y_1E(y_2) - y_2E(y_1) + E(y_1)E(y_2)) \\ &= E(y_1y_2) - 2E(y_1)E(y_2) + E(y_1)E(y_2) \\ &= E(y_1y_2) - E(y_1)E(y_2) \\ &= E(x_1x_2 + 4x_2^2) - E(x_1 + 4x_2)E(x_2) \\ &= E(x_1x_2) + 4E(x_2^2) - E(x_1)E(x_2) - 4E(x_2)E(x_2) \\ &= u^2 + 4(u^2 + \sigma_{x_2}^2) - u^2 - 4u^2 \\ &= 4\sigma_{x_2}^2 \\ &= 4. \end{aligned} \tag{76}$$

Here, we have used the fact that x_1 and x_2 are independent and, in one variable,

$$\begin{aligned} \sigma^2 &= E(x-u)^2 \\ &= E(x^2) - 2uE(x) + u^2 \\ &= E(x^2) - u^2 \end{aligned}$$

which implies that[18,chapter 4]

$$E(x^2) = u^2 + \sigma^2 \quad . \tag{77}$$

This gives us a correlation coefficient, ρ, of

$$\begin{aligned} \rho &= \frac{\sigma^2_{y_1,y_2}}{\sqrt{\sigma^2_{y_1}\sigma^2_{y_2}}} \\ &= 4/\sqrt{17} \\ &= 0.97014. \end{aligned}$$

The weights on a linear least squares combination of these two variables are, from Eq. 36,

$$\begin{aligned} w_1 &= \frac{1-4}{17+1-8} = -0.3 \\ w_2 &= \frac{17-4}{17+1-8} = 1.3 \quad . \end{aligned}$$

These equations produce a combined estimate of

$$y' = -0.3y_1 + 1.3y_2 \quad .$$

In a simulation involving 500 samples, the values of y_1, y_2, and y' are shown in Fig. 4. Each vertical line connects the values of the two individual estimates. The dots represent the combined estimate y'. Figure 4 clearly shows trends similar to our previous artificial example, namely, that both estimates may lie on one side of the true value and the combined estimate may lie outside the range of the individual estimates, closer to the true value. For 500 samples, the two individual estimates resided on the the same side of zero, the true answer, 91.6% of the time.

2. The Gauss-Markov Theorem and Halperin's Examination of the Variance

Halperin analyzes the performance of the combined estimator by comparing it with one of the individual estimators, $\mathbf{z}_1 = \mathbf{x}_1$. Unfortunately, the assignment of an estimator to $\mathbf{x}_1$ is not discussed, so it could be any estimator. He compares the unconditional variances (see Appendix F) and the confidence intervals, obtaining expressions ascertaining the superiority of the combined estimator. These expressions appear to indicate that, for three estimators, running more active cycles ensures the superiority of the three-combined estimator. Halperin is unable to make a definitive conclusion as to which estimator to use, saying it depends on the true covariance matrix and the number (desirably large) of samples, or, in our case, the number of active cycles. Due to the increased computational capabilities in the several years since Halperin's paper was written, the typical number of active cycles, usually much larger

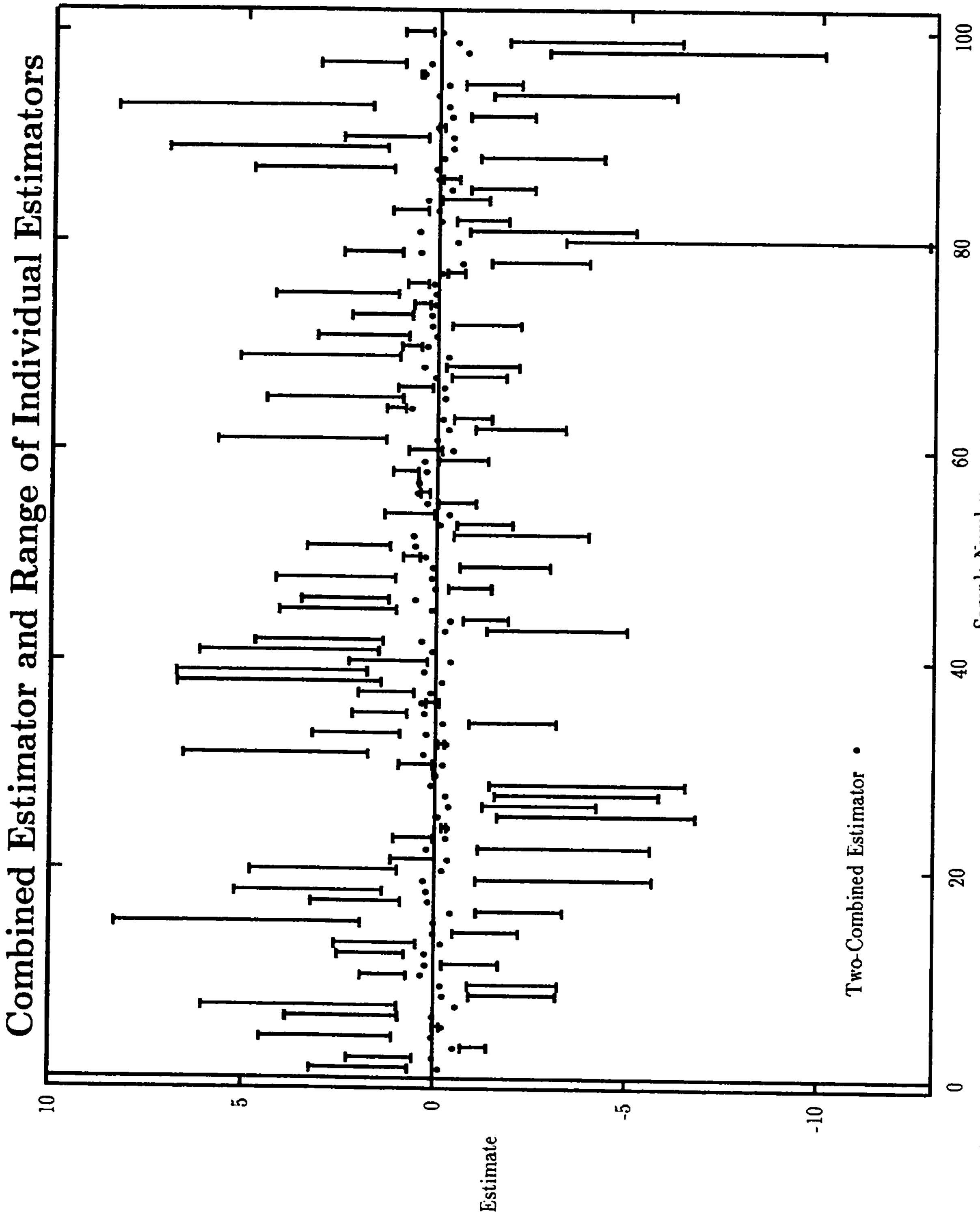

Fig. 4. Combination of two estimators.

than thirty–maybe on the order of one or two hundred or more–would seem to eradicate the fear of degradation in the performance of the combined estimator.

Providing a more solid theoretical foundation, we feel, is the Gauss-Markov Theorem, which says that the linear least squares parameters have minimum variance–linearly, they are the best possible–when the covariance matrix is known.[1,chapter VI;2,page 14;3,page 198] The estimate of the intercept in the regression equation is a least squares parameter and is, in fact, the combined k_{eff} estimator. Using a covariance matrix that is estimated by the data will not yield the absolutely minimum variance estimation of the least squares parameters, but, as our studies show, the best available.

The following subsection shows empirically that the combined estimator outperforms the individual variance with the smallest variance, while still providing confidence intervals with good coverage rates.

3. Statistical Studies for the Three-Combined k_{eff} Estimator

The purpose of this statistical study is two-fold. The first reason is to demonstrate the superior performance of the combined estimator. The second reason is to clarify some of the statistical qualities of a common test of MCNP's variance. Specifically, the variance of a Monte Carlo estimator is often checked by running several independent runs (each with a different random number seed) and comparing the average of the standard deviations from all the runs to the sample population standard deviation observed from the several estimates themselves.

A statistical simulation was performed to study the performance of the three-estimator combined estimator, especially under the condition of high correlation, and with an underlying multivariate normal distribution where each estimator had an expected value of zero. To study the performance of the combined estimator, its variance was examined. The covariance matrix is

$$\Sigma = \begin{pmatrix} 1 & 2 & 2 \\ 2 & 5 & 8 \\ 2 & 8 & 21 \end{pmatrix}. \tag{78}$$

The correlation coefficients are

$$\begin{aligned} \rho_{12} &= 0.8944 \\ \rho_{13} &= 0.4364 \\ \rho_{23} &= 0.7807. \end{aligned}$$

The next several figures show certain characteristics of the combined estimator for 100 samples. Each sample may be interpreted as an independent MCNP run. Figures 5, 6, and 7 show each individual estimator compared to one other and the combined estimate of those two values. In all three cases, the combined estimate is near the true value of zero, with less variance than either of the individual estimates and often outside the range of the two values. The same observations are made for Fig. 8, where all three estimators are combined, and that combination is plotted with the two extremes of the three individual values. Notice

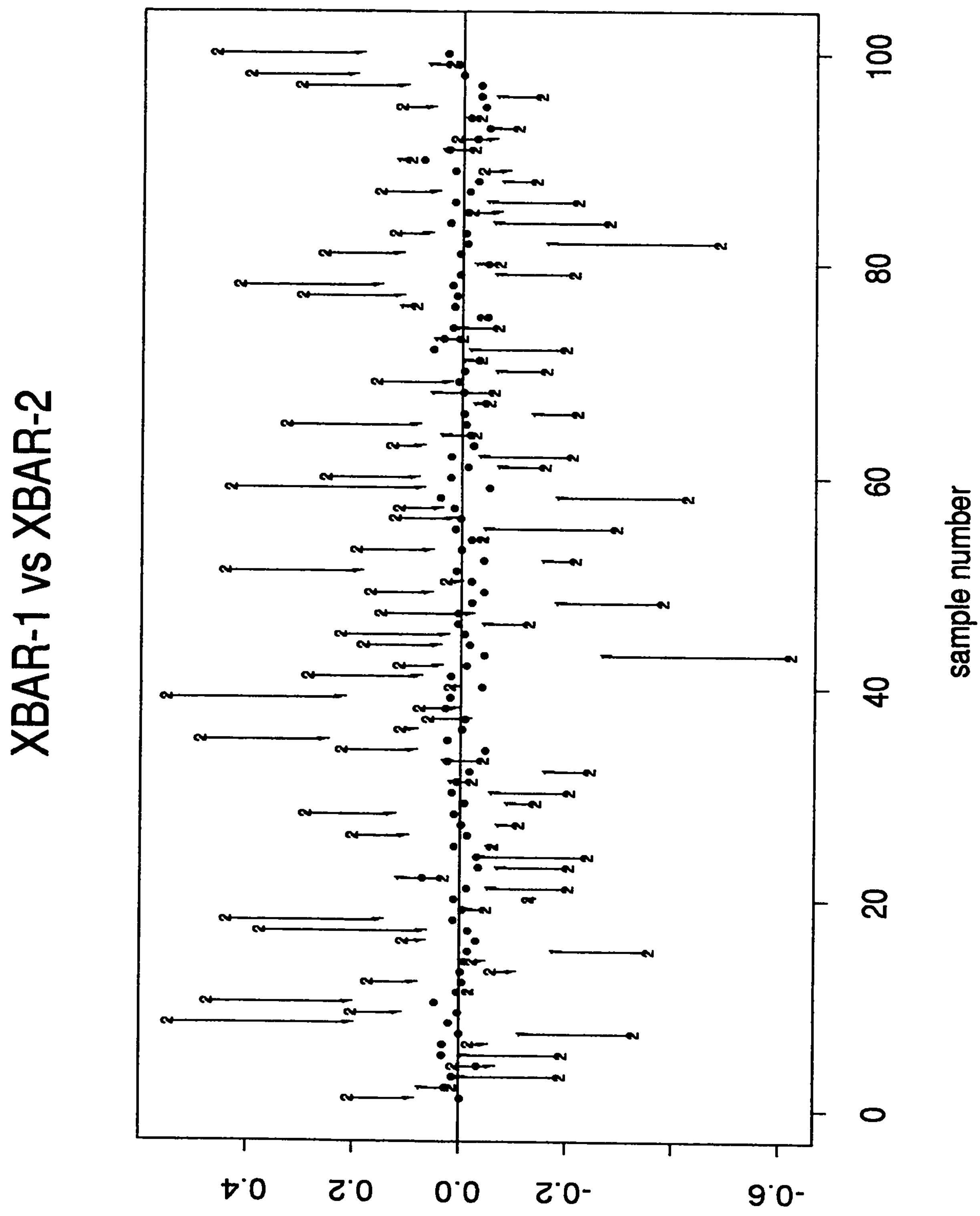

Fig. 5. The individual estimates $\bar{x}_1$ and $\bar{x}_2$, and the combination of the two.

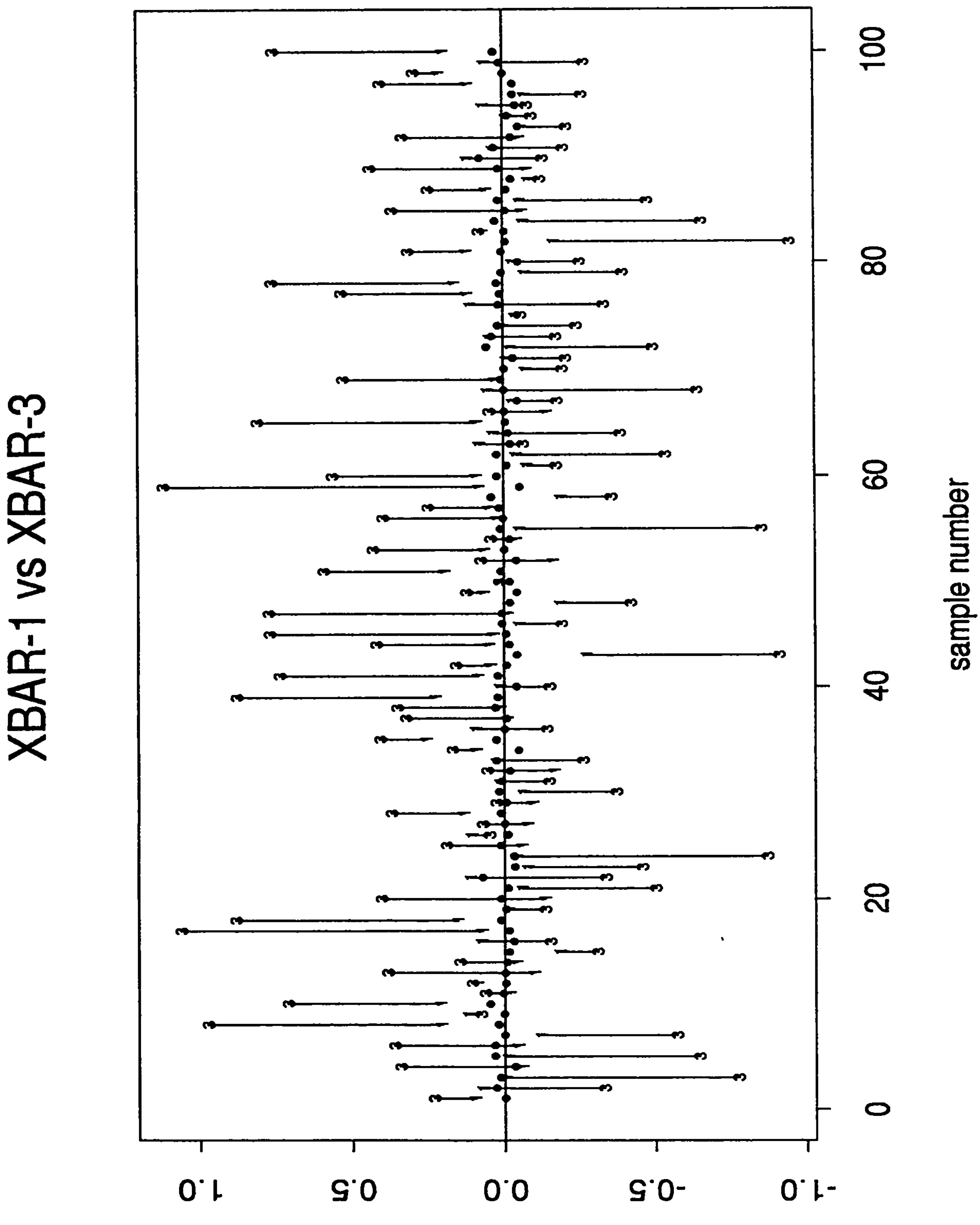

Fig. 6. The individual estimates $\bar{x}_1$ and $\bar{x}_3$, and the combination of the two.

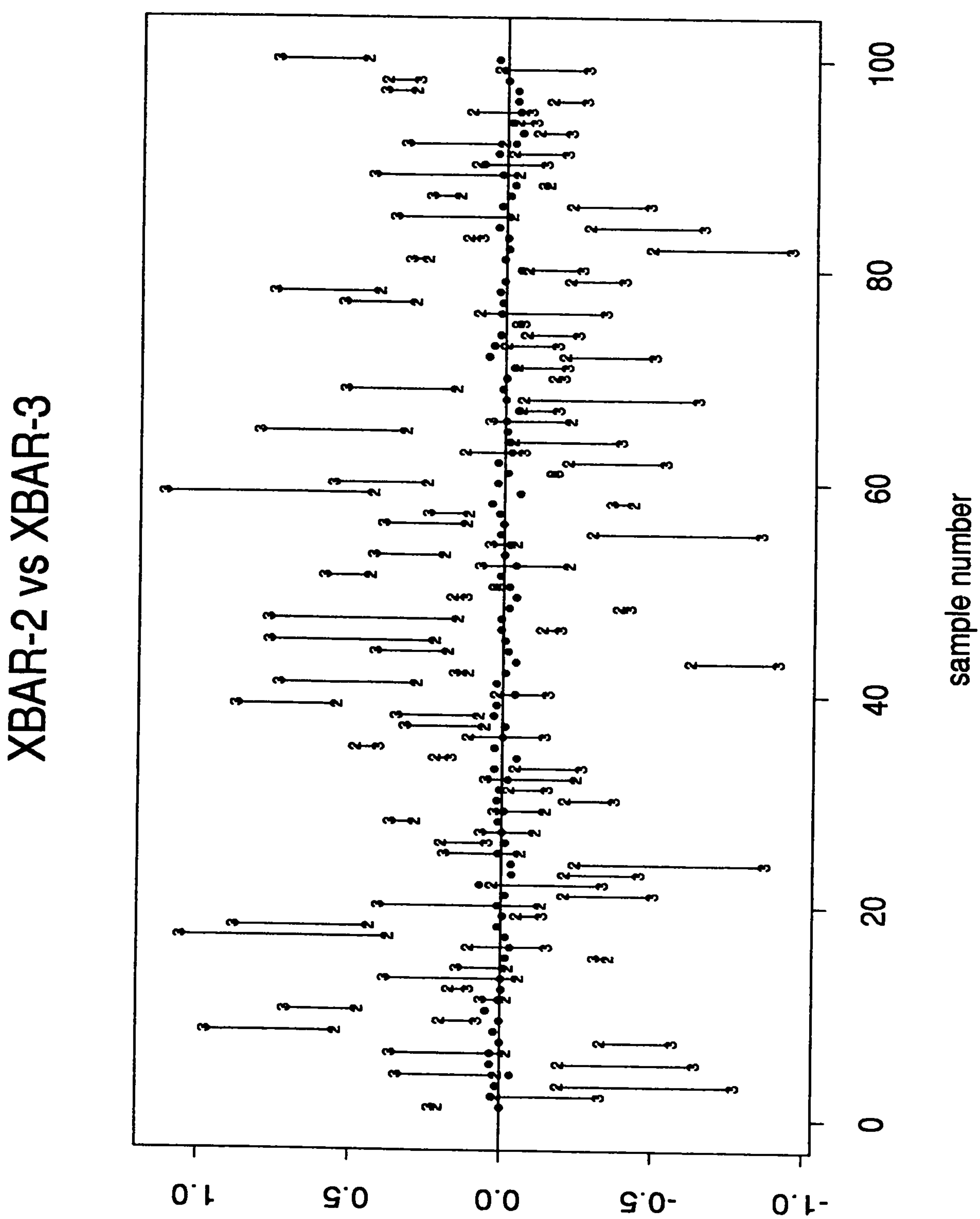

Fig. 7. The individual estimates $\bar{x}_2$ and $\bar{x}_3$, and the combination of the two.

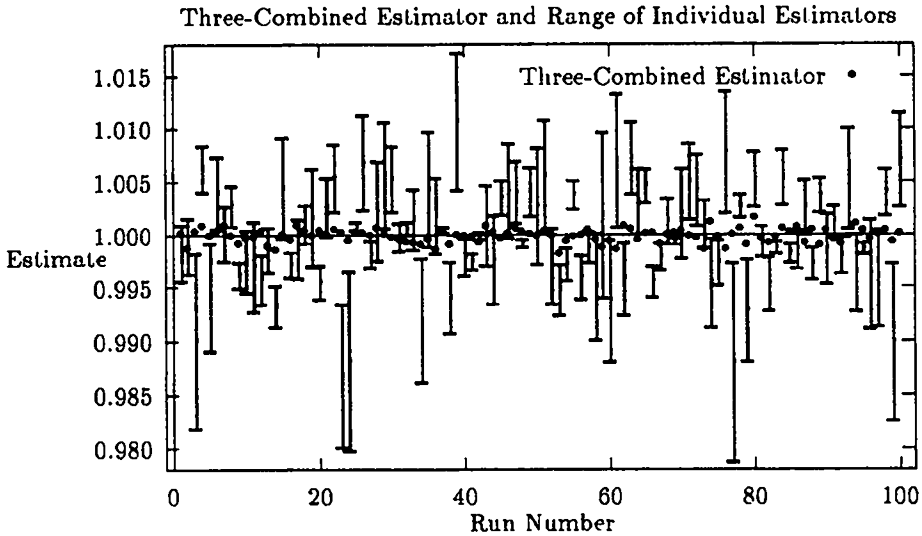

Fig. 8. The extreme valued individual estimates and the three-estimator combined estimate.

that the study was modified for Fig. 8—and Fig. 8 alone—so that it would appear more like a set of actual k_{eff}'s. The variances and covariances in Eq. 78 were multiplied by $(0.02)^2$ and the estimators were shifted so as to have expected values of 1.0. Of the 100 samples in Fig. 8, the range of the individual estimates does not cross the true value of zero 64 times. Of those 64, the three-estimator combined estimate lies closer to unity 54 times. The three-estimator combined estimate, with expected value zero and the covariance matrix in Eq. 78, is also plotted against the average of the three estimates and against the estimator with the minimum variance, whichever one it is, in Figs. 9 and 10, respectively. Once again, it is obvious to the naked eye that the combined estimator outperforms both of these estimates.

For 100 samples, the unconditional standard deviation of the combined estimator, using the equations given in Halperin's paper (see Appendix F) and the true covariance matrix, is 0.03046, where $\sigma_{opt} = 0.03015$. The simulation consisted of 10,000 trials of 20 runs of 100 samples each. The number of runs, 20, was chosen because it is a number of independent samples that a user would probably consider reasonable. The average of the estimated standard deviation of the combined estimate, using the estimated covariance matrix, was 0.03038. The average standard deviation obtained from 10,000 standard deviations derived from the population of the 20 samples themselves was 0.03005. This simulation, if it was a set of MCNP runs, would seem to indicate that MCNP was overestimating the true standard deviation.

There is, however, a flaw in this type of analysis. We know that the random variable τ, where

$$\tau = df\frac{s^2}{\sigma^2}, \tag{79}$$

is distributed as a χ^2 distribution with df degrees of freedom,[10,12] where s^2 was calculated with df degrees of freedom. (See Appendix A.) Consider the reported sample standard devi-

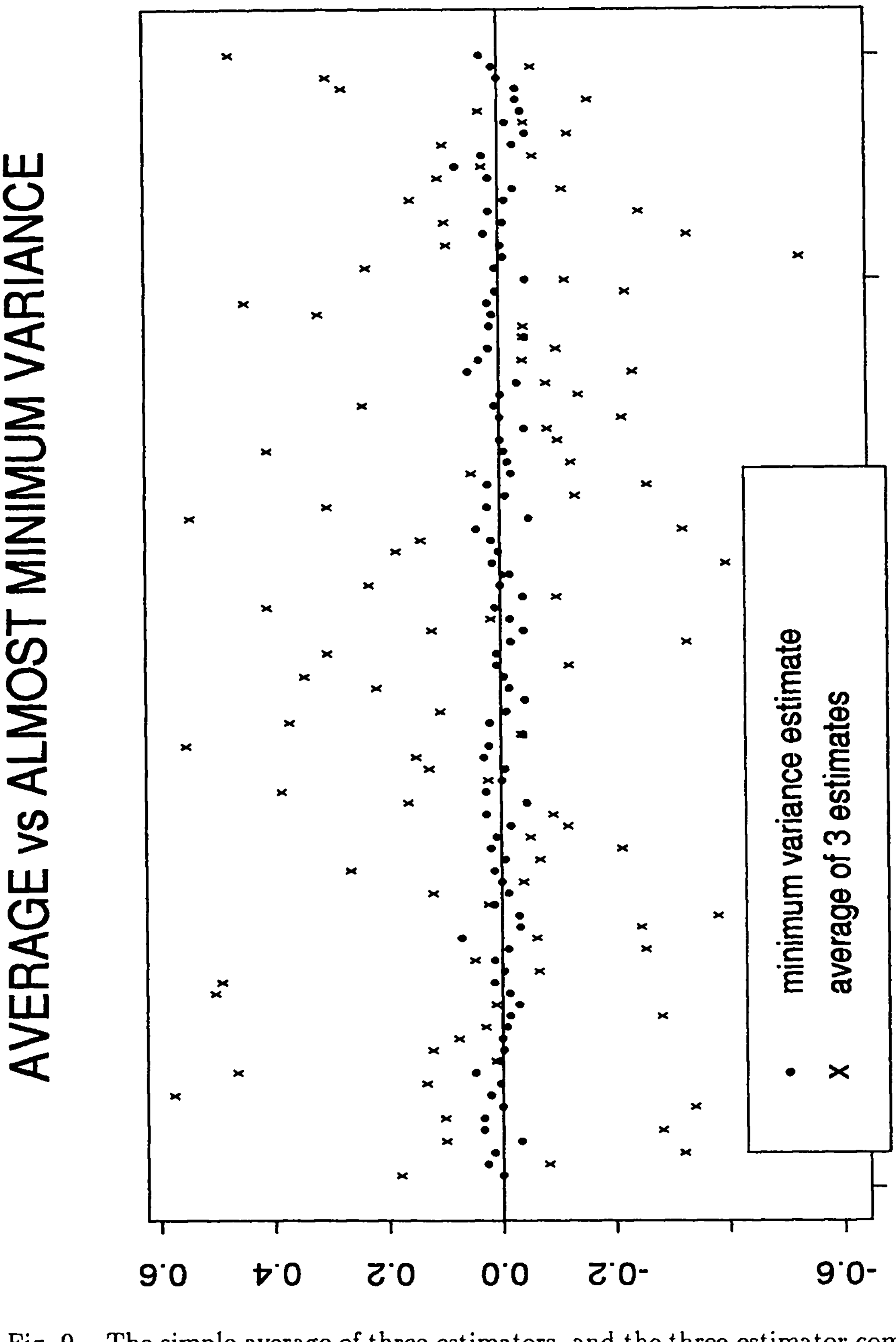

Fig. 9. The simple average of three estimators, and the three-estimator combined estimate.

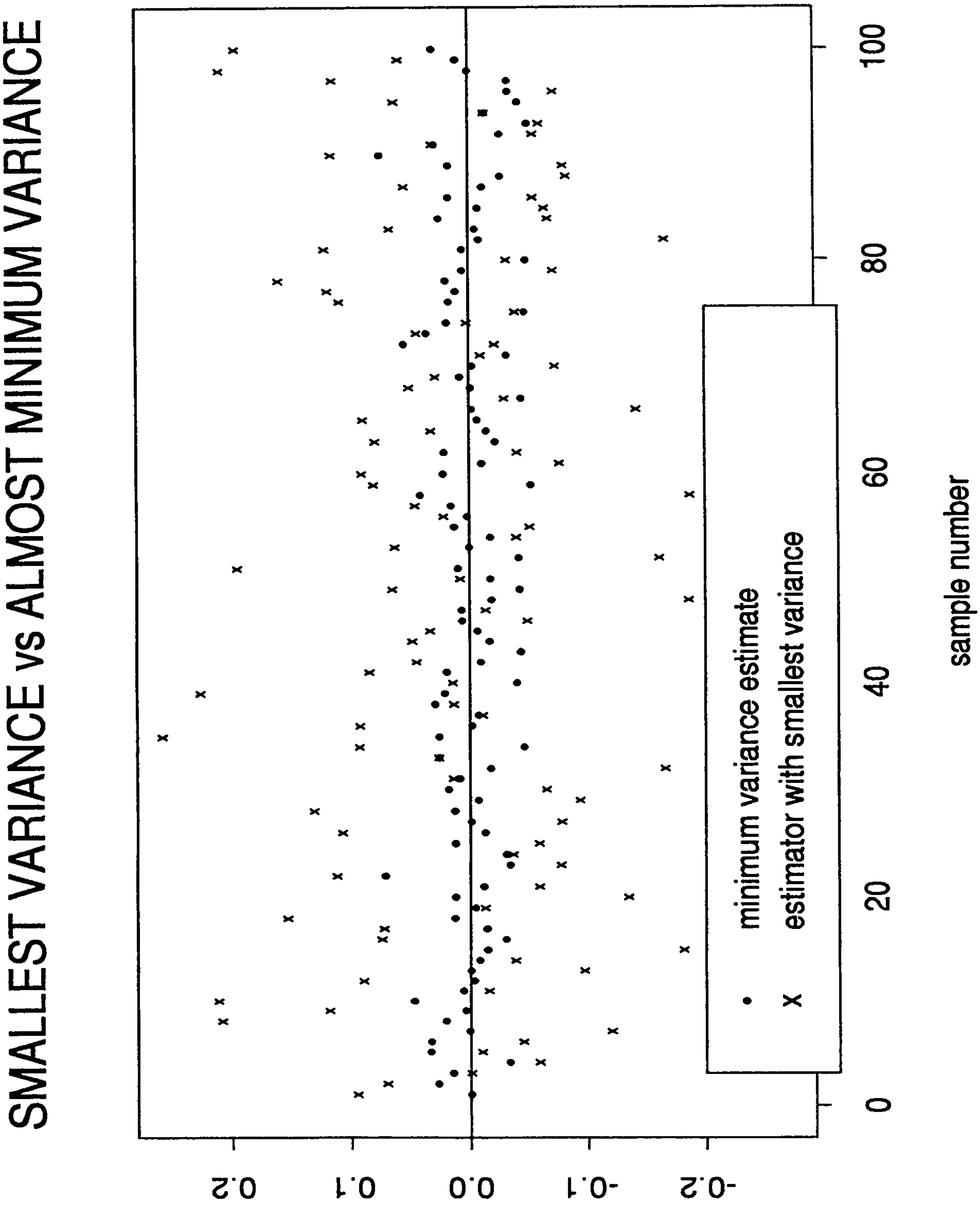

Fig. 10. Combined estimator and individual estimator with smallest variance.

ations, or, more appropriately, the sample variances, of the combined estimators for multiple MCNP runs. Since they are all independent of their associated estimators[1, page 148 and chapter 4] and of each other, we see that they are distributed, as expressed in Eq. 79, according to a χ^2 distribution with $n - k = 100 - 3 = 97$ degrees of freedom, where n is the number of active cycles in the problem and k is the number of estimators involved in the combined estimate. This assumes that the data–the k_{eff} estimates–are multivariate normal, which we believe to be a good assumption based on individual estimator normality checks and the good confidence interval coverage rates, as we will see later.

To investigate the effect of comparing values from two different χ^2 distributions, the simulation compared two different values: $\sigma^2(x_1), \ldots, \sigma^2(x_{20})$ distributed as $\sigma^2\frac{\chi^2_{97}}{97}$ and σ^2_{20} distributed as $\sigma^2\frac{\chi^2_{19}}{19}$. Thus, it was as if there were twenty independent MCNP runs, each with 100 active cycles. For the i^{th} run there is a mean, x_i, and an associated variance, $\sigma^2(x_i)$. The sample population variance observed from the twenty x_i's themselves is σ^2_{20}. Both $\frac{\chi^2_{97}}{97}$ and $\frac{\chi^2_{19}}{19}$ have expected value one since the expected value of a χ^2 distribution with *df* degrees of freedom is just *df*.[20] In 10,000 trials, the $\max(\sigma^2(x_i))$ was *less than* σ^2_{20} 16.8% of the time. This implies that, in our case, MCNP would evidently underestimate the apparent variance almost 17% of the time. This is a fairly significant percentage, and indicates that however the two compared values stack up, the fact remains that they are from two different distributions and not amenable to quantitative comparison. Figure 11 depicts distributions of the two variances we have just compared. The averaging of the reported variances results in a very peaked distribution.

If, as shown in Fig. 12, we look at the distribution of all 200000 reported variances, instead of the distribution of the run-averaged reported variances, we see how σ^2_{20} and $\sigma^2(x_i)$ are indeed distributed as $\sigma^2\frac{x^2_{19}}{19}$ and $\sigma^2\frac{x^2_{97}}{97}$, respectively.

Therefore, to compare the average of the reported variances of the combined estimator from twenty MCNP runs with the apparent sample population variance of the twenty estimators themselves is not necessarily a valid comparison. The two values will have the same expected value, but they come from two different distributions, so for them to be significantly different is not unexpected.

These observations indicated that, to make a legitimate analysis, the number of independent MCNP runs should be approximately equal to the number of cycles in each run. If 100 runs were performed per trial instead of 20, the apparent population variance, σ^2_{100}, would be distributed as $\sigma^2\frac{x^2_{99}}{99}$. Figure 13 shows that σ^2_{100} is more similarly distributed as $\sigma^2(x_i)$, thus allowing for a more legitimate comparison.

This is not meant to mislead anyone desiring to perform such a multiple run analysis. To run 200 active cycles and 200 independent runs may prove impractical. To run 5 active cycles and 5 independent runs is foolish. The proper way to perform this analysis, assuming access to not necessarily large computing resources and a desire for meaningful results, is to run a statistically significant number of active cycles, usually, say, 30 or more, and run enough independent problems to statistically approach a distribution similar to the one for each independent run. This suggestion is somewhat vague, but it hinges on the assumption that this type of analysis is usually performed to see that the reported standard deviation is in reasonable agreement with the sample population standard deviation.

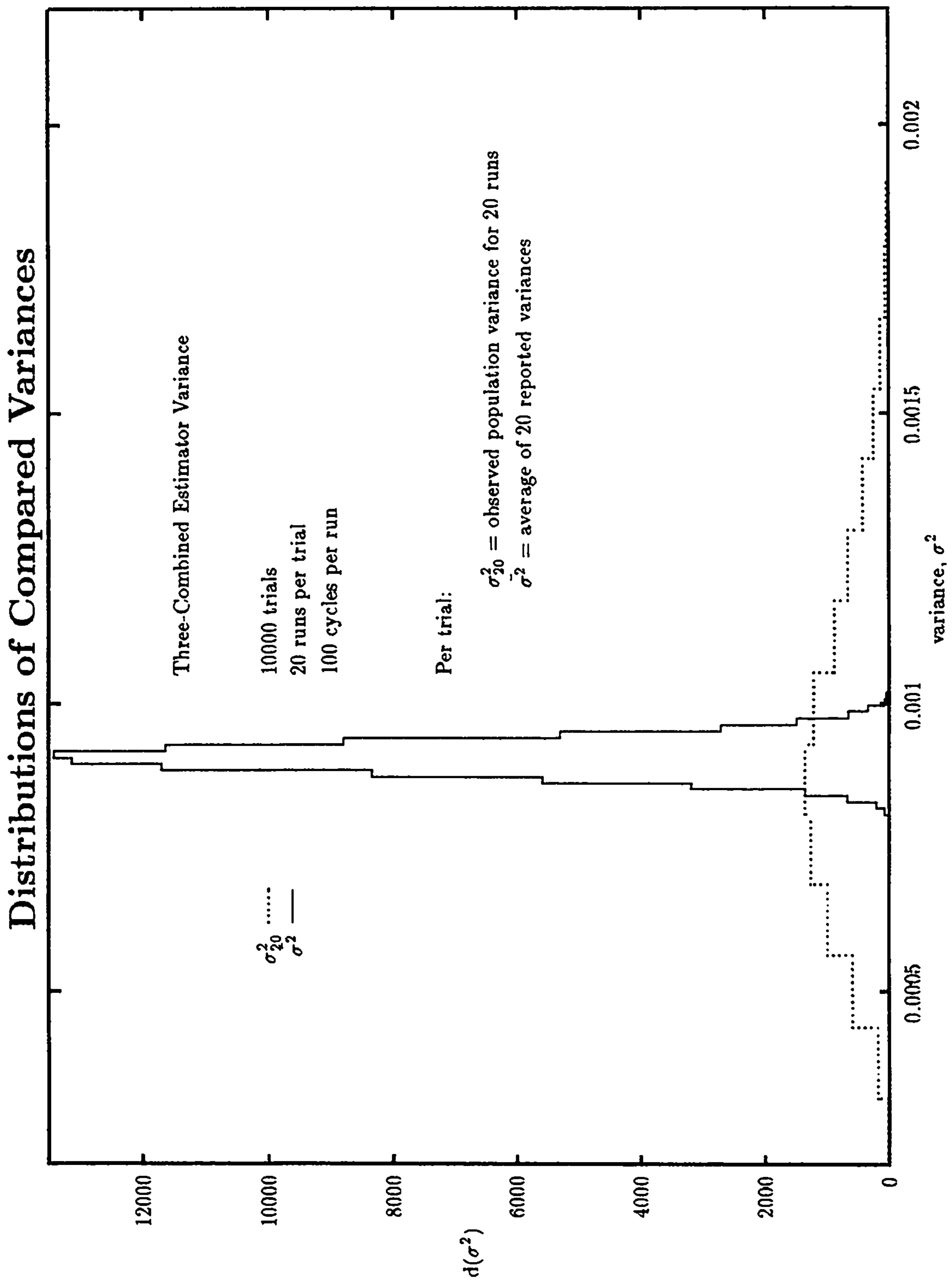

Fig. 11. Distribution of σ^2_{20} and $\overline{\sigma^2(x_i)}$ for 10000 trials.

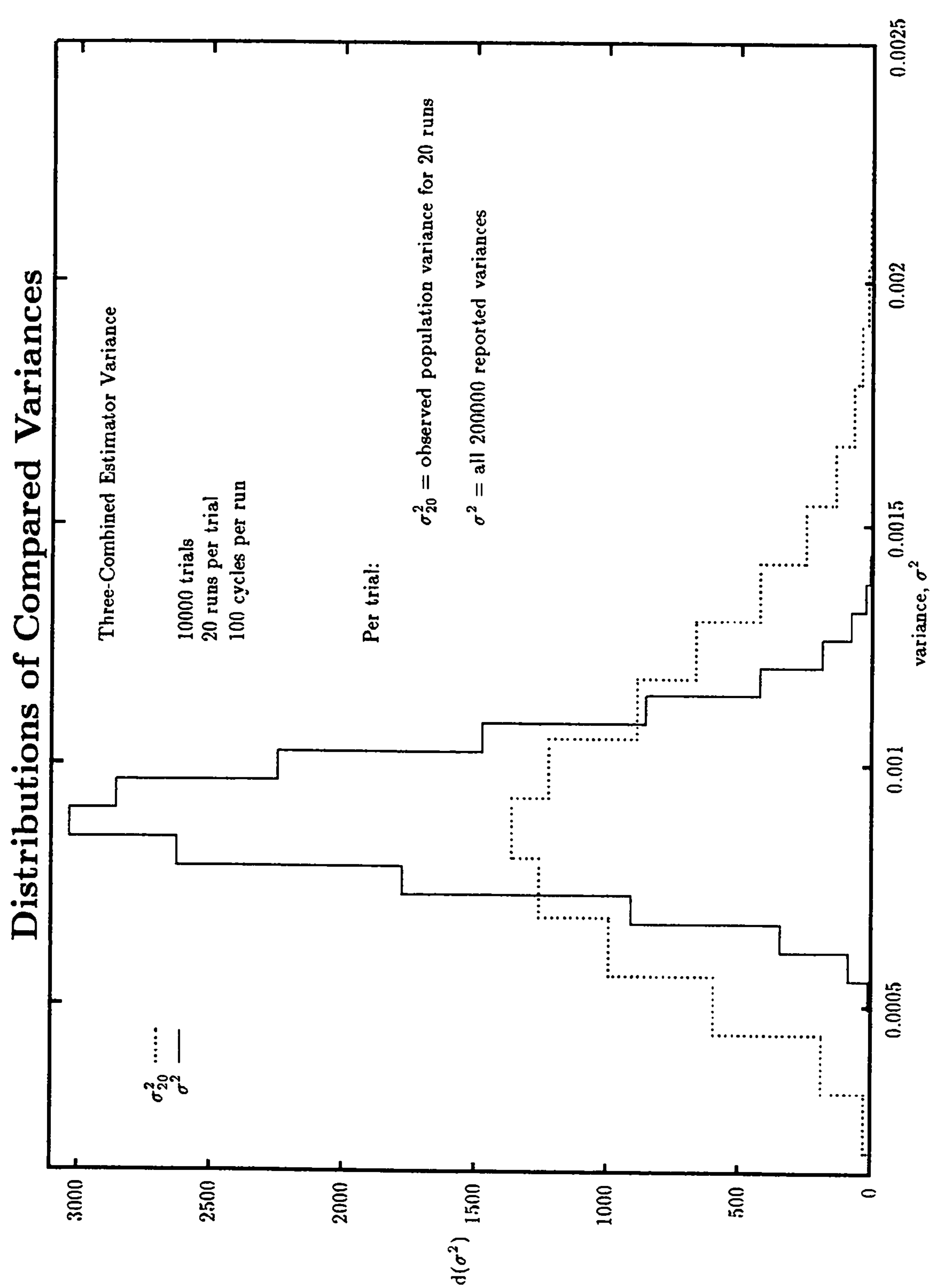

Fig. 12. Distribution of σ_{20}^2, for 10 000 trials, and the distribution of all 200 000 $\sigma^2(x_i)$.

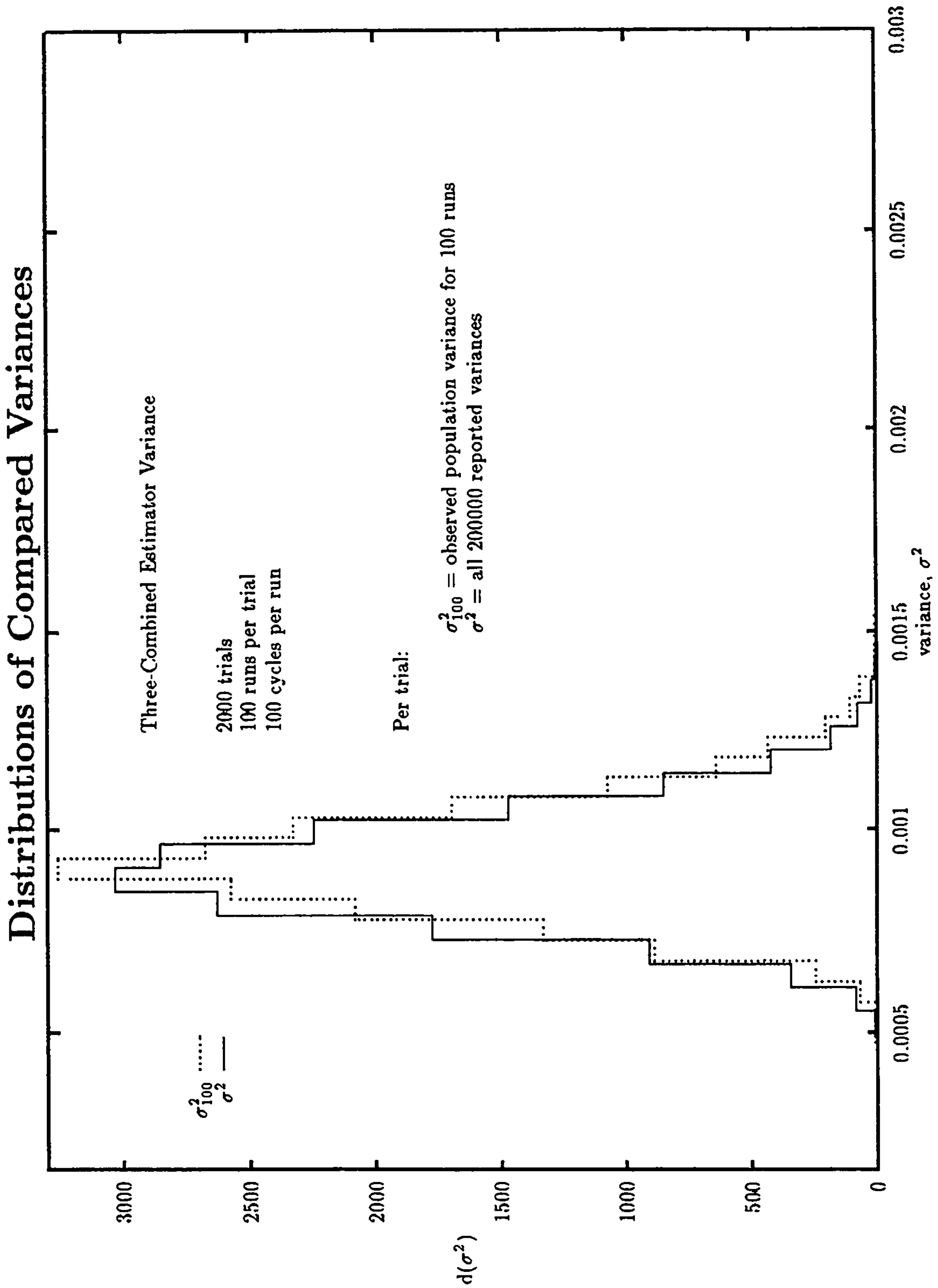

Fig. 13. Distribution of σ^2_{100}, for 2000 trials, and the distribution of all 200 000 $\sigma^2(x_i)$.

4. Estimator Combination in the Limit of Perfect Positive Correlation

We are interested in the behavior of the combined estimator as the correlation coefficient approaches unity, either positive or negative. The issue comes to mind of two estimates, from two separate estimators, that both have small variances and are fully and positively correlated, but are far apart. This issue is moot, since the individual estimators are assumed unbiased, which means that for infinite samples they will both be equal to the true value.

For presentation purposes, we'll consider the least squares combination of two estimates, x_1 and x_2, which is given by Eq. 36,

$$x' = w_1 x_1 + w_2 x_2, \tag{80}$$

where, substituting the expression for the correlation coefficient from Eq. 13, the weights are

$$w_1 = \frac{\sigma_{22}^2 - \rho\sigma_{11}\sigma_{22}}{\sigma_{11}^2 + \sigma_{22}^2 - 2\rho\sigma_{11}\sigma_{22}} \tag{81}$$

$$w_2 = \frac{\sigma_{11}^2 - \rho\sigma_{11}\sigma_{22}}{\sigma_{11}^2 + \sigma_{22}^2 - 2\rho\sigma_{11}\sigma_{22}}. \tag{82}$$

Since the denominator of the weights will vanish as the variances approach each other and the correlation coefficient approaches unity, we are led to investigate these limits jointly. To facilitate study of the variances, we introduce the variable, α,

$$\alpha = \frac{\sigma_{22}}{\sigma_{11}}. \tag{83}$$

Restricting α such that $\alpha \in [0,1]$ implies that σ_{11}^2 approaches σ_{22}^2 from $+\infty$, or, more correctly, σ_{22}^2 varies from zero to σ_{11}^2. The weights become

$$\begin{aligned} w_1 &= \frac{\alpha(\alpha - \rho)}{\alpha^2 - 2\rho\alpha + 1} \\ w_2 &= \frac{1 - \rho\alpha}{\alpha^2 - 2\rho\alpha + 1}. \end{aligned} \tag{84}$$

From Appendix D, we see that the denominator is greater than zero. Figure 14 shows the denominator of the weights, as given in Eq. 84, with various ρ from -1 limiting to 1, and in the limit as α goes to unity. We see that, for a correlation coefficient not near unity, the denominator of the weights will not become too small. However, the denominator will become arbitrarily small as the variances become equal and the correlation coefficient approaches unity.

Concerning the weights, we first look at the limit as the correlation coefficient approaches unity and the variances are not equal.

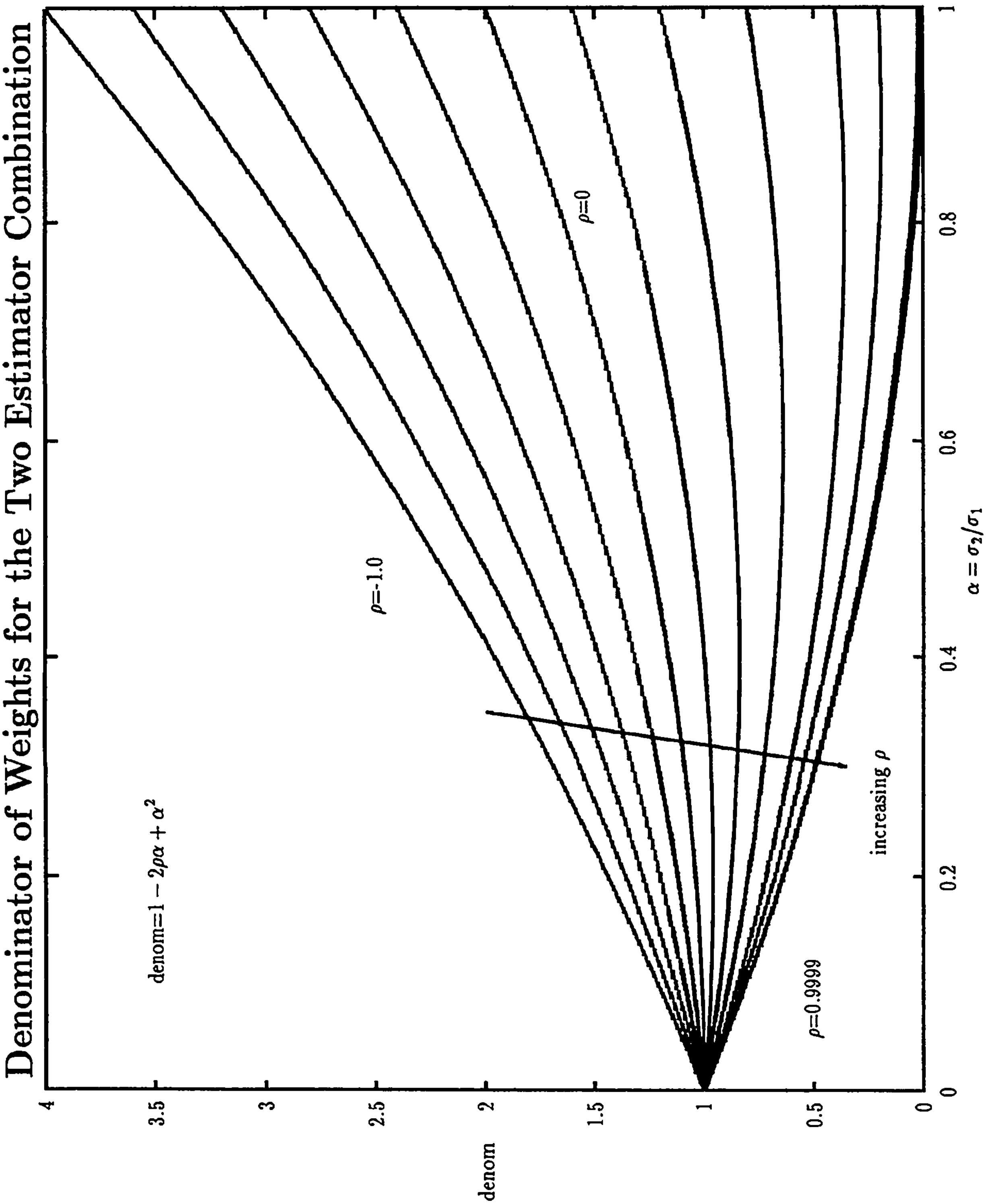

Fig. 14. Denominator of the weights in the least squares combination of two estimates.

$$
\begin{aligned}
\lim_{\rho \to 1, \alpha \neq 1} w_1 &= \frac{\alpha(\alpha - 1)}{\alpha^2 - 2\alpha + 1} \\
&= \frac{\alpha(\alpha - 1)}{(\alpha - 1)^2} \\
&= \frac{\alpha}{\alpha - 1},
\end{aligned} \tag{85}
$$

which will become negatively large for α close to unity. Also,

$$
\begin{aligned}
\lim_{\rho \to 1, \alpha \neq 1} w_2 &= \frac{1 - \alpha}{\alpha^2 - 2\alpha + 1} \\
&= \frac{(1 - \alpha)}{(1 - \alpha)^2} \\
&= \frac{1}{1 - \alpha},
\end{aligned} \tag{86}
$$

which will become positively large for α close to unity. If, for the moment, we back out of the alpha notation, we see from Eqs. 85 and 86, that, for perfect correlation and unequal variances, the combined estimate is a "one-over-standard deviation" weighted value:

$$
x' = \frac{\frac{1}{\sigma_{11}}\bar{x}_1 - \frac{1}{\sigma_{22}}\bar{x}_2}{\frac{1}{\sigma_{11}} - \frac{1}{\sigma_{22}}}. \tag{87}
$$

Compare this to the familiar "one-over-variance" weighting to which the combination reduces for zero correlation. Here, though, the standard deviations provide the weighting and there is a minus sign instead. Note that Eq. 87 is merely a limiting expression and would not be any more advantageous to use than the regular expression for the combination, especially since it is not applicable for equal variances ($\alpha = 1$).

Figure 15 shows the two least squares combination weights as α varies from zero to one, and for values of ρ from -1 to near unity.

The limit of the weights as α goes to unity, for any correlation coefficient, is

$$
\begin{aligned}
\lim_{\alpha \to 1} w_1 &= \lim_{\alpha \to 1} w_2 \\
&= \frac{1 - \rho}{1 - 2\rho + 1} \\
&= \frac{1 - \rho}{2(1 - \rho)} \\
&= \frac{1}{2},
\end{aligned} \tag{88}
$$

as shown in Fig. 15. Note that this equal weighting is only for *exactly* equal variances. It, too, is just a limiting expression. At some value of α slightly less than unity, the weights may

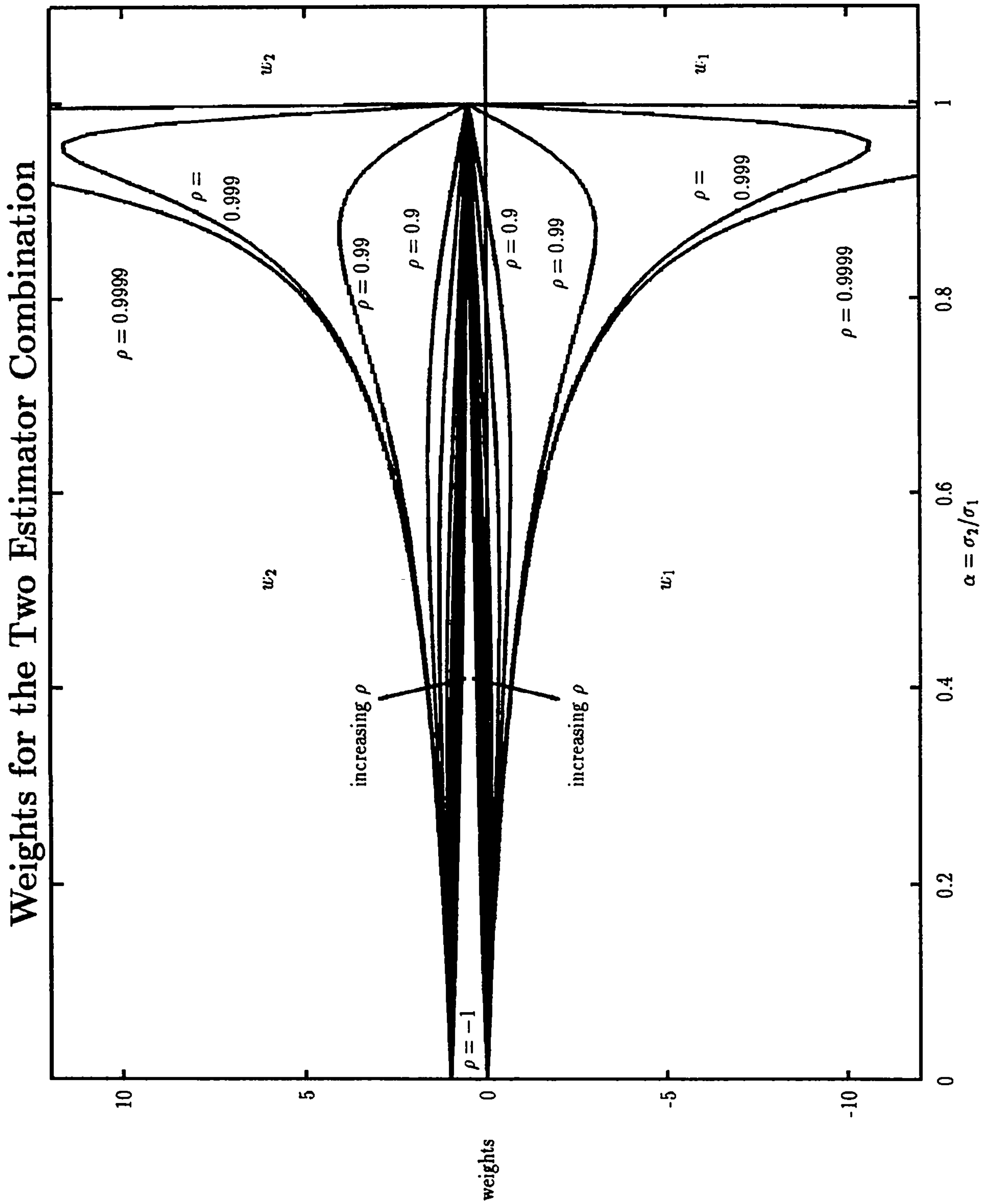

Fig. 15. Weights for the least squares combination of two estimates.

be quite different than 1/2, especially for correlation coefficients near unity, as evidenced in Fig. 15. In fact, for a correlation coefficient of unity, the curves depicting the weights, as in Fig. 15, would be discontinuous. They would approach infinity (plus infinity for w_2 and negative infinity for w_1) as $\alpha \to 1$ and would be 1/2 at $\alpha = 1$.

As α goes to zero, $w_1 \to 0$ and $w_2 \to 1$ as expected, since we want no part of an estimate with infinite variance, i.e., x_1, or, equivalently, we want the estimator with no variance.

The same analysis may be performed for the variance of the two-combined estimates. Introducing ρ and α into the equation for the variance of the combined estimator, Eq. 40 with the sums of squares replaced by variances, yields

$$\sigma_{x'}^2 = \frac{\alpha^2(1-\rho^2)}{n(n-1)}\left[\frac{(n-1)\sigma_{11}^2}{1-2\rho\alpha+\alpha^2} + \frac{n(\bar{x}_1-\bar{x}_2)^2}{(1-2\rho\alpha+\alpha^2)^2}\right]. \tag{89}$$

As $\alpha \to 0$ ($\sigma_{22} \to 0$), the variance of the combined estimate goes to zero, which is to say that the combination would reproduce any estimate with zero variance. If the two estimates are perfectly and negatively correlated, $\rho = -1$ and the variance of the combination is zero (meaning the combination reaps huge benefits).

Next, we look at the behavior of the variance as $\alpha \to 1$:

$$L = \lim_{\alpha\to 1} \sigma_{x'}^2 \tag{90}$$

$$= \frac{(1-\rho^2)}{n(n-2)}\left[\frac{(n-1)\sigma_{11}^2}{2(1-\rho)} + \frac{n(\bar{x}_1-\bar{x}_2)^2}{4(1-\rho)^2}\right] \tag{91}$$

$$\approx \frac{1+\rho}{n}\left[\frac{\sigma_{11}^2}{2} + \frac{(\bar{x}_1-\bar{x}_2)^2}{4(1-\rho)}\right]. \tag{92}$$

For a correlation coefficient of zero, L becomes

$$\lim_{\rho\to 0} L = \frac{\sigma_{11}^2}{2n} + \frac{(\bar{x}_1-\bar{x}_2)^2}{4n}. \tag{93}$$

For a correlation coefficient approaching unity, L is

$$\lim_{\rho\to 1} L = \frac{\sigma_{11}^2}{n} + \frac{1}{2n}\lim_{\rho\to 1}\frac{(\bar{x}_1-\bar{x}_2)^2}{1-\rho}. \tag{94}$$

We expect the $\bar{x}$'s to approach the true value as $1/\sqrt{n}$, so we would expect the remaining limit term to go as $1/(n^2(1-\rho))$, which could go to infinity or zero, depending on the relative values of n and ρ.

Any difference in $\bar{x}_1$ and $\bar{x}_2$ could possibly dominate the variance of the combined estimator, making it quite large. This is an automatic flag that demonstrates the correctness and robustness of the combination, since a large difference in x_1 and x_2 should translate into a larger variance in the combination.

VI. MCNP EXAMPLES

Five systems were modeled with MCNP to observe the behavior of the combined k_{eff} estimator. They are a sphere of a U-233 and water mixture with a water reflector, an infinite medium problem with a slightly modified mixture of U-233 and water, the Godiva reactor, a Jezebel reactor mock-up, and a two-component system consisting of the Godiva and Jezebel mock-up reactors, separated by a distance. Representative MCNP input files are in Appendix H.

A. U-233/Water Sphere

The first system was a sphere, 21.738 cm in diameter, made up of a U-233 metal/water mixture, where the U-233 density was 0.100 kg/l, the ratio H/U-233 was 256.781, and the reflector was 15.2 cm thick.[21] The estimates for implicit capture, 2000 neutrons per cycle, 10 inactive cycles, and 100 active cycles are shown in Table II. Table III shows the results for the same system except with analog capture.

Table III shows that analog capture only slightly decreases the correlation coefficient between the three estimators. As Table II shows, the three estimators are highly and positively correlated, especially the collision and track length estimators. The three-combined estimate has one of the smallest variances. In different independent runs, the combined estimate may

TABLE II. k_{eff} Estimates for the U-233/Water Sphere Using Implicit Capture

estimator	k_{eff}	standard deviation	correlation
collision	0.96798	0.00301	–
absorption	0.96263	0.00233	–
track length	0.96835	0.00314	–
collision/absorption	0.96379	0.00233	0.5744
absorption/track length	0.96369	0.00234	0.5642
collision/track length	0.96771	0.00301	0.9839
coll/abs/track length	0.96369	0.00233	–

TABLE III. k_{eff} Estimates for the U-233/Water Sphere Using Analog Capture

estimator	k_{eff}	standard deviation	correlation
collision	0.96230	0.00346	–
absorption	0.96500	0.00310	–
track length	0.96264	0.00359	–
collision/absorption	0.96398	0.00290	0.5558
absorption/track length	0.96418	0.00291	0.5354
collision/track length	0.96215	0.00347	0.9819
coll/abs/track length	0.96391	0.00291	–

not have exactly the smallest variance because of finite samples, because the covariance matrix is not known exactly, and because of the spread of all three individual estimates. Note, too, that the combination of the highly correlated collision and track length estimators produced an estimate outside the range of the two on the side of the estimator with the smaller variance. Figure 16 shows the three individual estimators (average of cycle estimates) and the three-estimator combination over the 100 active cycles. The combined estimator follows the absorption estimator very closely, lying on the side to which the other two estimators are situated. This was the general trend for all independent runs of this problem.

This problem was repeated using different random number sequences to produce 100 independent runs. (This particular set of runs was performed by C.T. Rombough.[21]) Comparing the sample population standard deviation of the 100 values for each estimator to the average of MCNP's reported standard deviations, MCNP was generally observed to conservatively estimate the population standard deviations, as shown in Table IV, where the first data column is the average k_{eff} for 100 runs, the second column is the sample population standard deviation for those k_{eff}'s, and the third column is the average of MCNP's reported standard deviations for the 100 runs. The combined estimator had the best performance overall. Figure 17 shows the distribution of the three-combined estimates from the 100 independent runs. They were not significantly different from a normal distribution at the 95% level. The solid line is a normal curve based on the average k_{eff} from the 100 runs and the average reported standard deviate. The histogram is the distribution of the 100 k_{eff}'s.

Of the 100 independent three-combined estimates, 70 percent of them covered the mean at the 68% confidence level, 95 percent of them covered the mean at the 95% confidence level, and 100 percent of them covered the mean at the 99% confidence level. Figure 18 shows the the 68% confidence intervals of each of the 100 independent runs compared to the 68% confidence interval of the mean of all 100 runs, which is the best estimate of the true k_{eff}. Seventy of the 100 confidence intervals cross the mean. Of particular importance is the fact that thirty of these confidence intervals do not cross the mean, which is expected. This result means that the confidence interval obtained from one independent MCNP run may not include the true value of k_{eff}. When criticality safety is an issue, a larger confidence interval should be used, such as the 99% confidence interval and perhaps another one larger than that. The raw data[21] are in Appendix G.

Initially, this problem was only repeated for 20 independent runs. The analysis seemed to indicate that MCNP was underestimating the standard deviation. It turns out that 20 runs were not enough to make an adequate analysis. See the discussions in Section 3.

There is an interesting observation to make in this analysis. We have been comparing standard deviations from a population of several runs to the average of the reported standard deviations from the several runs. For each estimator, then, we looked at the difference between these two values. Instead, let us look at the differences in the *variances.* For each of the individual estimators and the combined estimator, the magnitude of the variance difference for the combined estimator is not larger than the variance difference for the individual estimator with the largest magnitude. This held for every multiple run analysis we performed. The implication is that, if a bias did exist in the variance of one of the three individual estimators, the bias in the variance of the combined estimator would not exceed it, thus lending more credibility to the combined estimator. Appendix E examines the propagation of bias in the combined estimator and its variance.

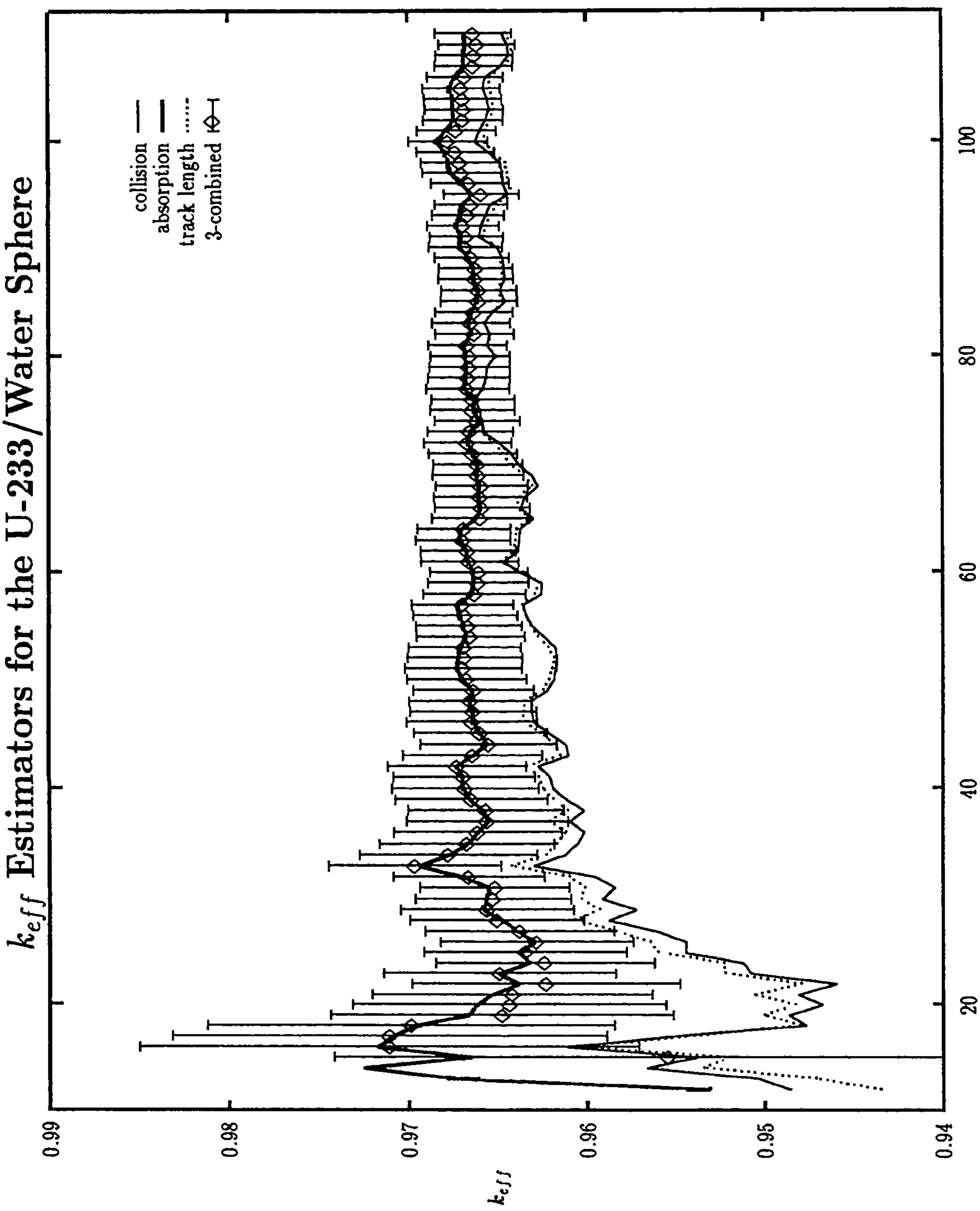

Fig. 16. Individual estimates and the combined estimate for the U-233/water sphere problem over 100 active cycles.

TABLE IV. k_{eff} Estimates for the U-233/Water Sphere and Their Associated Standard Deviations for 100 Independent Runs

k_{eff} estimator	$\bar{k}_{eff}$	$\sigma_{observed}$	$\bar{\sigma}_{calculated}$ $(\sigma_{\bar{\sigma}})$	coverage rates 68%	95%	99%
collision	0.96516	0.00293	0.00321 (0.00020)	72	97	99
absorption	0.96474	0.00228	0.00227 (0.00016)	68	95	99
track length	0.96509	0.00302	0.00324 (0.00020)	71	97	99
col/abs/trkl	0.96484	0.00216	0.00221 (0.00015)	70	95	100

B. U-233/Water Mixture In An Infinite Medium

The second system is an infinite medium, made up of a U-233 metal/water mixture, where the mixture density was 0.1 gm/cc and the ratio H/U-233 was 2220. The spatial distribution of the neutrons is not important in an infinite medium criticality calculation. For 2000 neutrons per cycle, 10 inactive cycles, 100 active cycles, and implicit capture, MCNP gave the estimates of k_∞ and its standard deviation as shown in Table V. The collision and track length estimators are highly correlated because the medium is infinite and there is no leakage. The combination of these two estimators yields an estimate slightly below their range. Both of those estimators are highly negatively correlated with the absorption estimator. A large contribution to the absorption estimator will result in a smaller contribution to the other two estimators and vice versa, thus explaining the negative correlation. The large negative correlation causes a large reduction in the variance when the estimators are combined. Figure 19 shows a plot (also available from MCNP using the "z" option) of the correlated data and the combination of them over the 100 active cycles. As the correlation coefficients indicate, when the track length estimator is low, so is the collision estimator, and when both of them are low, the absorption estimate is high.

Twenty independent runs were made of this problem in order to compare the observed population standard deviation with the average of the reported standard deviations. The data are listed in Table VI. The means of all four estimators are in excellent agreement. There is also excellent agreement between the MCNP estimation and the population estimation of the standard deviations. The population of combined k_{eff} estimators is much more compact than the individual estimators, showing that the combined error reduction from ~ 0.0015 to ~ 0.0005 is real. Although we know that twenty runs is probably not enough for this test, the observed standard deviation of the combined estimate is 0.00055, while the average of the reported standard deviation, at 0.00044, appears to underestimate it. The variance difference for the combined estimator is no larger than that of any individual estimator. The confidence intervals appear valid because the 68%, 95%, and 99% confidence intervals covered the mean 75%, 95%, and 100% of the time. Run number 7 had some difficulties in that the absorption and the track length estimators did not pass the normality check[22,23] at the 99% confidence level. The absorption estimator passed the normality check only at the 99% confidence level. One might expect this to happen about 1% of the time. The estimators of all other problems passed at the 95% confidence level, except the absorption estimator in

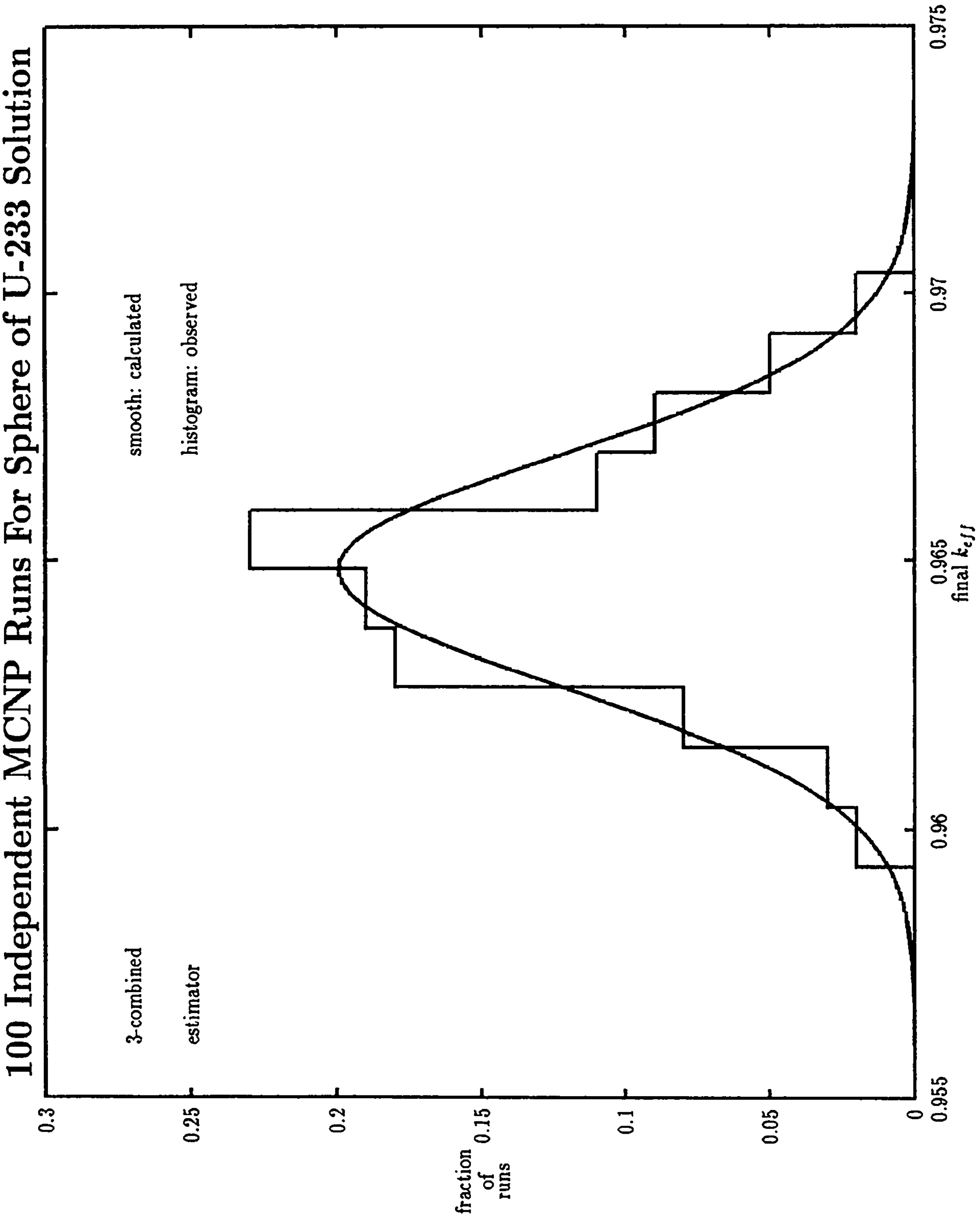

Fig. 17. Distribution of the three-combined estimator from 100 independent MCNP runs.

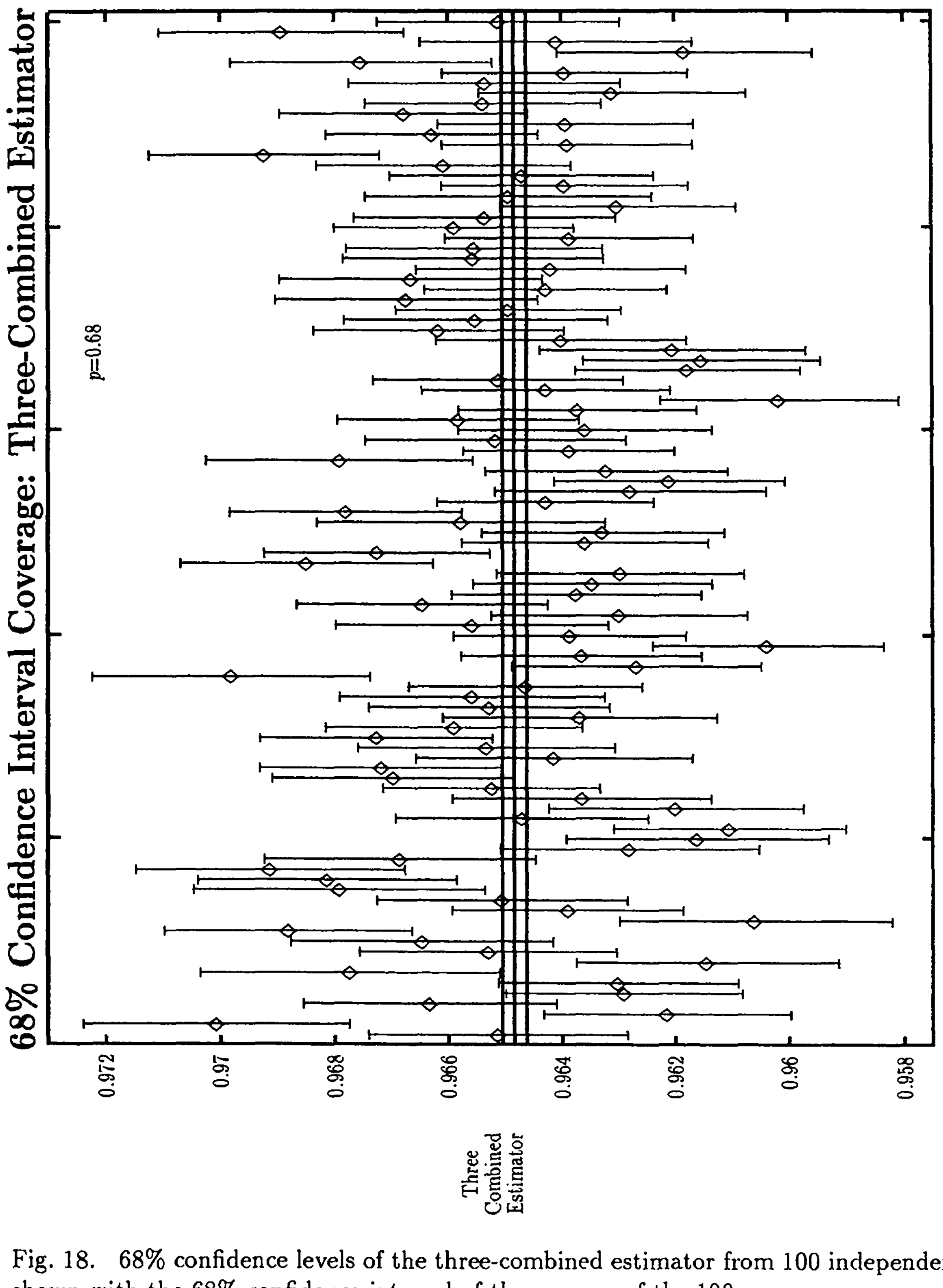

Fig. 18. 68% confidence levels of the three-combined estimator from 100 independent runs, shown with the 68% confidence interval of the average of the 100 runs.

TABLE V. k_∞ Estimates for U-233/Water Mixture in an Infinite Medium.

estimator	k_∞	standard deviation	correlation
collision	1.01332	0.00124	
absorption	1.01628	0.00171	
track length	1.01308	0.00123	
collision/absorption	1.01455	0.00039	-0.8545
absorption/track length	1.01439	0.00040	-0.8459
collision/track length	1.01307	0.00124	0.9876
coll/abs/track length	1.01451	0.00040	

run 9, which passed at 99%. Given the high positive and negative correlations, it is reasonable that, if one estimator does not appear to have cycle values distributed normally, the others will not either. Eliminating this run from the variance test yielded the results in Table VII, showing that the combined estimator variance was probably not underestimated. Here, the conglomerated data appeared sharper than normal since the 68%, 95%, and 99% confidence intervals covered the mean 79%, 100%, and 100% of the time. This demonstrates that the user should consider the information provided by the cycle k_{eff} normality checks.[22,23]

C. Godiva

MCNP modeled the Godiva reactor with 1000 neutrons per cycle, 10 inactive cycles, and 100 active cycles. Godiva is a highly enriched uranium bare sphere 8.741 cm in radius. For implicit capture, the results are in Table VIII and for analog capture, the results are in Table IX.

For implicit capture, the collision and absorption estimators are highly positively correlated and both are fairly highly correlated to the track length estimator. For analog capture, the absorption and track length estimators are almost uncorrelated, whereas the collision and track length estimators are relatively highly positively correlated. These results appear to be caused by a highly scattering medium. The variances are slightly smaller for implicit capture and the k_{eff} estimates agree.

One hundred independent runs were made using implicit capture, with the results in Table X (the one hundred independent run results are in Appendix G). The coverage rates were adequate, but not excellent for implicit capture. The quality of the coverage rates would likely pose little problem in a criticality safety study because of the use of safety margins. Another 100 runs were made, each with 500 active cycles. Batching the cycles into 50 batches of 10 cycles each resulted in much better coverage rates, as shown in Table XI. The use of batch statistics is discussed more thoroughly in the Two-Component Systems section.

One hundred independent runs were also performed using analog capture. Both implicit and analog capture gave basically the same answer. Those results are in Table XII.

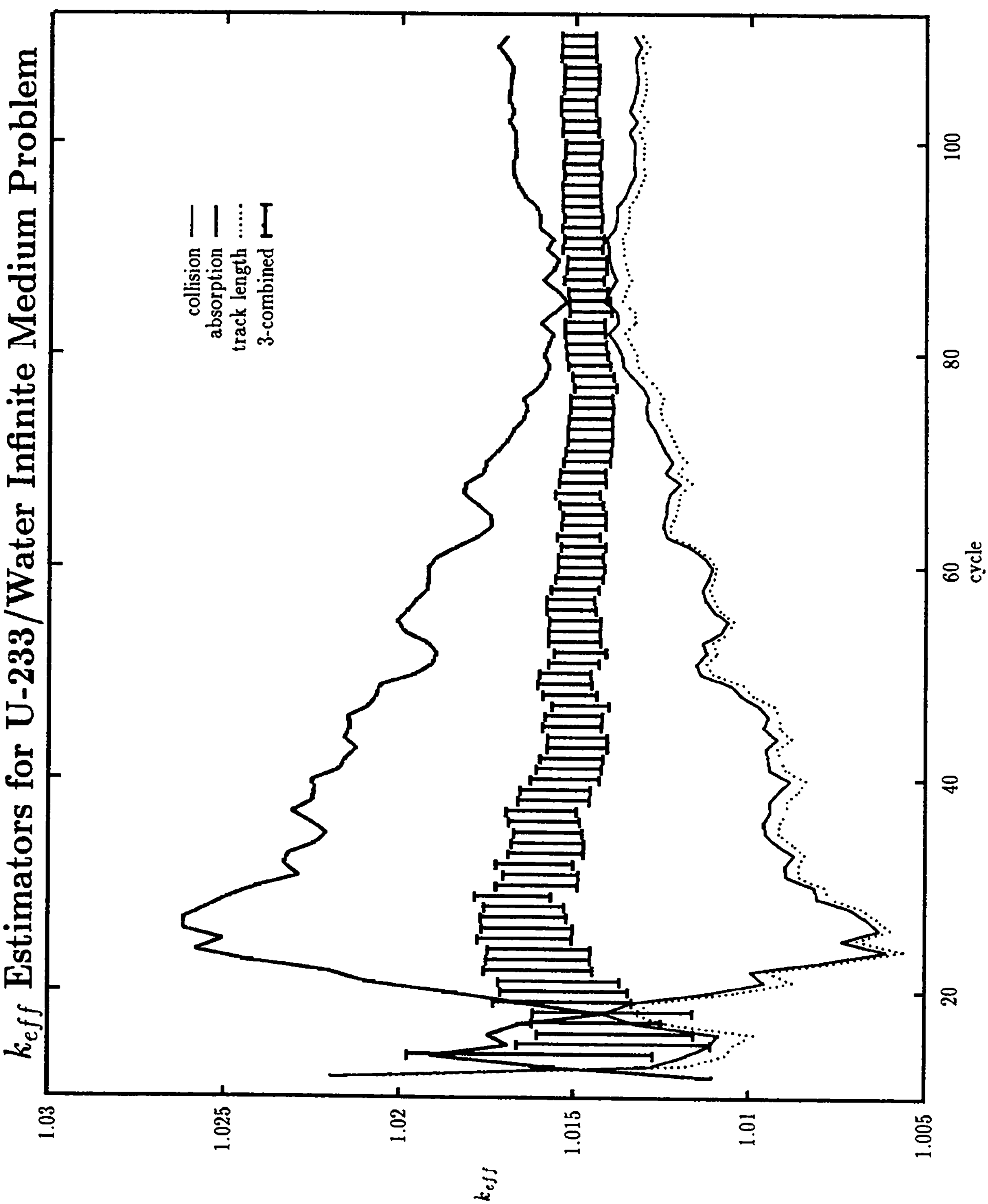

Fig. 19. Individual estimates and the combined estimate over 100 active cycles for the U-233/water mixture in an infinite medium.

TABLE VI. k_∞ Estimates for the U-233/water Mixture in an Infinite Medium and Their Associated Standard Deviations and Coverage Rates for 20 Independent Runs.

k_{eff} estimator	$\bar{k}_\infty$	$\sigma_{observed}$	$\bar{\sigma}_{calculated}$ ($\sigma_{\bar{\sigma}}$)	coverage rates		
				68%	95%	99%
collision	1.01490	0.00136	0.00125 (0.00006)	65	100	100
absorption	1.01440	0.00158	0.00160 (0.00011)	70	95	100
track length	1.01491	0.00137	0.00126 (0.00007)	65	100	100
col/abs/trkl	1.01467	0.00048	0.00044 (0.00004)	75	95	100

TABLE VII. k_∞ Estimates for the U-233/Water Mixture in an Infinite Medium and Their Associated Standard Deviations and Coverage Rates for 19 Independent Runs, Eliminating the Non-Normal Run.

k_{eff} estimator	$\bar{k}_\infty$	$\sigma_{observed}$	$\bar{\sigma}_{calculated}$ ($\sigma_{\bar{\sigma}}$)	coverage rates		
				68%	95%	99%
collision	1.01479	0.00131	0.00125 (0.00006)	68	100	100
absorption	1.01441	0.00162	0.00161 (0.00011)	68	95	100
track length	1.01479	0.00131	0.00126 (0.00007)	63	100	100
col/abs/trkl	1.01462	0.00043	0.00044 (0.00004)	79	100	100

TABLE VIII. k_{eff} Estimates for the Godiva Reactor with Implicit Capture

estimator	k_{eff}	standard deviation	correlation
collision	1.00100	0.00243	-
absorption	1.00078	0.00240	-
track length	0.99832	0.00199	-
collision/absorption	1.00076	0.00242	0.9908
absorption/track length	0.99891	0.00197	0.6572
collision/track length	0.99890	0.00198	0.6639
coll/abs/track length	0.99877	0.00198	-

TABLE IX. k_{eff} Estimates for the Godiva Reactor with Analog Capture

estimator	k_{eff}	standard deviation	correlation
collision	0.99924	0.00316	-
absorption	0.99837	0.00361	-
track length	0.99821	0.00287	-
collision/absorption	0.99889	0.00274	0.3122
absorption/track length	0.99827	0.00235	0.0907
collision/track length	0.99851	0.00282	0.7657
coll/abs/track length	0.99822	0.00237	-

TABLE X. k_{eff} Estimates for the Godiva Reactor and Their Associated Standard Deviations and Coverage Rates for 100 Independent Runs, Using Implicit Capture.

k_{eff} estimator	$\bar{k}_{eff}$	$\sigma_{observed}$	$\bar{\sigma}_{calculated}$ $(\sigma_{\bar{\sigma}})$	coverage rates 68%	95%	99%
collision	0.99695	0.00270	0.00234 (0.00018)	64	90	98
absorption	0.99699	0.00272	0.00234 (0.00017)	61	90	98
track length	0.99717	0.00236	0.00190 (0.00014)	57	86	97
col/abs/trkl	0.99717	0.00238	0.00188 (0.00014)	59	87	95

TABLE XI. k_{eff} Estimates for the Godiva Reactor and Their Associated Standard Deviations and Coverage Rates for 100 Independent Runs, Using Implicit Capture, 500 Active Cycles, and 50 Batches of 10 Cycles each.

k_{eff} estimator	$\bar{k}_{eff}$	$\sigma_{observed}$	$\bar{\sigma}_{calculated}$ $(\sigma_{\bar{\sigma}})$	coverage rates 68%	95%	99%
collision	0.99771	0.00099	0.00115 (0.00010)	75	98	99
absorption	0.99772	0.00101	0.00114 (0.00017)	75	97	99
track length	0.99781	0.00092	0.00096 (0.00010)	66	95	100
col/abs/trkl	0.99779	0.00092	0.00097 (0.00009)	71	95	100

TABLE XII. k_{eff} Estimates for the Godiva Reactor and Their Associated Standard Deviations and Coverage Rates for 100 Independent Runs, Using Analog Capture.

k_{eff} estimator	$\bar{k}_{eff}$	$\sigma_{observed}$	$\bar{\sigma}_{calculated}$ ($\sigma_{\bar{\sigma}}$)	coverage rates 68%	95%	99%
collision	0.99783	0.00329	0.00322 (0.00019)	63	95	99
absorption	0.99793	0.00385	0.00381 (0.00030)	69	95	99
track length	0.99787	0.00295	0.00280 (0.00020)	70	94	99
col/abs/trkl	0.99768	0.00216	0.00215 (0.00017)	76	90	100

D. Simplified Jezebel

Jezebel is a spherical reactor, about 6.385 cm in radius, made up of delta-phase Pu (4.5 at.% Pu-240, 1.02 wt.% Ga) at a density of 15.61 g/cm^3. MCNP was used to estimate the criticality of an idealized pure Pu-239 model of Jezebel with 2000 neutrons per cycle for 10 inactive cycles and 50 active cycles. The results using implicit capture are in Table XIII. With one isotope and implicit capture, the collision and absorption estimators are exactly the same, so no new information is gained by having both of them. Therefore, there is effectively only one combination of two estimators.

Table XIV shows the k_{eff} estimates for the Jezebel model with analog capture. The track length and absorption estimators are just slightly anticorrelated, probably because of the absence of competition for weight contribution between the two estimators as in implicit capture. The two estimators combine with a reduced standard deviation. The large gain in the reduction of the standard deviation is carried over to the three-combined estimate. The results of the two types of capture agree. Fifty independent MCNP runs were each made for implicit and analog capture. The results are shown in Tables XV and XVI, respectively.

E. Two-Component Systems

It has been shown that a system with a dominance ratio close to unity could produce an underestimation (bias) of the estimated standard deviation of k_{eff}.[24,25] The dominance ratio is the ratio of the second largest eigenvalue to the largest eigenvalue. The largest eigenvalue is k_{eff}. The general consensus among people in the field seems to be that this underestimation could be as large as a factor of two. Some studies have shown this, although the dependence on dominance ratio was not clear.[24] A straight power iteration method, as used in a Monte Carlo criticality calculation, may converge very slowly for a system with a high dominance ratio, since the higher order eigenmodes will not die out quickly from cycle to cycle. Such a calculation will have a high cycle-to-cycle correlation of the k_{eff} values and the estimated k_{eff} standard deviation calculated by MCNP could be smaller than the actual standard deviation. Such a bias would result in inadequate confidence interval coverage rates.

The effect of variance bias on the three-combined estimator is discussed and demonstrated in Appendix E. Specifically, if the biases (viewed as either additive or multiplicative) in the

TABLE XIII. k_{eff} Estimates for the Jezebel Model with Implicit Capture

estimator	k_{eff}	standard deviation	correlation
collision	1.01403	0.00289	-
absorption	1.01403	0.00289	-
track length	1.01084	0.00185	-
collision/absorption	1.01403	0.00289	1.0000
absorption/track length	1.01118	0.00188	0.5180
collision/track length	1.01118	0.00188	0.5180
coll/abs/track length	1.01118	0.00188	-

TABLE XIV. k_{eff} Estimates for the Jezebel Model with Analog Capture

estimator	k_{eff}	standard deviation	correlation
collision	1.01224	0.00383	-
absorption	1.01525	0.00490	-
track length	1.01233	0.00258	-
collision/absorption	1.01328	0.00338	0.2298
absorption/track length	1.01304	0.00219	-0.1206
collision/track length	1.01232	0.00260	0.6158
coll/abs/track length	1.01312	0.00218	-

TABLE XV. k_{eff} Estimates for the Jezebel Reactor Mock-up and Their Associated Standard Deviations and Coverage Rates for 50 Independent Runs, Using Implicit Capture.

k_{eff} estimator	$\bar{k}_{eff}$	$\sigma_{observed}$	$\bar{\sigma}_{calculated}$ ($\sigma_{\bar{\sigma}}$)	coverage rates 68%	95%	99%
collision	1.01304	0.00284	0.00279 (0.00033)	66	96	100
absorption	1.01304	0.00284	0.00279 (0.00033)	66	96	100
track length	1.01298	0.00231	0.00187 (0.00022)	56	86	96
col/abs/trkl	1.01302	0.00221	0.00184 (0.00022)	60	90	98

TABLE XVI. k_{eff} Estimates for the Jezebel Reactor Mock-up and Their Associated Standard Deviations and Coverage Rates for 50 Independent Runs, Using Analog Capture.

k_{eff} estimator	$\bar{k}_{eff}$	$\sigma_{observed}$	$\bar{\sigma}_{calculated}$ ($\sigma_{\bar{\sigma}}$)	coverage rates 68%	95%	99%
collision	1.01279	0.00321	0.00335 (0.00037)	72	98	100
absorption	1.01198	0.00351	0.00465 (0.00045)	84	100	100
track length	1.01308	0.00277	0.00261 (0.00025)	64	92	100
col/abs/trkl	1.01275	0.00195	0.00209 (0.00026)	72	100	100

individual estimator variances are the same, the three-combined estimator will not be affected (the biases will cancel out), but the variance of the three-combined estimator will retain the individual estimator variance bias. If the biases in the variances of the three individual estimators are not the same, an inaccuracy in the three-combined k_{eff} estimator may result, depending on the relative size of the variances.

Two types of systems that have large dominance ratios are large thermal reactors and multiple-component lattice-type systems. The latter are prevalently found in criticality safety considerations, such as the handling and storage of nuclear waste. In the interest of criticality safety, we looked at a two-component system consisting of an idealized Jezebel reactor and a Godiva reactor, 80 cm center to center. A fission matrix patch to MCNP[26] was used to estimate the dominance ratio at 0.985. A dominance ratio of 0.985 is not particularly high, but the Jezebel/Godiva system seemed to display more of a variance underestimation than a Jezebel/Jezebel system whose dominance ratio was 0.994. We infer, then, that ease and accuracy of calculation is not only a direct function of dominance ratio, but also system geometry and material.

To investigate the bias in the standard deviation, one hundred independent MCNP runs were made for the Jezebel/Godiva system, using 5000 histories per cycle, 20 inactive cycles, and 800 active cycles. The results of one of the runs are shown in Table XVII. The observed standard deviation, $\sigma_{observed}$, is the population standard deviation observed in the 100 k_{eff} values themselves from the 100 runs. This will be considered the best estimate of the true standard deviation of k_{eff}. The uncertainty in $\sigma_{observed}$ is estimated by the variance of the variance (see the MCNP manual). The standard deviation calculated by MCNP is $\sigma_{calculated}$. We assume that $\sigma_{observed}$, distributed as a χ^2 with ~100 degrees of freedom, and $\sigma_{calculated}$, distributed as a χ^2 with ~800 degrees of freedom, are, for comparison purposes, distributed similarly. Given 820 cycles per run, the output of the 100 runs seemed to indicate that twenty inactive cycles was adequate to effectively achieve the fundamental mode. The input deck is found in Appendix H, and the entire k_{eff} data is found in Appendix G. For 100 MCNP runs, the results are shown in Table XVIII. There is an underestimation in the standard deviations for this example, but nowhere near a factor of two. The $\sigma_{calculated}$ for the three-combined k_{eff} is 0.00030 with a population uncertainty of 0.00001. The $\sigma_{observed}$ is 0.00038, meaning that $\sigma_{calculated}$ underestimates $\sigma_{observed}$ by about 25%. The standard deviations in the collision and absorption estimators are underestimated by almost 30% and the track length estimator standard deviations by about 20%. This difference in underestimation between the individual estimator's standard deviation does not appear to adversely affect the

TABLE XVII. k_{eff} Estimates for the Two-Component System, Godiva and Jezebel Mock-up.

k_{eff} estimator type	k_{eff}	standard deviation	correlation
collision	1.01230	0.00043	-
absorption	1.01231	0.00043	-
track length	1.01252	0.00030	-
collision/absorption	1.01230	0.00043	0.9991
absorption/track length	1.01248	0.00030	0.4893
collision/track length	1.01248	0.00030	0.4914
coll/abs/track length	1.01249	0.00030	-

TABLE XVIII. 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	0.00040 (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

three-combined estimator itself, mainly because it is weighted much more to the track length estimator. In this problem, the correlation coefficient between the collision and absorption estimators is about 0.999, and the correlation coefficient between the track length estimator and the other two is about 0.48. The coverage rates for the three-combined k_{eff} estimator at the 68%, 95%, and 99% confidence levels were 54, 88, and 98 percent.

One way to detect and assess a correlation between k_{eff} cycles is to combine several k_{eff} cycles into one new k_{eff} batch cycle. For example, if the 800 active k_{eff} cycles were batched into 40 batch cycles of 20 k_{eff} cycles each, the batches would have a smaller batch-to-batch correlation, giving an improved estimate of $\sigma_{observed}$. MCNP provides this batch information. For 40 batches of 20 cycles each, the data from Table XIX were observed.

The $\sigma_{observed}$ for batch sizes of one cycle and 20 cycles for the combined estimator are the same. The average $\sigma_{calculated}$ is in excellent agreement with $\sigma_{observed}$. Batching resulted in a marked improvement in coverage rates. Forty batches with twenty cycles each produced confidence intervals at the 68%, 95%, and 99% confidence levels that covered the mean 70, 95, and 99 percent of the time.

The average calculated standard deviation increases with increasing batch size. Figure 20 shows that, for increasing batch size, the average of the 100 calculated standard deviations, $\bar{\sigma}_{calculated}$, approaches the population standard deviation observed from the 100

TABLE XIX. 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.

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

three-combined k_{eff} values, $\sigma_{observed}$. The individual estimators and their standard deviations had the same behavior. Note, though, that with larger correlated k_{eff} batch sizes there are fewer batch values of k_{eff} and, therefore, the variation, or spread, in the estimated batch $\sigma_{calculated}$ becomes larger, as verified in Fig. 20. The smaller biases in $\sigma_{calculated}$ lead to an improvement in the three-combined k_{eff} estimator.

This example clearly demonstrates that batched data in MCNP can be used to examine cycle-to-cycle correlation effects on $\sigma_{calculated}$. If these effects exist, the user can use the confidence intervals from a larger batch size. Additionally, 30 of the 100 runs had warning messages, mostly indicating that the ratio of the combined estimator from the first half of the problem to that of the second half was too large. This drifting effect can be visualized in the distributions, from 100 independent MCNP runs, of the three-combined k_{eff} estimator at 30, 100, and 800 active cycles, as shown in Fig. 21. The user can utilize both the batch data and warning messages to detect problems with spatial convergence, which may indicate a system with a large dominance ratio. If this appears to be a problem, the various MCNP k_{eff} tables and plots in the output should be examined for any drifting behavior in the k_{eff} estimates. If necessary, the user can make independent MCNP runs.

The dominance ratio of the modeled system need not be equal to that of the physical system itself. If, by symmetry, the odd eigenmodes can be eliminated, the dominance ratio can be reduced. This may result in an easier and more precise calculation. For these reasons, it is a recommended procedure for criticality calculations. An example is the Jezebel/Jezebel system, mentioned above, whose dominance ratio is 0.994. By putting a reflecting plane perpendicularly between the spheres, the second eigenmode, which is odd, is eliminated in the calculation, and the dominance ratio is reduced to 0.418.

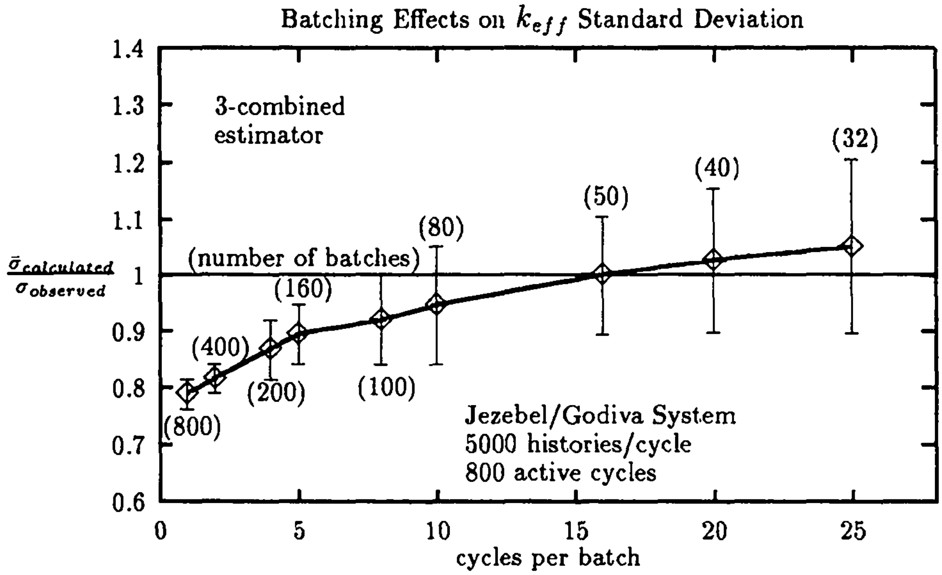

Fig. 20. For 800 active cycles and 100 independent runs, MCNP's batch data shows an underestimation in the calculated standard deviation for too few cycles per batch. The error bars represent the observed variation in $\bar{\sigma}_{calculated}$ at the one sigma level.

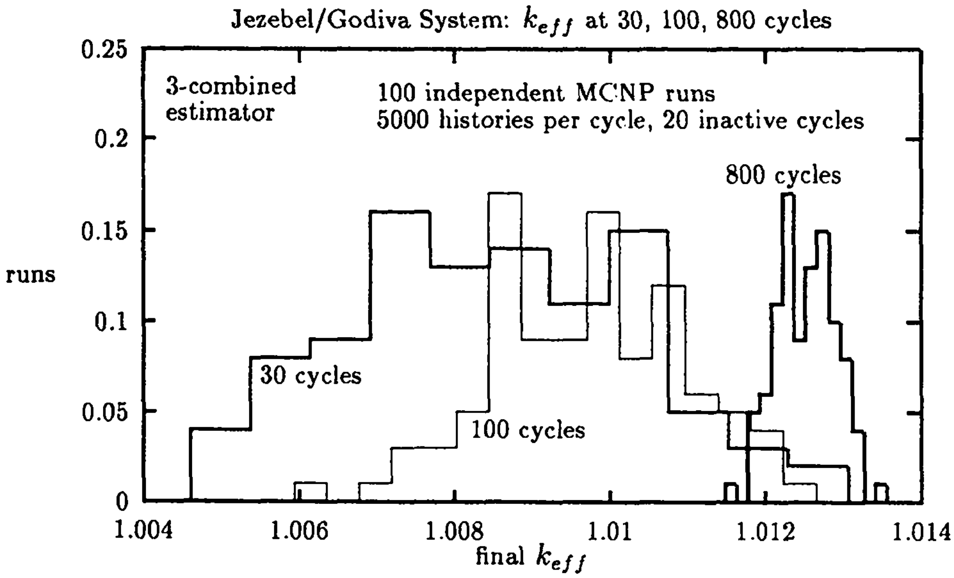

Fig. 21. The drifting of the three-combined estimator as seen in its distribution from 100 independent MCNP runs at 30, 100, and 800 active cycles.

VII. SUMMARY AND CONCLUSIONS

The process that MCNP employs in a criticality calculation has been presented, along with some basic statistics regarding the analysis of MCNP's three k_{eff} estimators: collision, absorption, and track length. Of utmost importance is the realization that MCNP does not give a single value for the estimate of k_{eff}. MCNP produces a range of values that should contain the true value with some specified confidence. The term *confidence interval* is given to this range. To increase the probability that a confidence interval includes the true value, either more cycles need to be run or the size of the interval must be increased. When criticality safety and human safety are at stake, high percentage confidence intervals are desired to increase the probability that the true value is in the intervals.

MCNP's best estimator for k_{eff} has been theoretically and empirically shown to be the three-combined estimator. The combination of the three estimators is performed essentially by the least squares method, taking into account observed covariances, and is based mainly on a paper by M. Halperin.[4] MCNP's coding has been verified to be correct. The Halperin method produces the estimate with the least variance, as specified by the Gauss-Markov Theorem.[1,chapter VI;2,page 14;3,page 198] This method assumes that the covariance matrix of the estimators is known. In MCNP (as in Halperin's paper), the covariance matrix is estimated from the data, therefore the three-combined estimator is the "almost" optimum estimator, yet, in practice, it is still the best estimator.

The behavior of the combined estimate has been described and demonstrated. The correlation between estimators plays a large role in the combined estimator; negative correlation results in a much reduced variance in the combined estimator, whereas a high positive correlation may result in a combined estimate outside the range of the estimates from the individual estimators. In a statistical simulation, the combined estimate outperformed both the simple average of the individual estimators and the individual estimator with the smallest variance.

For multiple independent runs, the coverage rates of the k_{eff} confidence intervals were verified for several real systems. The confidence intervals nominally covered the mean the appropriate percentage of time for problems with low dominance ratios. For high dominance ratio problems, the estimated k_{eff} standard deviations may be underestimated, resulting in inadequate coverage rates. The three-combined k_{eff} estimator remains minimally affected when the relative underestimation in the individual k_{eff} standard deviation is about the same. MCNP provides batched k_{eff} cycle data that assist the user in detecting and alleviating an underestimation in standard deviations that is caused by the cycle-to-cycle correlations typically found in high dominance ratio problems. MCNP's warning messages also alert the user to non-normal data or a drift in the fundamental eigenmode.

For an adequate number of cycles, usually much greater than thirty (see manual for MCNP version 4A), the three-combined k_{eff} estimator is MCNP's best estimate for building k_{eff} confidence intervals.

ACKNOWLEDGMENTS

Many thanks to Ann Nagy for preparing the several "final" versions of this manuscript.

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VIII. APPENDIX A: COMMON DISTRIBUTIONS

The normal distribution and Student's t-distribution were described in Section III. Whereas a distribution such as the normal distribution describes the sums of samples of random variables, the χ^2-distribution describes the sums of the squares of samples of random variables where the underlying data are independent and normally distributed. Particularly, for the sample variance, s^2, calculated with $n-1$ degrees of freedom, estimating the true variance, σ^2, the random variable

$$\frac{(n-1)s^2}{\sigma^2} \tag{95}$$

is called "chi-squared" (χ^2) and is distributed as a χ^2-distribution with $n-1$ degrees of freedom. Figure 22 shows the χ^2 distribution for 1, 3, and 10 degrees of freedom. The expected value of χ^2 is the number of degrees of freedom, here $n-1$.[10,page 109]

The F-distribution describes the distribution of a random variable of the form

$$\frac{C_1/d_1}{C_2/d_2}, \tag{96}$$

where C_1 has a χ^2-distribution with d_1 degrees of freedom and C_2 has an independent χ^2-distribution with d_2 degrees of freedom. With the χ^2-distribution identified, we see that the F-distribution, with (n_1-1) and (n_2-1) degrees of freedom, describes the random variable

$$\frac{\frac{(n_1-1)s_1^2}{\sigma_1^2}(n_2-1)}{\frac{(n_2-1)s_2^2}{\sigma_2^2}(n_1-1)} = \frac{s_1^2/\sigma_1^2}{s_2^2/\sigma_2^2}, \tag{97}$$

where the underlying data in each of sets 1 and 2 are independent and normally distributed. Since the expected value of the χ^2-statistic is the degrees of freedom, the F-statistic, Equation 96, has an expected value of unity.

Both the χ^2-distribution and F-distribution are non-symmetric and rightwardly skewed from zero to ∞. As the degrees of freedom, d, approach infinity, $\sqrt{2\chi^2}$ approaches a normal distribution with mean $\sqrt{2d-1}$ and unit variance.[11]

Hotelling's T^2-distribution is a multivariate extension of Student's t distribution.[3,page 123] Suppose we have n mutually independent vectors, $\mathbf{x}_i$ of length p and that each is distributed normally with mean Θ and covariance matrix Σ. Then the sample mean and variance are

$$\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i \tag{98}$$

$$\mathbf{S} = \frac{1}{n-1}\sum_{i=1}^{n}(\mathbf{x}_k - \bar{\mathbf{x}})(\mathbf{x}_k - \bar{\mathbf{x}})' \tag{99}$$

where $\bar{\mathbf{x}}$ and $\mathbf{S}$ are of dimension $(n \times 1)$ and $(n \times n)$, respectively. Hotelling's T^2-statistic for some known Θ_o is

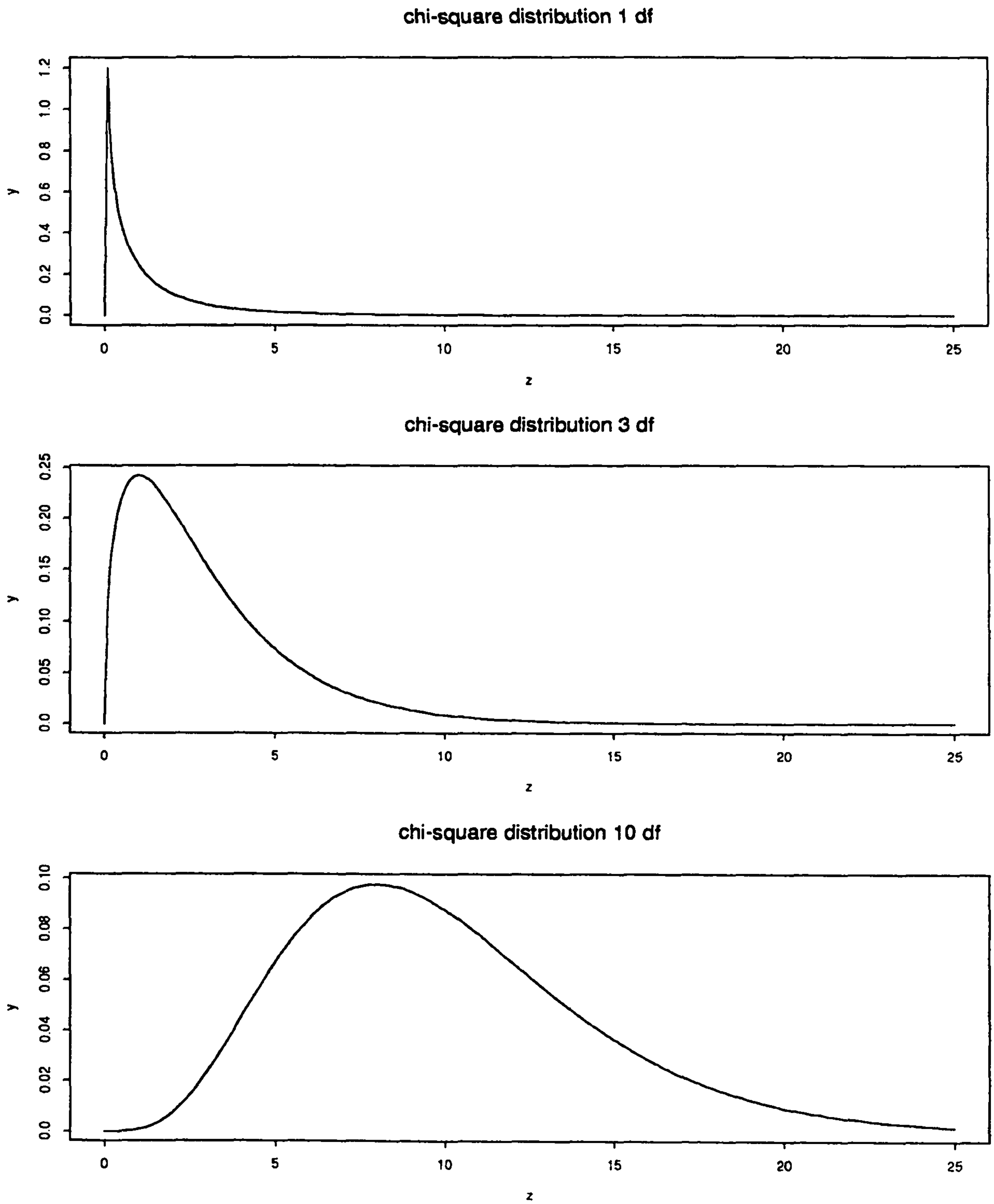

Fig. 22. χ^2-distributions.

$$T^2_{p,n-p} = n(\mathbf{x}_k - \mathbf{\Theta}_o)'\mathbf{S}^{-1}(\mathbf{x}_k - \mathbf{\Theta}_o) \tag{100}$$

and reduces to the Student's t-statistic for the univariate case, $p = 1$.

The statistic U,[3,page 123]

$$U = \left(\frac{T^2}{n-1}\right)\left(\frac{n-p}{p}\right) \tag{101}$$

is distributed as $F_{p,n-p}(\lambda)$ where λ is the noncentrality parameter,[2,page 418]

$$\lambda = n(\mathbf{\Theta} - \mathbf{\Theta}_o)'\mathbf{\Sigma}^{-1}(\mathbf{\Theta} - \mathbf{\Theta}_o). \tag{102}$$

If $\mathbf{\Theta} = \mathbf{\Theta}_o$, then U is distributed as a central F-distribution. This means that the expected value of U is one. Therefore, the expected value of Hotelling's T-statistic is

$$E(T^2) = \frac{p(n-1)}{n-p}. \tag{103}$$

IX. APPENDIX B: REGRESSION ANALYSIS

Univariate Regression Analysis is a statistical study where the relationship between one dependent variable and one or more independent variables is estimated.[7] The functional describing the relation between the dependent and independent variables is called a regression. For one independent variable, we have $y = f(x)$, which is called the regression of y on x[1] and the coefficients that constitute f are called the regression parameters.

There are many ways to estimate the regression parameters, such as the Least Squares Method, the Principle of Maximum Likelihood, and the Method of Moments. It is stunning that the Maximum Likelihood Principle with assumption of normality produces the same parameter estimation as the Least Squares Method. Given that, we will concentrate on the Least Squares Method and briefly examine the Maximum Likelihood Principle.

A. Least Squares Method

Legendre proposed in 1805 that the best value gleaned from observations would have the least value of the sum of squared deviations of the observations.[1] This is the Least Squares principle. The goal of the Least Squares Method is to produce the best fit to a set of scattered data points. By "best fit" we mean that the deviations of the data points from the fit are a minimum. From the method, then, we obtain the least squares parameters, which, for the equation of a line, are the slope and intercept. The least squares method can be derived in many ways (several of the books in the references contain this information). We are interested in the least squares method applied to the univariate linear regression model[3]

$$y_i = a_0 + a_1 x_{i1} + a_2 x_{i2} + \cdots + a_{k-1} x_{i,k-1} + e_i \tag{104}$$

where the x's and y are observable scalar variables for $i = 1, \ldots, n$, the a's are unknown coefficients, and the e's are random errors. Equation 104 is a univariate model since there is only one dependent variable y that is observed n times. When the univariate model has several independent variables, x, it is sometimes called a multi-linear regression model. If there are several dependent variables, it is called a multivariable linear regression. Equation 104 is quite amenable to matrix form:

$$\mathbf{y} = \mathbf{X}\beta + \mathbf{e} \tag{105}$$

where

$\mathbf{e}$ is the $(n \times 1)$ vector of errors,
β is the $(k \times 1)$ vector of unknown coefficients a_i,
$\mathbf{y}$ is the $(n \times 1)$ vector of dependent variables, and
$\mathbf{X}$ is the $(n \times k)$ regressor matrix:

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1,k-1} \\ \vdots & \vdots & & \vdots \\ 1 & x_{n1} & \cdots & x_{n,k-1} \end{bmatrix}. \tag{106}$$

Several assumptions are employed in the least squares method.[3]

- $\mathbf{y}$ is a vector of independent observations on a random variable, which is observed with no error in measurement.
- $\mathbf{X}$ is a matrix of known independent constants.
- $\mathbf{e}$ is a vector of unobservables that take into account measurement errors and possibly model errors.
- the covariance matrix of $\mathbf{e}$, $\mathbf{\Sigma}$, is represented as $\sigma^2\mathbf{I}$. In other words, the errors are uncorrelated and homoscedastic (they all have the same variance, σ^2).
- $E(\mathbf{e}) = 0$. It is not necessary for the errors to be multivariate normally distributed in order to obtain least squares solutions. It *is* necessary, though, in order to obtain confidence intervals for the solutions.
- $E(\mathbf{y}) = \mathbf{X}\beta$, or, in other words, there is a true linear relationship between the dependent and independent variables.
- $\text{var}(\mathbf{y}) = \text{var}(\mathbf{e}) = \mathbf{\Sigma}$.

Lest pandemonium erupt amongst the Monte Carlo practitioners, we must put to bed any alarm stemming from these stated assumptions. Yes, these assumptions may seem to preclude the combination of Monte Carlo eigenvalue estimators which are stochastic in nature, but if $\mathbf{X}$ does not depend upon β or $\mathbf{\Sigma}$ (the regression parameters), stochasticity in $\mathbf{X}$ will not affect the least squares solution.[3] If y is also stochastic, the problem becomes very complicated, so reliance is made upon the assumption that the measurement errors pale in comparison to those of the linear model.[3] We will soon see that we can also modify any data where the errors are correlated and heteroscedastic in order to meet the assumptions listed above.

Let us derive the least squares solutions for the simple model with one dependent variable and one independent variable:

$$y_{true} = a_0 + a_1 x. \tag{107}$$

The observations y_i on y_{true} are then

$$y_i = a_0 + a_1 x_i + e_i, \tag{108}$$

whose parameters, a_0 and a_1, will be estimated by the least squares estimates, b_0 and b_1, so that y may be predicted by the fitted equation

$$\hat{y} = b_0 + b_1 x. \tag{109}$$

Obtaining b_0 and b_1 follows from minimizing the sums of the squares of the errors, Q,

$$
\begin{aligned}
Q &= \sum_{i=1}^{n} e_i^2 \\
&= \sum_{i=1}^{n} (y_i - y_{true})^2 \\
&= \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2 \qquad (110)
\end{aligned}
$$

with respect to a_0 and a_1. We find

$$
\begin{aligned}
\frac{\partial Q}{\partial a_0} &= -2 \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) = 0, \\
\frac{\partial Q}{\partial a_1} &= -2 \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) x_i = 0, \qquad (111)
\end{aligned}
$$

from which we determine the estimates b_0 and b_1 as

$$
\begin{aligned}
b_0 &= \bar{y} - b_1 \bar{x}, \qquad (112) \\
b_1 &= \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} \\
&= \frac{\sum (x_i - \bar{x}) y_i}{\sum (x_i - \bar{x})^2}. \qquad (113)
\end{aligned}
$$

Equations 111 are called the *normal equations*. We shall also estimate the variance of the least squares parameter estimates, b_0 and b_1. For b_1, the x's act as coefficients on the y's, so if the variance of y is σ^2, the variance of b_1 is

$$
\sigma_{b_1}^2 = \frac{\sigma^2}{\sum (x_i - \bar{x})^2}. \qquad (114)
$$

The variance of b_0 is found as[27]

$$
\begin{aligned}
\sigma_{b_0}^2 &= var(\bar{y} - b_1 \bar{x}) \\
&= \frac{\sigma^2}{n} + \frac{\sigma^2 \bar{x}^2}{\sum (x_i - \bar{x})^2} \\
&= \frac{\sigma^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2}. \qquad (115)
\end{aligned}
$$

We estimate σ^2 by the sum of squares of deviations of the observed y_i from the mean $\bar{y}$, divided by the degrees of freedom:

$$\hat{\sigma}^2 = \frac{\sum(y_i - \bar{y})^2}{n-2}. \tag{116}$$

To proceed to the point of building confidence intervals, we need to make the assumption that the errors e_i–the deviations of the observations about the regression line–are normally distributed with mean zero and variance σ^2. We may use $\hat{\sigma}^2$ in the variance expressions for b_0 and b_1, Eqs. 115 and 114, and thusly build $100(1-\alpha)\%$ confidence intervals for each:

$$b_1 \pm t_{n-2,1-\frac{\alpha}{2}} \frac{\sigma}{\sqrt{\sum(x_i - \bar{x})^2}} \tag{117}$$

and

$$b_0 \pm t_{n-2,1-\frac{\alpha}{2}} \left[\frac{\hat{\sigma}^2 \sum x_i^2}{n\sum(x_i - \bar{x})^2}\right]^{\frac{1}{2}}. \tag{118}$$

Here, $t_{n-2,1-\frac{\alpha}{2}}$ is the Student's t distribution for $n-2$ degrees of freedom at the $100(1-\alpha)\%$ confidence level.

Now that the regression parameters are estimated, a predicted value of y, $\hat{y}_k$, for some specific x_k is

$$\begin{aligned} \hat{y}_k &= b_0 + b_1 x_k \\ &= \bar{y} - b_1\bar{x} + b_1 x_k \\ &= \bar{y} + b_1(x_k - \bar{x}) \end{aligned} \tag{119}$$

and the variance of $\hat{y}_k$ is, since $\bar{y}$ and b_1 are uncorrelated,[3]

$$\begin{aligned} \sigma^2_{\hat{y}_k} &= var(\bar{y}) + (x_k - \bar{x})^2 var(b_1) \\ &= \sigma^2\left[\frac{1}{n} + \frac{(x_k - \bar{x})^2}{\sum(x_i - \bar{x})^2}\right], \end{aligned} \tag{120}$$

which is estimated by replacing σ^2 by $\hat{\sigma}^2$.

Now, that we've seen the least squares solution for one dependent and one independent variable, let us look at the multi-linear model, where there are two or more independent variables,

$$\mathbf{y}_{true} = \mathbf{X}\beta. \tag{121}$$

Written for the observations $\mathbf{y}$ on $\mathbf{y}_{true}$ it becomes

$$\mathbf{y} = \mathbf{X}\beta + \mathbf{e}, \tag{122}$$

whose parameter vector, β, will be estimated by $\hat{\beta}$, so that the fitted equation is

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\beta}, \tag{123}$$

As in the simple case, we want to minimize the sums of squares of the errors,

$$\begin{aligned} \mathbf{Q} &= (\mathbf{y}-\mathbf{y}_{true})'(\mathbf{y}-\mathbf{y}_{true}), \\ &= (\mathbf{y}-\mathbf{X}\beta)'(\mathbf{y}-\mathbf{X}\beta), \end{aligned} \tag{124}$$

with respect to β, whereupon we find[3]

$$-\mathbf{2X}'(\mathbf{y}-\mathbf{X}\beta) = \mathbf{0}, \tag{125}$$

which implies that the estimate of β is

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}, \tag{126}$$

assuming that $(\mathbf{X}'\mathbf{X})^{-1}$ exists. Again, Eq. 126 represents the *normal equations.* The Gauss-Markov Theorem says that $\hat{\beta}$ is an unbiased estimator of the parameter vector β for the linear least squares method, and that it has minimum variance among all linear parameter estimators.[1,chapter VI;2,page 14;3,page 198]

The true variance, σ^2, is estimated, in an unbiased fashion, by

$$\hat{\sigma}^2 = \frac{1}{n-k}(\mathbf{y}-\mathbf{X}\hat{\beta})'(\mathbf{y}-\mathbf{X}\hat{\beta}), \tag{127}$$

which may be used to estimate the variance in $\hat{\beta}$,

$$var(\hat{\beta}) = (\mathbf{X}'\mathbf{X})^{-1}\sigma^2, \tag{128}$$

as

$$\hat{\sigma}^2_{\hat{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\hat{\sigma}^2. \tag{129}$$

The predicted value, $\hat{\mathbf{y}}_k$, for a certain $\mathbf{X}_k$, and its variance are calculated as follows:[27]

$$\hat{\mathbf{y}}_k = \mathbf{X}'_k\hat{\beta} = \hat{\beta}'\mathbf{X}_k \tag{130}$$

$$var(\hat{\mathbf{y}}_k) = \mathbf{X}'_k(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}_k\sigma^2, \tag{131}$$

with σ^2 appropriately replaced with its estimate, $\hat{\sigma}^2$.

Just as in the simple case, confidence intervals may be built for any element of the estimated parameter vector, $\hat{\beta}$.

The issue of correlation remains. The least squares method has the assumption of uncorrelated errors such that covariance matrix of $\mathbf{e}$ is written as $\sigma^2\mathbf{I}$, but, if the errors are correlated, the matrix is written as $\sigma^2\mathbf{\Sigma}$, where Σ is a full matrix, and the assumption is violated. Most unfortunately, the Gauss-Markov Theorem no longer applies, and the estimators, $\hat{\beta}$, may not have the minimum variance among all estimators. Fear not, though, for this is almost painlessly remedied by multiplying the model $(\mathbf{y}, \mathbf{X}, \mathbf{e})$ by $\mathbf{\Sigma}^{-1/2}$. This remedy results in what is termed the generalized least squares method:[3]

$$\tilde{\beta} = (\mathbf{X}'\mathbf{\Sigma}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{\Sigma}^{-1}\mathbf{y}, \tag{132}$$

$$\hat{\sigma}^2 = \frac{1}{n-k}(\mathbf{y} - \mathbf{X}\tilde{\beta})'(\mathbf{y} - \mathbf{X}\tilde{\beta}), \tag{133}$$

$$var(\tilde{\beta}) = \sigma^2(\mathbf{X}'\mathbf{\Sigma}^{-1}\mathbf{X})^{-1}. \tag{134}$$

A joint confidence region for all the parameters is found from,[27,page 79]

$$\frac{k}{n-k}(\mathbf{y}'\mathbf{\Sigma}^{-1}\mathbf{y} - \mathbf{y}'\mathbf{\Sigma}^{-1}\mathbf{X}(\mathbf{X}'\mathbf{\Sigma}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{\Sigma}^{-1}\mathbf{y})F_{k,n-k,1-\alpha}. \tag{135}$$

The least squares method assumes a linear relationship between the independent variables and the dependent variable.[28] If this is not a reasonable assumption, we have two choices:[7,page 242] change the model, say, to nonlinear least squares, or transform the variables such that a linear relationship does exist. The latter option requires that the model be intrinsically linear and may require some additional knowledge of the variables under study.[27]

The combination of estimators, as MCNP does, is a specific application of the least squares method and has no unique approach. One approach is to just consider observations on a true value. Then Eq. 122 becomes simply, in elemental form

$$y_i = a_0 + e_i, i = 1, \ldots, n, \tag{136}$$

where the true value a_0 will be estimated by b_0 for the n observations, y_i. For a full $(n \times n)$ covariance matrix for the e's, or equivalently, the y's, the least squares estimate b_0 is found from Eq. 132. There is one parameter and n observations, so the regressor matrix $\mathbf{X}$ is an $(n \times 1)$ matrix of ones. Here we see that, instead of independent variables, $\mathbf{X}$ contains design, or specified, parameters.

We now derive the combination least squares equations for two estimators, x_1 and x_2, treated as observations on a true value x. The covariance matrix is

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_{11}^2 & \sigma_{12}^2 \\ \sigma_{12}^2 & \sigma_{22}^2 \end{pmatrix}, \tag{137}$$

the regressor matrix is

$$\mathbf{X} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{138}$$

the vector of the two estimators is

$$\mathbf{y} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \tag{139}$$

and the inverse covariance matrix is

$$\mathbf{\Sigma}^{-1} = \frac{1}{\sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2} \begin{pmatrix} \sigma_{22}^2 & -\sigma_{12}^2 \\ -\sigma_{12}^2 & \sigma_{11}^2 \end{pmatrix}. \tag{140}$$

Notice that σ^2 has been absorbed into $\mathbf{\Sigma}$. Equation 132 stipulates the combination of the estimators:

$$\begin{aligned} b_0 &= (\mathbf{X}'\mathbf{\Sigma}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{\Sigma}^{-1}\mathbf{y} && (141) \\ &= \left[\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} \sigma_{22}^2 & -\sigma_{12}^2 \\ -\sigma_{12}^2 & \sigma_{11}^2 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\right]^{-1} \\ &\times \begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} \sigma_{22}^2 & -\sigma_{12}^2 \\ -\sigma_{12}^2 & \sigma_{11}^2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ &= \frac{\sigma_{22}^2 - \sigma_{12}^2}{\sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2}x_1 + \frac{\sigma_{11}^2 - \sigma_{12}^2}{\sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2}x_2 && (142) \\ &= w_1x_1 + w_2x_2. && (143) \end{aligned}$$

and the estimated variance of b_0, from Eq. 134, is

$$\begin{aligned} \hat{\sigma}_b^2 &= \sigma^2(\mathbf{X}'\mathbf{\Sigma}^{-1}\mathbf{X})^{-1} \\ &= \frac{\sigma_{11}^2\sigma_{22}^2 - (\sigma_{12}^2)^2}{\sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2}. && (144) \end{aligned}$$

B. The Principle of Maximum Likelihood

The Principle of Maximum Likelihood says that, given a set of hypotheses that could have produced an observed result, the *one* that most likely caused it is selected as the correct one.[8]

The likelihood function is dependent upon the true value and represents the probability of getting the observed value. We will briefly look at how the maximum likelihood estimators of the regression parameters are obtained[29] for the simple case of one dependent and one independent variable.[10] Given the linear regression model

$$y_{true} = a_0 + a_1 x, \tag{145}$$

and $\{y_i, i = 1, \ldots, n\}$ are observations on y_{true}, we have

$$y_i = a_0 + a_1 x_i + e_i, \tag{146}$$

where e_i are errors, assumed to be normally distributed with mean zero and variance σ^2 (this is equivalent to assuming y_i to be distributed with mean y_{true} and variance σ^2). When a_0 and a_1 are estimated by b_0 and b_1 we are able to predict y for a specific x_k,

$$\hat{y} = b_0 + b_1 x. \tag{147}$$

The method of maximum likelihood proceeds as follows to estimate the regression parameters. The density function of the y_i is

$$p_i = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\frac{(y_i - a_0 - a_1 x_1)^2}{2\sigma^2} \right\}. \tag{148}$$

The likelihood function is defined as

$$\begin{aligned} \prod_{i=1}^{n} p_i &= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\frac{(y_i - a_0 - a_1 x_1)^2}{2\sigma^2} \right\} \\ &= \frac{1}{(\sqrt{2\pi}\sigma)^n} exp\left\{ -\sum \frac{(y_i - a_0 - a_1 x_1)^2}{2\sigma^2} \right\}. \end{aligned} \tag{149}$$

It is easier to work with the logarithm of the likelihood, L,

$$L = -n \ln \sqrt{2\pi}\sigma - \sum_{i=1}^{n} \frac{(y_i - a_0 - a_1 x_1)^2}{2\sigma^2}. \tag{150}$$

Replacing the parameters a_0 and a_1 with their estimates, b_0 and b_1, and setting equal to zero the partial derivative of L with respect to each, gives the following equations:

$$\frac{\partial L}{\partial a_0} = -2 \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) = 0, \tag{151}$$

$$\frac{\partial L}{\partial a_1} = -2 \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) x_i = 0. \tag{152}$$

These are the *normal equations*! It is utterly remarkable (or just somewhat remarkable, if you're jaded by the numerous phenomena in mathematics) that the principle of maximum likelihood, with the assumption of normality, produces the normal equations, just as those coming from the least squares method.

X. APPENDIX C: PEELLE'S PERTINENT PUZZLE

A. Introduction

In October 1987, R.W. Peelle put out an informal memorandum[20, as recounted] that documented his strange results obtained from combining two correlated measurements from two foil activation experiments. The experiment consisted of two independent activations of the same foil in an attempt to determine the activation cross section, x, which is the ratio of the activation to the mass of the foil; $x = a/m$. The activations were $a_1 = 1.0$ and $a_2 = 1.5$ and the mass of the foil was 1.0. The variance of each quantity was to be the sum of two parts that had standard error relative to the quantity, an independent 10% and a fully positively correlated 20%. This would presumably correspond to a 10% uncertainty in the activations and a 20% uncertainty in the foil mass. This, then, is Peelle's problem. It is desired to obtain one final answer from these data.

B. Combining Correlated Data

Given Peelle's data, what is the proper way to proceed? Peelle proceeded by calculating an activation cross section for each activation, $x_1 = a_1/m$ and $x_2 = a_2/m$, calculating a full variance-covariance matrix, and applying the least squares method to x_1 and x_2 to get the best estimate $x' =< x_1, x_2 >$, where $< y, z >$ denotes the least squares combination of y and z.[20]

$$x_1 = 1.0 \tag{153}$$

$$x_2 = 1.5 \tag{154}$$

$$var(x_1) = [(0.1)(x_1)]^2 + [(0.2)(x_1)]^2 = 0.01 + 0.04 = 0.05 \tag{155}$$

$$var(x_2) = [(0.1)(x_2)]^2 + [(0.2)(x_2)]^2 = 0.0225 + 0.09 = 0.1125 \tag{156}$$

$$cov(x_1, x_2) = [(0.2)(x_1)][(0.2)(x_2)] = (0.2)(0.3) = 0.06 \tag{157}$$

The resulting x', from Eqs. 143 and 144, is 0.882 ± 0.218, which, surprisingly enough, lies *outside* the range of x_1 and x_2. This is incorrect, not necessarily because of its outlying position, but because of the data preparation before applying least squares.[30] The fact that the equations for the variances of x_1 and x_2 look very similar, yet give different results, is a clue to the incorrect preparation of the data and, therefore, the incorrect application of the least squares method. To estimate one quantity, the same experiment was performed twice, each using the same equipment and the same materials. Therefore the variances should be the same for both measurements and the covariance should not depend on the size of either one of the measurements alone.[30]

The correct way of combining these data, for this problem, is to combine the independently measured activations with least squares, then use the mass to obtain an activation cross section[31] and regular propagation of errors to estimate the standard deviation, thus the combined average is

$$x' = \frac{< a_1, a_2 >}{m} = \frac{a'}{m} \tag{158}$$

where a' is the least squares combination of a_1 and a_2. Since they are independent and uncorrelated, the combination is simply an inverse variance weighting scheme, which results in

$$a' = 1.154 \pm 0.083. \tag{159}$$

Then, using standard propagation of errors with no correlation between a' and m,[9] we find,

$$x' = 1.154 \pm 0.245. \tag{160}$$

This, then, is believed to be the correct solution to Peelle's Pertinent Puzzle. Zhao and Perey[32] explained that Peelle's incorrect result came from trying to combine derived quantities, where the derived quantities were nonlinear functions of the observed quantities. They showed that, when fitting derived data, an iterative procedure–necessary since the covariance matrix is known only approximately–would converge to the correct solution, that of fitting the observed data. Perel, Wagschal, and Yeivin[19] show that nonlinearity is not an issue, merely the observation that the mass of the foil in Peelle's experiment is an explicit quantity, since it causes the correlation. They point out that before applying least squares, one must know the cause of the correlations in the problem. If the cause is unknown, then the only way to proceed *is* as Peelle did in his experiment. A general statement from the nuclear data community on the applicability of the least squares method is apparently yet to come.[31,19]

Chiba[33] came to similar conclusions by giving a criterion where the least squares solution was invariant before and after a transformation of the data vector that doesn't reduce its dimension. Chiba begins with the correct least squares solution, as above, and transforms the data differently to show the invariance of the solution. When Chiba transformed the data improperly, the solution Peelle had originally obtained was produced.

Chiba also showed that truncation of the data, thus reducing its dimension, was a transformation that produced different least squares solutions than those before the transformation. Peelle's two-dimensioned problem with nonzero covariances should indicate the presence of another quantity causing the correlation and that the problem is really of at least three dimensions. However, as noted earlier, this requires explicit knowledge of the cause of the correlation. If this knowledge is not available, then the extra dimension will remain unavailable.

C. Summary

In summary, the method of least squares is very powerful and, as with anything powerful, should be used carefully, as shown by the response to Peelle's Pertinent Puzzle. We've seen that the covariance of an observation cannot depend upon the value of that observation. If the cause of correlation is explicitly known, it must also be modeled to obtain the correct results. To do otherwise is a truncation of parameter space, and the least squares solution is not invariant under such an operation, and therefore, incorrect. When the cause of correlation is not explicitly known, the full parameter space is assumed, and the least squares method is applied with little reservation. Any time the combined estimate falls outside the range of highly and positively correlated individual estimates, surprise and suspicion should be displaced by understanding and appreciation.

XI. APPENDIX D: DETAILED OBSERVATIONS OF THE TWO-ESTIMATOR COMBINED ESTIMATE

Given the two-combined estimator

$$\hat{x} = w_1 x_1 + w_2 x_2$$

where the weights are, from Eq. 36,

$$\begin{aligned} w_1 &= \frac{\sigma_{22}^2 - \sigma_{12}^2}{\sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2} \\ w_2 &= \frac{\sigma_{11}^2 - \sigma_{12}^2}{\sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2}, \end{aligned}$$

we see that they sum to unity, and their denominator is positive, since

$$\begin{aligned} \sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2 &= \sigma_{11}^2 + \sigma_{22}^2 - 2\rho\sigma_{11}\sigma_{22} \\ &= (\sigma_{11} - \sigma_{22})^2 + 2\sigma_{11}\sigma_{22}(1-\rho) > 0. \end{aligned} \tag{161}$$

If $x_2 > x_1$ and $\sigma_{11}^2 < \sigma_{12}^2 < \sigma_{22}^2$, then $w_1 > 0$ and $w_2 < 0$, and

$$\begin{aligned} w_2(x_2 - x_1) &< 0 \\ (w_1 - 1)x_1 + w_2 x_2 &< 0 \\ w_1 x_1 + w_2 x_2 &< x_1 \\ \hat{x} &< x_1, \end{aligned}$$

where $\hat{x}$ is the two-estimator combined estimate. Similarly, if $x_2 > x_1$ and $\sigma_{22}^2 < \sigma_{12}^2 < \sigma_{11}^2$, then $w_1 < 0$ and $w_2 > 0$, and

$$\begin{aligned} w_1(x_1 - x_2) &> 0 \\ w_1 x_1 + (w_2 - 1)x_2 &> 0 \\ w_1 x_1 + w_2 x_2 &> x_2 \\ \hat{x} &> x_2, \end{aligned}$$

where, again, $\hat{x}$ is the two-estimator combined estimate.

Also, given that the denominator of the weights is positive, then the covariance is less than the average of the variances:

$$\begin{aligned} 0 &< \sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2 \\ \sigma_{12}^2 &< \frac{\sigma_{11}^2 + \sigma_{22}^2}{2}. \end{aligned} \tag{162}$$

Of course, this limit is less restrictive than that obtained from the expression of the correlation coefficient:

$$\sigma_{12}^2 < \sigma_{11}^2 \sigma_{22}^2. \tag{163}$$

XII. APPENDIX E: BIAS IN LEAST SQUARES

A negligible amount of bias, b_k exists in the Monte Carlo k-effective estimator. It is negligible since it is a function of M^{-1}, where M is the number of histories per cycle,[34] and will be less than a true standard deviation, σ, per the following equation:[6]

$$\frac{|\, b_k \,|}{\sigma} < \frac{N}{2}\frac{\sigma}{k}, \tag{164}$$

where N is the number of cycles and k is the true eigenvalue. Gelbard and Gu[6] found that the observed bias was insensitive to the dominance ratio, but Gelbard and Prael[24] found the variances, as commonly calculated, were sensitive to the dominance ratio. They found that increasing the batch size–groups of more than one cycle–decreased the bias in the variance.

In what follows, we empirically see that the estimated variance of the combined estimator will, at worst, preserve the bias in an individual estimator variance, but not magnify it.

A. Bias in the Estimator

If, for a two estimator case, with both estimates having the same expected value (unbiased), the variances are equal and they are perfectly correlated, the Least Squares method will produce a singular matrix and break down. There is no need to fret, because, in this case, the estimators are exactly the same and you may confidently select either one of them. If, on the other hand, both fully correlated estimators had the same variance, but different values, then the Least Squares method will still break down, but without additional information, you cannot justify selecting one estimate over the other. Actually, for a combination of two estimators, this situation will reduce to the average of the two estimates but with infinite variance. This latter situation would seem to indicate a bias in one of the estimators. In general, bias in the estimated least squares parameters is due to both bias in the independent values and incorrectness of the model.[27,page 81]

Having a bias in one of the estimators invalidates a major assumption behind our application of the least squares method. This is easily visualized by considering Halperin's transformation,[4] which, for a two estimator case, transforms the unbiased variables x_1 and x_2 to $z_1 = x_1$ and $z_2 = x_1 - x_2$. Any linear transformation will not destroy the multivariate normal qualities of a distribution.[2,page 417] The expected value of z_1 is the true answer and the expected value of z_2 is zero. If we plot the distributions, where z_1 is the ordinate and z_2 is the abscissa, we will find the points clustered around the ordinate axis, at a value near z_1. Linear regression–least squares–will best fit the data to a line and estimate the best combination of the two values, x_1 and x_2, as the y-intercept. If one of the estimates was biased, then the expected value of z_2 would not be zero, but some constant equal to $\pm$ the bias. Our handy plot would now have data points clustered, not around the ordinate axis, but around z_2 equal to a constant. Finding a y-intercept would prove rather difficult, since both the slope and intercept of the linear best fit could be up to either plus or minus infinity.

If both estimators were biased equally, then this numerical–and graphical–problem would not exist, and least squares would produce the best biased estimate. Without further information, the true unbiased value is unobtainable in this case. So, for our application of the least squares method with Halperin's transformation, the assumption of unbiased estimators translates to the assumption that all the estimators have the same expected value. That is not a very appealing relaxation of the assumptions, though, from the standpoint of a desirable estimator.

B. Bias in the Variances and Covariances

We first look at the matrix equations for the combination of estimators and determine the effect of a variance-covariance bias on them. For a bias matrix, $\mathbf{B}$, we have the following relations, where the hat indicates a biased value and the subscript z indicates Halperin's transformation:[4]

$$\hat{\mathbf{\Sigma}} = \mathbf{\Sigma} + \mathbf{B} \tag{165}$$

$$\hat{\mathbf{\Sigma}}_z = \mathbf{A}\hat{\mathbf{\Sigma}}\mathbf{A}'. \tag{166}$$

Substituting Eqs. 166 into the equation for the combined estimator, Eq. H2.14 in Halperin's paper, the bias on the combined estimate is found, in terms of unbiased quantities, as

$$\left(\mathbf{\Sigma}_{z12}\mathbf{Q}_{z22}^{-1} + \mathbf{B}_{z12}(\mathbf{Q}_{z22}^{-1} - \mathbf{\Sigma}_{z22}^{-1})\right)(z_2, \ldots, z_k)', \tag{167}$$

where the numeric subscripts indicate the matrix partitioning as in Halperin's paper,

$$\mathbf{Q}_z^{-1} = \mathbf{A}'\mathbf{\Sigma}^{-1}\mathbf{B}(\mathbf{B} + \mathbf{B}\mathbf{\Sigma}^{-1}\mathbf{B})^{-1}\mathbf{B}\mathbf{\Sigma}^{-1}\mathbf{A}, \tag{168}$$

and

$$\hat{\mathbf{\Sigma}}_z^{-1} = \mathbf{\Sigma}_z^{-1} - \mathbf{Q}_z^{-1}. \tag{169}$$

The bias in the estimated variance of the combined estimator, in terms of unbiased quantities, is

$$\begin{aligned} - \; & n\sigma_{opt}^2(n-1)\bar{\mathbf{d}}\mathbf{Q}_{z22}^{-1}\bar{\mathbf{d}}' \\ + \; & [\mathbf{B}_{z12} - \mathbf{\Sigma}_{z12}\mathbf{\Sigma}_{z22}^{-1}\mathbf{B}_{z21} + \mathbf{\Sigma}_{z12}\mathbf{Q}_{z22}^{-1}(\mathbf{\Sigma}_{z21} + \mathbf{B}_{z21}) \\ - \; & \mathbf{B}_{z12}(\mathbf{\Sigma}_{z22}^{-1} - \mathbf{Q}_{z22}^{-1})(\mathbf{\Sigma}_{z21} + \mathbf{B}_{z21})] \\ \times \; & \left[\frac{1}{n} + \bar{\mathbf{d}}\mathbf{S}_{z22}^{-1}\bar{\mathbf{d}}' - (n-1)\bar{\mathbf{d}}\mathbf{Q}_{z22}^{-1}\bar{\mathbf{d}}'\right]. \end{aligned} \tag{170}$$

Biases, b_{ij}, in the individual covariances, σ_{ij}^2, yield, for the two-estimator combined estimate, a bias of

$$\frac{(Dr_2 - s_2B)\bar{x}_1 + (Dr_1 - s_1B)\bar{x}_2}{D(D+B)}, \tag{171}$$

where

$$
\begin{aligned}
D &= \sigma_{11}^2 + \sigma_{22}^2 - 2\sigma_{12}^2, &(172)\\
B &= b_{11} + b_{22} - 2b_{12}, &(173)\\
s_i &= \sigma_{ii}^2 - \sigma_{12}^2, &(174)\\
r_i &= b_{ii} - b_{12}. &(175)
\end{aligned}
$$

There will be no bias in the two-combined estimate if

- $b_{ij} = 0$, for all i,j,
- b_{ij}'s are all equal, or
- $b_{ij} = \sigma_{ij}^2$, for all i,j.

The bias in the asymptotic part of the estimated variance of the two-estimator combined estimate is

$$
b_{11} - \frac{Dr_1(2s_1 - r_1) - Bs_1^2}{D(D+B)}. \qquad (176)
$$

We can computationally examine the effect of a variance bias on the least squares solution for the two estimator combined case. This case was programmed up for the example in the "Peelle's Pertinent Puzzle" section:

$$
\begin{aligned}
x_1 &\sim N(0,1)\\
x_2 &\sim N(0,1)
\end{aligned}
$$

$$
\begin{aligned}
y_1 = x_1 + 4x_2 &\sim N(0,17)\\
y_2 = x_2 &\sim N(0,1)
\end{aligned}
$$

$$
\begin{aligned}
\sigma_{11}^2 &= 17\\
\sigma_{22}^2 &= 1\\
\sigma_{12}^2 &= 4
\end{aligned}
$$

and the linear least squares weights for the two estimator case are ($i \neq j$)

$$
w_i = \frac{\sigma_{ii}^2 - \sigma_{ij}^2}{\sigma_{ii}^2 + \sigma_{jj}^2 - 2\sigma_{ij}^2}.
$$

From the section on Halperin's paper, the expression for the variance of the combined estimator, $\hat{\sigma}_{\hat{\mu}}^2$, is

$$\frac{1}{n(n-2)}\left[\frac{(\hat{\sigma}_{11}^2\hat{\sigma}_{22}^2 - \hat{\sigma}_{12}^4)\left((n-1)(\hat{\sigma}_{11}^2 + \hat{\sigma}_{22}^2 - 2\hat{\sigma}_{12}^2) + n(\bar{x}_1 - \bar{x}_2)^2\right)}{(\hat{\sigma}_{11}^2 + \hat{\sigma}_{22}^2 - 2\hat{\sigma}_{12}^2)^2}\right].$$

Here, too, we see by inspection that if both variances and the covariance have the same bias, the weights, and hence the combined estimator, will remain unaffected. The variance of the combined estimator will, however, be affected. Both of these statements hold if the bias is viewed as a multiplicative bias instead of an additive bias—at least for the combination of two estimators.

Table XX shows, for one hundred samples, these bias effects.

As seen in Table XX, the combined mean is, referenced to zero bias, unaffected if all the biases are the same, whereas the standard deviation of the combined mean is not unaffected. A lone bias in the larger variance will weight the estimator with the smaller variance, thus having a relatively small effect on the combined mean. A lone bias in the smaller variance will weight the estimator with the larger variance and will have a more dramatic effect on the combined mean. If a bias, commensurate with the lone bias on one of the variances, is present in the covariance, these effects are even more drastic in both the combined mean and standard deviation.

TABLE XX. Bias Effects on the Two-Estimator Combined Estimate

absolute bias in			combined estimate	
σ_{11}^2	σ_{22}^2	σ_{12}^2	mean	standard deviation
0	0	0	-0.02	0.00
-1	-1	-1	-0.02	0.12
1	1	1	-0.02	0.12
1	0	1	0.29	0.11
0	1	1	0.05	0.10
0	1	0	0.23	0.04
1	0	0	0.04	0.01

XIII. APPENDIX F: UNCONDITIONAL VARIANCE OF THE COMBINED ESTIMATOR IN HALPERIN'S PAPER

The variance of the combined estimator, as presented on the bottom of page 39 of Halperin's paper,[4] is a conditional variance in that it is based on the conditional distribution of $\{z_{1j}\}$ given $\{z_{2j}, \ldots, z_{kj}\}$. The expected value of a conditional expression is the unconditional expression, so Halperin looks at the expected value of the variance. First, note the expression for Hotelling's T^2-statistic (see Appendix A):

$$T^2_{p,n-p} \;=\; n(\mathbf{x}_k - \Theta_o)'\mathbf{S}^{-1}(\mathbf{x}_k - \Theta_o), \tag{177}$$

where there are n vectors $\mathbf{x}_k$, each of length p. Comparing Eq. 177 with the second term in the brackets of the variance, we see the following relation,

$$\mathbf{d}'\mathbf{S}_d^{-1}\bar{\mathbf{d}} \;=\; \frac{T^2_{k-1,n-(k-1)}}{n(n-1)}, \tag{178}$$

where we note that $\mathbf{S}_d^{-1}$ is a $(k-1) \times (k-1)$ matrix containing only sums of squares, thus explaining the $(k-1)$ and $(n-1)$ terms. The expected value of Hotelling's T^2-statistic is $p(n-1)/(n-p)$, so that the expected value of the conditional variance, the unconditional variance, is

$$\sigma^2_{opt}\left[1 + \frac{k-1}{n-k+1}\right].$$

As Halperin points out, this gives the speed of convergence to σ^2_{opt}. (The speed of convergence for the conditional variance is known only to a desired confidence level since it relies upon Hotelling's T-statistic, which is a random variable.) For our case of three estimators and, say, 100 active cycles, the unconditional variance would be about $1.02\sigma^2_{opt}$.

XIV. APPENDIX G: DATA

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3. Results of 100 independent MCNP runs as performed by Mr. Charles T. Rombough of CTR Technical Services, Inc., Arlington, Texas.
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   (a) 800 batches of 1 k_{eff} cycle each
   (b) 40 batches of 20 k_{eff} cycles each

Results for 100 independent Godiva runs with *implicit* capture:

Godiva: Implicit Absorption

run	k(col)	std	k(abs)	std	k(trk ln)	std	k(c/a/t)	std
1	1.00100	0.00240	1.00080	0.00240	0.99830	0.00200	0.99877	0.00198
2	0.99590	0.00220	0.99580	0.00220	0.99830	0.00200	0.99743	0.00188
3	0.99210	0.00230	0.99220	0.00230	0.99290	0.00200	0.99269	0.00195
4	0.99250	0.00210	0.99320	0.00210	0.99320	0.00180	0.99285	0.00175
5	0.99660	0.00220	0.99650	0.00230	0.99640	0.00160	0.99643	0.00159
6	0.99760	0.00260	0.99780	0.00260	0.99760	0.00190	0.99755	0.00194
7	0.99870	0.00240	0.99890	0.00240	0.99860	0.00190	0.99870	0.00192
8	1.00170	0.00220	1.00180	0.00220	0.99940	0.00180	1.00023	0.00176
9	0.99370	0.00250	0.99370	0.00250	0.99530	0.00200	0.99508	0.00197
10	0.99620	0.00240	0.99670	0.00240	0.99570	0.00190	0.99578	0.00193
11	0.99580	0.00240	0.99620	0.00240	0.99730	0.00190	0.99738	0.00189
12	1.00120	0.00240	1.00060	0.00240	0.99910	0.00180	0.99907	0.00182
13	0.99830	0.00210	0.99820	0.00220	1.00070	0.00190	0.99974	0.00175
14	0.99660	0.00230	0.99680	0.00230	0.99800	0.00190	0.99774	0.00189
15	0.99570	0.00260	0.99560	0.00260	0.99580	0.00230	0.99567	0.00228
16	0.99500	0.00230	0.99450	0.00240	0.99510	0.00200	0.99549	0.00202
17	1.00250	0.00230	1.00300	0.00230	0.99990	0.00190	1.00095	0.00194
18	0.99450	0.00250	0.99430	0.00250	0.99310	0.00190	0.99327	0.00189
19	0.99680	0.00290	0.99600	0.00290	0.99800	0.00210	0.99791	0.00215
20	0.99840	0.00220	0.99830	0.00220	0.99880	0.00200	0.99863	0.00189
21	0.99720	0.00260	0.99640	0.00260	1.00010	0.00190	0.99996	0.00189
22	0.99890	0.00210	0.99920	0.00210	0.99950	0.00200	0.99959	0.00183
23	0.99820	0.00230	0.99830	0.00230	0.99690	0.00220	0.99740	0.00209
24	0.99430	0.00210	0.99380	0.00210	0.99320	0.00180	0.99332	0.00178
25	0.99510	0.00220	0.99510	0.00220	0.99580	0.00170	0.99570	0.00164
26	0.99630	0.00230	0.99610	0.00240	0.99680	0.00200	0.99666	0.00198
27	0.99920	0.00220	0.99930	0.00220	0.99860	0.00180	0.99870	0.00181
28	0.99540	0.00220	0.99540	0.00220	0.99560	0.00170	0.99563	0.00166
29	0.99890	0.00260	0.99890	0.00250	0.99660	0.00200	0.99678	0.00204
30	0.99860	0.00270	0.99890	0.00270	0.99830	0.00210	0.99840	0.00215
31	0.99560	0.00230	0.99540	0.00240	0.99700	0.00190	0.99672	0.00188
32	0.99620	0.00210	0.99670	0.00210	0.99690	0.00180	0.99661	0.00176
33	1.00120	0.00220	1.00130	0.00210	0.99990	0.00190	1.00044	0.00178
34	0.99410	0.00240	0.99480	0.00230	0.99730	0.00190	0.99769	0.00181
35	1.00260	0.00240	1.00270	0.00230	0.99960	0.00190	0.99984	0.00192
36	0.99680	0.00240	0.99730	0.00240	0.99800	0.00190	0.99756	0.00191
37	0.99680	0.00230	0.99670	0.00230	1.00070	0.00180	0.99994	0.00179
38	0.99470	0.00230	0.99450	0.00230	0.99670	0.00190	0.99616	0.00192
39	0.99190	0.00240	0.99200	0.00250	0.99350	0.00170	0.99331	0.00175
40	0.99520	0.00240	0.99570	0.00240	0.99290	0.00190	0.99337	0.00196

41	0.99855	0.00257	0.99851	0.00260	0.99834	0.00195	0.99836	0.00196
42	0.99759	0.00226	0.99708	0.00224	1.00011	0.00179	0.99916	0.00178
43	0.99483	0.00217	0.99516	0.00221	0.99594	0.00161	0.99571	0.00163
44	0.99679	0.00226	0.99694	0.00229	0.99491	0.00184	0.99533	0.00184
45	0.99927	0.00238	0.99920	0.00240	0.99859	0.00187	0.99865	0.00187
46	0.99874	0.00234	0.99905	0.00235	0.99880	0.00206	0.99882	0.00203
47	0.99924	0.00246	0.99922	0.00252	0.99850	0.00174	0.99845	0.00176
48	0.99778	0.00270	0.99796	0.00268	0.99999	0.00213	0.99991	0.00208
49	0.99389	0.00248	0.99430	0.00248	0.99467	0.00214	0.99465	0.00215
50	0.99436	0.00221	0.99388	0.00223	0.99428	0.00178	0.99404	0.00173
51	0.99208	0.00238	0.99257	0.00237	0.99639	0.00191	0.99612	0.00198
52	0.99942	0.00211	0.99963	0.00209	0.99823	0.00190	0.99875	0.00186
53	0.99750	0.00231	0.99759	0.00230	0.99776	0.00191	0.99772	0.00187
54	0.99371	0.00208	0.99369	0.00207	0.99364	0.00177	0.99365	0.00172
55	0.99682	0.00210	0.99687	0.00216	0.99770	0.00187	0.99735	0.00177
56	0.99470	0.00200	0.99459	0.00202	0.99410	0.00186	0.99425	0.00165
57	0.99852	0.00221	0.99855	0.00224	0.99669	0.00177	0.99712	0.00174
58	0.99825	0.00259	0.99845	0.00263	0.99832	0.00189	0.99834	0.00191
59	0.99585	0.00256	0.99646	0.00255	0.99653	0.00199	0.99677	0.00204
60	1.00364	0.00245	1.00370	0.00244	1.00280	0.00199	1.00300	0.00197
61	0.99676	0.00228	0.99645	0.00229	0.99976	0.00168	0.99934	0.00171
62	0.99184	0.00261	0.99189	0.00257	0.99237	0.00213	0.99232	0.00212
63	0.99155	0.00259	0.99153	0.00258	0.99400	0.00196	0.99400	0.00199
64	0.99849	0.00231	0.99772	0.00231	0.99680	0.00199	0.99704	0.00200
65	0.99763	0.00260	0.99768	0.00257	0.99699	0.00201	0.99707	0.00202
66	0.99402	0.00241	0.99388	0.00237	0.99507	0.00174	0.99483	0.00173
67	0.99882	0.00249	0.99900	0.00248	1.00030	0.00188	1.00034	0.00186
68	0.99802	0.00238	0.99800	0.00234	0.99958	0.00186	0.99925	0.00184
69	1.00033	0.00255	1.00070	0.00249	1.00214	0.00206	1.00254	0.00203
70	0.99765	0.00249	0.99800	0.00242	0.99557	0.00210	0.99656	0.00207
71	0.99603	0.00202	0.99598	0.00202	0.99426	0.00174	0.99481	0.00169
72	1.00548	0.00217	1.00555	0.00220	1.00153	0.00173	1.00247	0.00171
73	0.99279	0.00236	0.99291	0.00240	0.99303	0.00192	0.99301	0.00190
74	0.99440	0.00221	0.99339	0.00221	0.99583	0.00196	0.99382	0.00194
75	0.99618	0.00226	0.99608	0.00225	0.99381	0.00210	0.99462	0.00206
76	0.99465	0.00222	0.99505	0.00221	0.99722	0.00176	0.99674	0.00174
77	0.99677	0.00224	0.99665	0.00226	0.99917	0.00199	0.99844	0.00197
78	0.99566	0.00231	0.99499	0.00227	0.99687	0.00190	0.99611	0.00188
79	0.99741	0.00251	0.99704	0.00252	0.99790	0.00200	0.99765	0.00200
80	0.99835	0.00282	0.99833	0.00280	0.99832	0.00201	0.99831	0.00202
81	0.99954	0.00208	0.99990	0.00208	0.99734	0.00223	0.99895	0.00198
82	0.99424	0.00208	0.99429	0.00217	0.99880	0.00170	0.99740	0.00166
83	0.99822	0.00215	0.99832	0.00217	1.00032	0.00173	1.00000	0.00173
84	1.00116	0.00233	1.00129	0.00230	1.00238	0.00190	1.00228	0.00186
85	0.99617	0.00239	0.99629	0.00231	0.99693	0.00205	0.99683	0.00194
86	1.00103	0.00236	1.00137	0.00236	0.99944	0.00176	0.99980	0.00177
87	0.99717	0.00242	0.99685	0.00251	0.99718	0.00190	0.99744	0.00190
88	0.99743	0.00238	0.99765	0.00244	0.99781	0.00190	0.99764	0.00189
89	0.99713	0.00206	0.99733	0.00208	0.99798	0.00185	0.99760	0.00176
90	0.99387	0.00239	0.99381	0.00241	0.99177	0.00185	0.99213	0.00181
91	0.99910	0.00220	0.99920	0.00220	0.99590	0.00191	0.99698	0.00183
92	0.99865	0.00226	0.99869	0.00223	0.99797	0.00189	0.99817	0.00184
93	0.99678	0.00226	0.99698	0.00225	0.99698	0.00160	0.99711	0.00156
94	0.99681	0.00249	0.99707	0.00253	0.99539	0.00178	0.99553	0.00180
95	0.99861	0.00221	0.99827	0.00222	0.99814	0.00179	0.99803	0.00179
96	0.99286	0.00227	0.99352	0.00229	0.99429	0.00194	0.99362	0.00194
97	0.99760	0.00219	0.99772	0.00227	0.99817	0.00176	0.99795	0.00169
98	0.99854	0.00244	0.99897	0.00241	0.99768	0.00212	0.99833	0.00206
99	0.99390	0.00242	0.99416	0.00241	0.99561	0.00204	0.99540	0.00202
100	0.99391	0.00229	0.99383	0.00228	0.99510	0.00176	0.99505	0.00178
mean	0.99695	0.00234	0.99699	0.00234	0.99717	0.00190	0.99717	0.00188
sigma	0.00270	0.00018	0.00272	0.00017	0.00236	0.00014	0.00238	0.00014
difference in variance	-0.1816E-05		-0.1899E-05		-0.1932E-05		-0.2140E-05	
difference in stnd dev	-0.3605E-03		-0.3751E-03		-0.4539E-03		-0.5025E-03	

the results of the w test for normality applied to the collision, absorption,

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track-length, and combined keff values are:
the k( collision) values appear normally distributed at the 95 percent confidence level
the k(absorption) values appear normally distributed at the 95 percent confidence level
the k(trk length) values appear normally distributed at the 95 percent confidence level
the k(co/abs/trl) values appear normally distributed at the 95 percent confidence level
For  100 values of the  collision estimator
with average   0.996951 the data were:
confidence level      % of the time
-----------------     -------------
      0.680               64.0000
      0.950               90.0000
      0.990               98.0000
 Largest deviation =     3.93047
For  100 values of the absorption estimator
with average   0.996991 the data were:
confidence level      % of the time
-----------------     -------------
      0.680               61.0000
      0.950               90.0000
      0.990               98.0000
 Largest deviation =     3.89029
For  100 values of the trk length estimator
with average   0.997174 the data were:
confidence level      % of the time
-----------------     -------------
      0.680               57.0000
      0.950               86.0000
      0.990               97.0000
 Largest deviation =     2.92111
For  100 values of the 3-combined estimator
with average   0.997168 the data were:
confidence level      % of the time
-----------------     -------------
      0.680               59.0000
      0.950               87.0000
      0.990               95.0000
 Largest deviation =     3.10066
```

Results for 100 independent Godiva runs with *analog* capture:

Godiva: Analog Absorption

run	k(col)	std	k(abs)	std	k(trk ln)	std	k(c/a/t)	std
1	0.99920	0.00320	0.99840	0.00360	0.99820	0.00290	0.99822	0.00237
2	1.00160	0.00330	1.00080	0.00380	1.00210	0.00270	1.00172	0.00224
3	0.99480	0.00300	0.99120	0.00370	0.99790	0.00270	0.99555	0.00201
4	0.99590	0.00330	0.99270	0.00460	0.99380	0.00270	0.99289	0.00224
5	0.99060	0.00340	0.99300	0.00370	0.99100	0.00270	0.99187	0.00233
6	0.99630	0.00320	0.99920	0.00340	0.99600	0.00260	0.99728	0.00186
7	0.99410	0.00300	1.00340	0.00400	0.99120	0.00270	0.99513	0.00224
8	0.99730	0.00330	1.00030	0.00360	0.99420	0.00260	0.99591	0.00218
9	0.99470	0.00300	0.99230	0.00410	0.99840	0.00260	0.99738	0.00194
10	0.99360	0.00330	1.00030	0.00370	0.99390	0.00290	0.99677	0.00219
11	0.99710	0.00310	0.99220	0.00380	0.99520	0.00270	0.99359	0.00184
12	0.99930	0.00340	0.99830	0.00360	0.99820	0.00270	0.99793	0.00194
13	0.99890	0.00330	0.99130	0.00360	1.00040	0.00280	0.99689	0.00199
14	0.99660	0.00300	1.00250	0.00400	0.99610	0.00290	0.99852	0.00209
15	0.99380	0.00300	0.99910	0.00420	0.99560	0.00250	0.99688	0.00222
16	1.00020	0.00330	0.99860	0.00320	0.99870	0.00290	0.99834	0.00201
17	0.99450	0.00340	0.99480	0.00380	0.99560	0.00300	0.99550	0.00219
18	1.00320	0.00340	0.99580	0.00370	1.00000	0.00270	0.99820	0.00225
19	0.99660	0.00310	1.00210	0.00370	0.99600	0.00260	0.99821	0.00200
20	0.99310	0.00320	1.00390	0.00380	0.99420	0.00320	0.99891	0.00209
21	0.99210	0.00360	0.99850	0.00410	0.99390	0.00310	0.99645	0.00246
22	0.99640	0.00340	0.99400	0.00360	0.99730	0.00300	0.99595	0.00220
23	0.99680	0.00310	1.00190	0.00330	0.99880	0.00260	1.00056	0.00188
24	1.00480	0.00290	0.99710	0.00410	1.00080	0.00260	0.99960	0.00232
25	1.00120	0.00330	0.99110	0.00380	1.00130	0.00290	0.99702	0.00220
26	0.99790	0.00350	0.99330	0.00320	0.99980	0.00320	0.99665	0.00224
27	0.99930	0.00340	0.99620	0.00320	0.99740	0.00310	0.99641	0.00198
28	1.00020	0.00310	0.99590	0.00360	1.00020	0.00270	0.99851	0.00198
29	0.99790	0.00320	0.99640	0.00420	0.99870	0.00290	0.99805	0.00243
30	0.99700	0.00310	0.98820	0.00370	0.99820	0.00270	0.99453	0.00211
31	0.99710	0.00300	0.99960	0.00390	0.99770	0.00280	0.99848	0.00218
32	0.99660	0.00300	0.99610	0.00370	0.99650	0.00270	0.99631	0.00225
33	1.00370	0.00310	0.99990	0.00420	1.00040	0.00250	0.99963	0.00223
34	0.99940	0.00340	0.99360	0.00380	1.00220	0.00300	0.99916	0.00237
35	0.99560	0.00320	0.98660	0.00370	1.00190	0.00290	0.99708	0.00225
36	0.99730	0.00320	0.99650	0.00410	0.99840	0.00280	0.99805	0.00213
37	0.99600	0.00340	0.99710	0.00380	0.99440	0.00260	0.99496	0.00203
38	0.99490	0.00320	0.99710	0.00410	1.00260	0.00290	1.00288	0.00245
39	0.99960	0.00340	0.99770	0.00320	1.00040	0.00270	0.99937	0.00201
40	1.00130	0.00320	0.99720	0.00360	0.99860	0.00250	0.99741	0.00200
41	1.00208	0.00337	1.00203	0.00415	0.99921	0.00276	0.99939	0.00201
42	0.99881	0.00329	0.99533	0.00366	0.99777	0.00284	0.99647	0.00209
43	0.99818	0.00298	0.99446	0.00364	1.00013	0.00279	0.99801	0.00198
44	0.99829	0.00344	0.99621	0.00366	0.99779	0.00286	0.99699	0.00223
45	1.00055	0.00325	1.00035	0.00472	1.00249	0.00263	1.00239	0.00228
46	1.00149	0.00354	0.98870	0.00373	1.00285	0.00294	0.99687	0.00226
47	1.00230	0.00299	0.99748	0.00378	1.00412	0.00261	1.00192	0.00206
48	0.99968	0.00346	0.99915	0.00353	1.00283	0.00265	1.00232	0.00211
49	0.99704	0.00319	1.00544	0.00362	0.99472	0.00278	0.99881	0.00207
50	1.00006	0.00313	0.99293	0.00398	1.00046	0.00279	0.99774	0.00221
51	0.99707	0.00304	1.00118	0.00436	0.99805	0.00264	0.99922	0.00227
52	1.00311	0.00304	1.00419	0.00369	1.00016	0.00254	1.00117	0.00205
53	1.00156	0.00279	1.00136	0.00427	0.99685	0.00267	0.99800	0.00210
54	1.00134	0.00319	0.99424	0.00403	0.99965	0.00297	0.99729	0.00236
55	0.99368	0.00306	0.99759	0.00432	0.99666	0.00292	0.99760	0.00207
56	0.99815	0.00310	0.99919	0.00322	0.99605	0.00270	0.99693	0.00188
57	1.00118	0.00310	0.99662	0.00392	0.99937	0.00271	0.99794	0.00211
58	1.00015	0.00329	0.99813	0.00398	0.99875	0.00299	0.99824	0.00247
59	0.99613	0.00334	0.99261	0.00373	0.99818	0.00286	0.99646	0.00239
60	0.99621	0.00348	0.99979	0.00401	0.99415	0.00341	0.99639	0.00250
61	0.99539	0.00332	0.99821	0.00406	0.99812	0.00273	0.99899	0.00217

62	0.99828	0.00329	0.99969	0.00394	0.99766	0.00265	0.99829	0.00193
63	0.99524	0.00314	0.99585	0.00371	0.99626	0.00256	0.99629	0.00207
64	1.00139	0.00322	1.00218	0.00380	0.99951	0.00300	1.00043	0.00221
65	1.00090	0.00315	0.99747	0.00399	0.99951	0.00267	0.99859	0.00222
66	1.00311	0.00343	1.00045	0.00317	1.00178	0.00283	1.00096	0.00188
67	1.00041	0.00303	0.99882	0.00384	0.99931	0.00269	0.99886	0.00203
68	0.99804	0.00317	0.99909	0.00383	0.99806	0.00309	0.99848	0.00232
69	0.99260	0.00311	1.00202	0.00368	0.99378	0.00257	0.99700	0.00199
70	0.99854	0.00317	0.99967	0.00347	0.99551	0.00286	0.99709	0.00210
71	1.00197	0.00389	0.99768	0.00423	0.99818	0.00298	0.99675	0.00225
72	0.99722	0.00338	0.99346	0.00420	0.99717	0.00276	0.99581	0.00217
73	0.99857	0.00318	0.99649	0.00332	1.00010	0.00285	0.99864	0.00207
74	0.99667	0.00306	1.00134	0.00398	0.99656	0.00283	0.99847	0.00190
75	0.99592	0.00312	0.99899	0.00380	0.99536	0.00265	0.99668	0.00185
76	0.99122	0.00274	1.00163	0.00411	0.99564	0.00239	0.99826	0.00201
77	0.99566	0.00297	0.98995	0.00399	0.99926	0.00292	0.99571	0.00217
78	0.99406	0.00325	1.00050	0.00386	0.99240	0.00287	0.99545	0.00209
79	0.99627	0.00325	0.99999	0.00341	0.99642	0.00289	0.99807	0.00218
80	0.99834	0.00353	1.00602	0.00363	0.99512	0.00279	0.99861	0.00215
81	0.99949	0.00313	0.99711	0.00401	0.99820	0.00310	0.99754	0.00223
82	0.99528	0.00305	0.99132	0.00351	0.99596	0.00258	0.99436	0.00214
83	0.99778	0.00320	0.99610	0.00391	0.99891	0.00293	0.99809	0.00221
84	0.99766	0.00349	0.99189	0.00399	0.99999	0.00317	0.99697	0.00260
85	0.99306	0.00349	0.99499	0.00386	0.99748	0.00318	0.99800	0.00244
86	1.00054	0.00338	1.00116	0.00398	1.00013	0.00279	1.00042	0.00215
87	0.99288	0.00312	0.99465	0.00359	0.99210	0.00307	0.99321	0.00225
88	0.99762	0.00328	1.00108	0.00361	0.99653	0.00258	0.99797	0.00199
89	0.99248	0.00309	0.99854	0.00409	0.98992	0.00252	0.99206	0.00227
90	1.00274	0.00317	0.99252	0.00360	1.00209	0.00305	0.99684	0.00211
91	1.00840	0.00367	0.99956	0.00422	1.00484	0.00315	1.00163	0.00246
92	1.00113	0.00329	0.99443	0.00360	1.00079	0.00304	0.99787	0.00218
93	0.99902	0.00348	0.99755	0.00348	0.99895	0.00300	0.99830	0.00223
94	0.99491	0.00309	0.99650	0.00426	0.99514	0.00277	0.99561	0.00218
95	0.99624	0.00338	0.99620	0.00358	0.99844	0.00316	0.99778	0.00221
96	1.00123	0.00325	1.00451	0.00403	1.00157	0.00264	1.00273	0.00196
97	0.99565	0.00307	0.99914	0.00395	0.99680	0.00293	0.99812	0.00180
98	0.99365	0.00290	0.99797	0.00352	0.99170	0.00260	0.99371	0.00207
99	0.99125	0.00325	0.99698	0.00356	0.99810	0.00260	0.99976	0.00212
100	0.99885	0.00296	0.99636	0.00365	0.99703	0.00260	0.99642	0.00184
mean	0.99783	0.00322	0.99739	0.00381	0.99787	0.00280	0.99768	0.00215
sigma	0.00329	0.00019	0.00385	0.00030	0.00295	0.00020	0.00216	0.00017
difference in variance	-0.4438E-06		-0.3788E-06		-0.8624E-06		-0.5341E-07	
difference in stnd dev	-0.6817E-04		-0.4945E-04		-0.1498E-03		-0.1241E-04	

the results of the w test for normality applied to the collision, absorption, track-length, and combined keff values are:

the k(collision) values appear normally distributed at the 95 percent confidence level
the k(absorption) values appear normally distributed at the 95 percent confidence level
the k(trk length) values appear normally distributed at the 95 percent confidence level
the k(co/abs/trl) values appear normally distributed at the 99 percent confidence level, but not at 95 percent

For 100 values of the collision estimator
with average 0.997832 the data were:

confidence level	% of the time
0.680	63.0000
0.950	95.0000
0.990	99.0000

Largest deviation = 2.87954

For 100 values of the absorption estimator
with average 0.997393 the data were:

confidence level	% of the time
0.680	69.0000
0.950	95.0000
0.990	99.0000

Largest deviation = 2.91694

For 100 values of the trk length estimator with average 0.997868 the data were:

confidence level	% of the time
0.680	70.0000
0.950	94.0000
0.990	99.0000

Largest deviation = 3.15413

For 100 values of the 3-combined estimator with average 0.997678 the data were:

confidence level	% of the time
0.680	76.0000
0.950	90.0000
0.990	100.0000

Largest deviation = 2.57763

These are the results of 100 independent MCNP runs as performed by Mr. Charles T. Rombough of CTR Technical Services, Inc., Arlington, Texas, and relayed to Art Forster in a letter dated July 8, 1993.[21] (Used with permission, 19 August 1993).

Charles T. Rombough's Data

run	k(col)	std	k(abs)	std	k(trk ln)	std	k(c/a/t)	std
1	0.96031	0.00322	0.96585	0.00230	0.95928	0.00331	0.96513	0.00228
2	0.96709	0.00338	0.97110	0.00233	0.96626	0.00342	0.97007	0.00233
3	0.96145	0.00296	0.96278	0.00231	0.96211	0.00308	0.96215	0.00218
4	0.96536	0.00304	0.96580	0.00240	0.96659	0.00288	0.96633	0.00222
5	0.96071	0.00338	0.96326	0.00209	0.96045	0.00340	0.96291	0.00209
6	0.96286	0.00303	0.96324	0.00220	0.96258	0.00307	0.96301	0.00211
7	0.97016	0.00341	0.96679	0.00262	0.96916	0.00348	0.96773	0.00263
8	0.96468	0.00321	0.96016	0.00238	0.96397	0.00335	0.96145	0.00230
9	0.96219	0.00327	0.96604	0.00229	0.96212	0.00330	0.96530	0.00226
10	0.96959	0.00366	0.96703	0.00226	0.96831	0.00370	0.96646	0.00231
11	0.97141	0.00311	0.96734	0.00227	0.97266	0.00306	0.96881	0.00217
12	0.96081	0.00333	0.96047	0.00244	0.96058	0.00339	0.96060	0.00239
13	0.96375	0.00304	0.96364	0.00214	0.96345	0.00322	0.96390	0.00203
14	0.96091	0.00314	0.96551	0.00214	0.95961	0.00326	0.96506	0.00221
15	0.96717	0.00337	0.96824	0.00261	0.96688	0.00342	0.96792	0.00255
16	0.96913	0.00307	0.96730	0.00249	0.96849	0.00312	0.96814	0.00227
17	0.96479	0.00341	0.97081	0.00240	0.96422	0.00335	0.96912	0.00235
18	0.96874	0.00346	0.96612	0.00242	0.96938	0.00354	0.96685	0.00238
19	0.96375	0.00312	0.96263	0.00234	0.96308	0.00313	0.96281	0.00228
20	0.96077	0.00301	0.96141	0.00244	0.96153	0.00300	0.96162	0.00230
21	0.95842	0.00286	0.96139	0.00202	0.95766	0.00289	0.96105	0.00204
22	0.96761	0.00324	0.96437	0.00220	0.96793	0.00330	0.96471	0.00222
23	0.96071	0.00339	0.96209	0.00224	0.96111	0.00341	0.96200	0.00224
24	0.96613	0.00334	0.96319	0.00230	0.96615	0.00340	0.96365	0.00228
25	0.96692	0.00340	0.96469	0.00198	0.96735	0.00338	0.96524	0.00191
26	0.96765	0.00317	0.96684	0.00215	0.96842	0.00319	0.96696	0.00212
27	0.96478	0.00317	0.96748	0.00214	0.96493	0.00313	0.96717	0.00213
28	0.96359	0.00303	0.96471	0.00256	0.96397	0.00309	0.96414	0.00244
29	0.96332	0.00300	0.96583	0.00233	0.96342	0.00302	0.96533	0.00226
30	0.96634	0.00296	0.96731	0.00210	0.96669	0.00301	0.96727	0.00203
31	0.96561	0.00339	0.96606	0.00236	0.96552	0.00334	0.96591	0.00226
32	0.96630	0.00336	0.96298	0.00247	0.96643	0.00347	0.96369	0.00242
33	0.96371	0.00327	0.96562	0.00217	0.96365	0.00327	0.96528	0.00212
34	0.96605	0.00301	0.96530	0.00255	0.96618	0.00309	0.96558	0.00234
35	0.96761	0.00293	0.96381	0.00209	0.96683	0.00295	0.96464	0.00206
36	0.97510	0.00312	0.96823	0.00247	0.97423	0.00307	0.96981	0.00243
37	0.96471	0.00312	0.96203	0.00230	0.96464	0.00320	0.96269	0.00220
38	0.96459	0.00307	0.96332	0.00225	0.96444	0.00312	0.96366	0.00212
39	0.96482	0.00299	0.95973	0.00201	0.96502	0.00311	0.96038	0.00202
40	0.96227	0.00338	0.96389	0.00203	0.96239	0.00347	0.96387	0.00205
41	0.96773	0.00340	0.96488	0.00245	0.96833	0.00336	0.96558	0.00240
42	0.96457	0.00356	0.96283	0.00225	0.96441	0.00361	0.96299	0.00226
43	0.96722	0.00349	0.96613	0.00227	0.96746	0.00354	0.96646	0.00220
44	0.96085	0.00329	0.96392	0.00237	0.96124	0.00319	0.96374	0.00220
45	0.96273	0.00278	0.96397	0.00227	0.96250	0.00281	0.96346	0.00211
46	0.96356	0.00316	0.96250	0.00237	0.96334	0.00326	0.96297	0.00219
47	0.97043	0.00280	0.96720	0.00241	0.97081	0.00289	0.96849	0.00221
48	0.96767	0.00306	0.96722	0.00210	0.96800	0.00325	0.96726	0.00198
49	0.96526	0.00295	0.96264	0.00231	0.96568	0.00294	0.96359	0.00217
50	0.96112	0.00302	0.96437	0.00232	0.96043	0.00311	0.96328	0.00214
51	0.96958	0.00343	0.96447	0.00261	0.96979	0.00345	0.96577	0.00254
52	0.96965	0.00322	0.96779	0.00211	0.96922	0.00326	0.96780	0.00204
53	0.96371	0.00299	0.96382	0.00216	0.96316	0.00310	0.96429	0.00191
54	0.96408	0.00335	0.96210	0.00239	0.96506	0.00336	0.96279	0.00240
55	0.96587	0.00324	0.96110	0.00206	0.96637	0.00327	0.96211	0.00203
56	0.96541	0.00321	0.96279	0.00217	0.96546	0.00330	0.96322	0.00214
57	0.96599	0.00304	0.96797	0.00249	0.96693	0.00302	0.96791	0.00234
58	0.96425	0.00291	0.96374	0.00189	0.96436	0.00283	0.96387	0.00186

59	0.96889	0.00306	0.96361	0.00243	0.96905	0.00315	0.96517	0.00230
60	0.96293	0.00323	0.96358	0.00228	0.96368	0.00326	0.96359	0.00224
61	0.96679	0.00325	0.96565	0.00216	0.96715	0.00331	0.96583	0.00213
62	0.96244	0.00298	0.96464	0.00220	0.96136	0.00295	0.96373	0.00210
63	0.96135	0.00334	0.96016	0.00212	0.96106	0.00334	0.96018	0.00209
64	0.96261	0.00318	0.96460	0.00220	0.96247	0.00322	0.96429	0.00219
65	0.96342	0.00303	0.96627	0.00236	0.96278	0.00305	0.96512	0.00220
66	0.95954	0.00321	0.96235	0.00206	0.95952	0.00325	0.96178	0.00198
67	0.96281	0.00372	0.96163	0.00204	0.96198	0.00371	0.96154	0.00209
68	0.96450	0.00328	0.96211	0.00239	0.96309	0.00328	0.96205	0.00234
69	0.96441	0.00284	0.96439	0.00233	0.96564	0.00290	0.96401	0.00221
70	0.96923	0.00322	0.96551	0.00223	0.96926	0.00328	0.96617	0.00221
71	0.96520	0.00355	0.96561	0.00233	0.96469	0.00359	0.96552	0.00233
72	0.96547	0.00302	0.96482	0.00201	0.96493	0.00307	0.96494	0.00198
73	0.96566	0.00320	0.96711	0.00234	0.96518	0.00329	0.96673	0.00231
74	0.96858	0.00291	0.96183	0.00233	0.96903	0.00292	0.96428	0.00214
75	0.96327	0.00362	0.96695	0.00228	0.96348	0.00368	0.96665	0.00231
76	0.96300	0.00331	0.96471	0.00241	0.96260	0.00333	0.96419	0.00238
77	0.96502	0.00311	0.96551	0.00242	0.96527	0.00308	0.96556	0.00230
78	0.96763	0.00321	0.96508	0.00228	0.96768	0.00320	0.96554	0.00226
79	0.96204	0.00337	0.96420	0.00223	0.96155	0.00342	0.96387	0.00219
80	0.96621	0.00301	0.96629	0.00221	0.96570	0.00299	0.96590	0.00211
81	0.96504	0.00316	0.96502	0.00242	0.96538	0.00313	0.96535	0.00231
82	0.96343	0.00334	0.96296	0.00206	0.96388	0.00334	0.96301	0.00208
83	0.96509	0.00344	0.96521	0.00262	0.96476	0.00346	0.96493	0.00253
84	0.96282	0.00331	0.96403	0.00223	0.96308	0.00331	0.96394	0.00218
85	0.96382	0.00307	0.96533	0.00241	0.96333	0.00310	0.96470	0.00233
86	0.96579	0.00341	0.96611	0.00223	0.96594	0.00342	0.96608	0.00224
87	0.96877	0.00321	0.96934	0.00208	0.96853	0.00326	0.96923	0.00202
88	0.96677	0.00322	0.96311	0.00223	0.96712	0.00317	0.96390	0.00221
89	0.96613	0.00329	0.96614	0.00185	0.96545	0.00339	0.96628	0.00187
90	0.96925	0.00321	0.96251	0.00227	0.96903	0.00332	0.96392	0.00225
91	0.96820	0.00325	0.96653	0.00221	0.96834	0.00327	0.96677	0.00218
92	0.96626	0.00327	0.96559	0.00221	0.96562	0.00330	0.96538	0.00208
93	0.96632	0.00339	0.96289	0.00233	0.96599	0.00342	0.96311	0.00236
94	0.96765	0.00373	0.96636	0.00245	0.96671	0.00367	0.96535	0.00239
95	0.96251	0.00317	0.96426	0.00218	0.96225	0.00312	0.96394	0.00217
96	0.96418	0.00362	0.96804	0.00227	0.96359	0.00362	0.96752	0.00229
97	0.96762	0.00309	0.96113	0.00217	0.96787	0.00320	0.96183	0.00225
98	0.96016	0.00320	0.96463	0.00238	0.96111	0.00325	0.96409	0.00240
99	0.96858	0.00294	0.96908	0.00228	0.96871	0.00303	0.96892	0.00215
100	0.96470	0.00309	0.96527	0.00233	0.96470	0.00306	0.96511	0.00214
	---------------		---------------		---------------		---------------	
mean	0.96516	0.00321	0.96474	0.00227	0.96509	0.00324	0.96484	0.00221
sigma	0.00293	0.00020	0.00228	0.00016	0.00302	0.00020	0.00216	0.00015
difference in variance	0.1700E-05		-0.3118E-07		0.1398E-05		0.2178E-06	
difference in stnd dev	0.2769E-03		-0.6845E-05		0.2233E-03		0.4978E-04	

the results of the w test for normality applied to the collision, absorption, track-length, and combined keff values are:

the k(collision) values appear normally distributed at the 95 percent confidence level
the k(absorption) values appear normally distributed at the 95 percent confidence level
the k(trk length) values appear normally distributed at the 95 percent confidence level
the k(co/abs/trl) values appear normally distributed at the 95 percent confidence level

For 100 values of the collision estimator
with average 0.965156 the data were:

confidence level	% of the time
0.680	72.0000
0.950	97.0000
0.990	99.0000

Largest deviation = 3.18701

```
For  100 values of the absorption estimator
with average   0.964740 the data were:
 confidence level      % of the time
 ----------------     ------------
       0.680             68.0000
       0.950             95.0000
       0.990             99.0000

 Largest deviation =     2.72964

For  100 values of the trk length estimator
with average   0.965088 the data were:
 confidence level      % of the time
 ----------------     ------------
       0.680             71.0000
       0.950             97.0000
       0.990             99.0000

 Largest deviation =     2.97790

For  100 values of the 3-combined estimator
with average   0.964840 the data were:
 confidence level      % of the time
 ----------------     ------------
       0.680             70.0000
       0.950             95.0000
       0.990            100.0000

 Largest deviation =     2.24474
```

100 runs Godiva/Jezebel: 800 batches, 1 cyc/batch

run	k(col)	std	k(abs)	std	k(trk ln)	std	k(c/a/t)	std
1	1.01210	0.00040	1.01210	0.00040	1.01270	0.00030	1.01258	0.00031
2	1.01250	0.00040	1.01250	0.00040	1.01230	0.00030	1.01236	0.00030
3	1.01290	0.00040	1.01290	0.00040	1.01310	0.00030	1.01303	0.00030
4	1.01170	0.00040	1.01170	0.00040	1.01230	0.00030	1.01217	0.00030
5	1.01230	0.00040	1.01230	0.00040	1.01220	0.00030	1.01225	0.00030
6	1.01250	0.00040	1.01260	0.00040	1.01230	0.00030	1.01232	0.00029
7	1.01260	0.00040	1.01260	0.00040	1.01280	0.00030	1.01277	0.00030
8	1.01290	0.00050	1.01290	0.00050	1.01230	0.00030	1.01240	0.00030
9	1.01150	0.00040	1.01150	0.00040	1.01200	0.00030	1.01193	0.00032
10	1.01230	0.00040	1.01230	0.00040	1.01250	0.00030	1.01249	0.00030
11	1.01280	0.00040	1.01290	0.00040	1.01270	0.00030	1.01274	0.00030
12	1.01290	0.00040	1.01280	0.00040	1.01290	0.00030	1.01284	0.00031
13	1.01200	0.00040	1.01200	0.00040	1.01250	0.00030	1.01240	0.00029
14	1.01210	0.00040	1.01210	0.00040	1.01280	0.00030	1.01271	0.00030
15	1.01330	0.00040	1.01330	0.00040	1.01270	0.00030	1.01286	0.00029
16	1.01180	0.00040	1.01180	0.00040	1.01210	0.00030	1.01203	0.00029
17	1.01250	0.00040	1.01250	0.00040	1.01250	0.00030	1.01253	0.00029
18	1.01190	0.00040	1.01190	0.00040	1.01230	0.00030	1.01220	0.00030
19	1.01240	0.00040	1.01240	0.00040	1.01260	0.00030	1.01259	0.00029
20	1.01230	0.00040	1.01230	0.00040	1.01290	0.00030	1.01279	0.00030
21	1.01220	0.00040	1.01210	0.00040	1.01220	0.00030	1.01217	0.00030
22	1.01280	0.00040	1.01280	0.00040	1.01250	0.00030	1.01254	0.00029
23	1.01200	0.00040	1.01200	0.00040	1.01210	0.00030	1.01206	0.00030
24	1.01330	0.00040	1.01330	0.00040	1.01290	0.00030	1.01297	0.00029
25	1.01310	0.00040	1.01310	0.00040	1.01310	0.00030	1.01310	0.00029
26	1.01230	0.00040	1.01230	0.00040	1.01220	0.00030	1.01223	0.00029
27	1.01280	0.00040	1.01280	0.00040	1.01270	0.00030	1.01273	0.00030
28	1.01260	0.00040	1.01260	0.00040	1.01300	0.00030	1.01288	0.00030
29	1.01250	0.00040	1.01250	0.00040	1.01240	0.00030	1.01242	0.00029
30	1.01280	0.00040	1.01290	0.00040	1.01270	0.00030	1.01274	0.00031
31	1.01170	0.00040	1.01170	0.00040	1.01180	0.00030	1.01182	0.00028
32	1.01360	0.00040	1.01360	0.00040	1.01310	0.00030	1.01321	0.00029
33	1.01360	0.00040	1.01360	0.00040	1.01300	0.00030	1.01309	0.00030
34	1.01200	0.00040	1.01200	0.00040	1.01270	0.00030	1.01256	0.00029
35	1.01280	0.00040	1.01270	0.00040	1.01290	0.00030	1.01293	0.00030
36	1.01300	0.00040	1.01300	0.00040	1.01270	0.00030	1.01278	0.00029
37	1.01270	0.00040	1.01270	0.00040	1.01270	0.00030	1.01271	0.00029
38	1.01310	0.00040	1.01300	0.00040	1.01250	0.00030	1.01262	0.00028
39	1.01230	0.00040	1.01230	0.00040	1.01240	0.00030	1.01237	0.00029
40	1.01210	0.00040	1.01210	0.00040	1.01240	0.00030	1.01233	0.00029
41	1.01310	0.00040	1.01310	0.00040	1.01270	0.00030	1.01276	0.00029
42	1.01210	0.00040	1.01210	0.00040	1.01230	0.00030	1.01230	0.00030
43	1.01160	0.00040	1.01160	0.00040	1.01190	0.00030	1.01189	0.00029
44	1.01230	0.00040	1.01230	0.00040	1.01200	0.00030	1.01211	0.00030
45	1.01290	0.00040	1.01290	0.00040	1.01270	0.00030	1.01273	0.00029
46	1.01270	0.00040	1.01270	0.00040	1.01280	0.00030	1.01279	0.00030
47	1.01260	0.00040	1.01260	0.00040	1.01260	0.00030	1.01262	0.00030
48	1.01300	0.00040	1.01300	0.00040	1.01280	0.00030	1.01285	0.00029
49	1.01320	0.00040	1.01320	0.00040	1.01270	0.00030	1.01281	0.00030
50	1.01200	0.00040	1.01200	0.00040	1.01250	0.00030	1.01237	0.00029
51	1.01230	0.00050	1.01230	0.00050	1.01270	0.00030	1.01263	0.00031
52	1.01310	0.00040	1.01310	0.00040	1.01300	0.00030	1.01303	0.00031
53	1.01200	0.00040	1.01200	0.00040	1.01240	0.00030	1.01233	0.00030
54	1.01310	0.00040	1.01310	0.00040	1.01290	0.00030	1.01293	0.00029
55	1.01290	0.00040	1.01290	0.00040	1.01240	0.00030	1.01249	0.00028
56	1.01230	0.00040	1.01230	0.00040	1.01200	0.00030	1.01210	0.00030
57	1.01350	0.00040	1.01350	0.00040	1.01280	0.00030	1.01294	0.00029
58	1.01220	0.00040	1.01220	0.00040	1.01300	0.00030	1.01287	0.00030
59	1.01270	0.00040	1.01270	0.00040	1.01230	0.00030	1.01238	0.00031
60	1.01200	0.00040	1.01190	0.00040	1.01270	0.00030	1.01254	0.00031
61	1.01240	0.00040	1.01240	0.00040	1.01230	0.00030	1.01234	0.00029
62	1.01240	0.00040	1.01240	0.00040	1.01270	0.00030	1.01265	0.00031
63	1.01230	0.00040	1.01220	0.00040	1.01220	0.00030	1.01219	0.00029

64	1.01360	0.00040	1.01360	0.00040	1.01340	0.00030	1.01347	0.00029
65	1.01290	0.00040	1.01290	0.00040	1.01280	0.00030	1.01283	0.00031
66	1.01240	0.00040	1.01240	0.00040	1.01260	0.00030	1.01254	0.00031
67	1.01340	0.00040	1.01340	0.00040	1.01310	0.00030	1.01317	0.00031
68	1.01220	0.00040	1.01220	0.00040	1.01190	0.00030	1.01200	0.00030
69	1.01200	0.00040	1.01200	0.00040	1.01280	0.00030	1.01268	0.00030
70	1.01190	0.00040	1.01190	0.00040	1.01200	0.00030	1.01202	0.00029
71	1.01400	0.00040	1.01400	0.00040	1.01270	0.00030	1.01295	0.00030
72	1.01190	0.00040	1.01190	0.00040	1.01250	0.00030	1.01234	0.00031
73	1.01270	0.00050	1.01270	0.00050	1.01220	0.00030	1.01225	0.00030
74	1.01230	0.00040	1.01230	0.00040	1.01230	0.00030	1.01235	0.00029
75	1.01240	0.00040	1.01240	0.00040	1.01230	0.00030	1.01231	0.00030
76	1.01160	0.00040	1.01160	0.00040	1.01190	0.00030	1.01181	0.00029
77	1.01150	0.00040	1.01150	0.00040	1.01190	0.00030	1.01181	0.00030
78	1.01250	0.00040	1.01240	0.00040	1.01290	0.00030	1.01279	0.00030
79	1.01210	0.00040	1.01210	0.00040	1.01260	0.00030	1.01251	0.00030
80	1.01240	0.00040	1.01240	0.00040	1.01240	0.00030	1.01244	0.00029
81	1.01240	0.00040	1.01240	0.00040	1.01210	0.00030	1.01216	0.00030
82	1.01310	0.00050	1.01310	0.00050	1.01270	0.00030	1.01278	0.00030
83	1.01220	0.00040	1.01220	0.00040	1.01220	0.00030	1.01218	0.00028
84	1.01220	0.00040	1.01220	0.00040	1.01210	0.00030	1.01213	0.00031
85	1.01290	0.00040	1.01290	0.00040	1.01310	0.00030	1.01304	0.00029
86	1.01320	0.00040	1.01320	0.00040	1.01300	0.00030	1.01302	0.00029
87	1.01140	0.00040	1.01140	0.00040	1.01230	0.00030	1.01215	0.00030
88	1.01270	0.00040	1.01280	0.00040	1.01260	0.00030	1.01263	0.00030
89	1.01180	0.00040	1.01170	0.00050	1.01210	0.00030	1.01204	0.00030
90	1.01280	0.00040	1.01280	0.00040	1.01230	0.00030	1.01243	0.00029
91	1.01300	0.00040	1.01300	0.00040	1.01320	0.00030	1.01320	0.00032
92	1.01310	0.00040	1.01310	0.00040	1.01320	0.00030	1.01316	0.00028
93	1.01250	0.00040	1.01250	0.00040	1.01260	0.00030	1.01259	0.00030
94	1.01110	0.00040	1.01110	0.00040	1.01160	0.00030	1.01152	0.00030
95	1.01220	0.00040	1.01220	0.00040	1.01230	0.00030	1.01226	0.00030
96	1.01200	0.00040	1.01200	0.00040	1.01190	0.00030	1.01191	0.00030
97	1.01180	0.00040	1.01180	0.00040	1.01220	0.00030	1.01215	0.00030
98	1.01220	0.00040	1.01210	0.00040	1.01240	0.00030	1.01230	0.00030
99	1.01260	0.00040	1.01260	0.00040	1.01230	0.00030	1.01233	0.00029
100	1.01280	0.00050	1.01280	0.00050	1.01310	0.00030	1.01307	0.00029
mean	1.01249	0.00040	1.01249	0.00041	1.01252	0.00030	1.01252	0.00030
sigma	0.00055	0.00002	0.00055	0.00002	0.00037	0.00000	0.00038	0.00001
std of std	0.00009		0.00009		0.00023		0.00001	
difference in variance	-0.1362E-06		-0.1396E-06		-0.4725E-07		-0.5603E-07	
difference in stnd dev	-0.1429E-03		-0.1458E-03		-0.7047E-04		-0.8277E-04	

the results of the w test for normality applied to the collision, absorption, track-length, and combined keff values are:

the k(collision) values appear normally distributed at the 95 percent confidence level
the k(absorption) values appear normally distributed at the 95 percent confidence level
the k(trk length) values appear normally distributed at the 95 percent confidence level
the k(co/abs/trl) values appear normally distributed at the 95 percent confidence level

For 100 values of the collision estimator with average 1.01249 the data were:

confidence level	% of the time
0.680	52.0000
0.950	86.0000
0.990	94.0000

Largest deviation = 3.77268

For 100 values of the absorption estimator with average 1.01249 the data were:

confidence level	% of the time
0.680	51.0000
0.950	86.0000
0.990	94.0000

Largest deviation = 3.78519

For 100 values of the trk length estimator with average 1.01252 the data were:

confidence level	% of the time
0.680	57.0000
0.950	90.0000
0.990	98.0000

Largest deviation = 3.08315

For 100 values of the 3-combined estimator with average 1.01252 the data were:

confidence level	% of the time
0.680	54.0000
0.950	88.0000
0.990	98.0000

Largest deviation = 3.34064

100 runs Godiva/Jezebel: 40 batches, 20 cyc/batch

run	k(col)	std	k(abs)	std	k(trk ln)	std	k(c/a/t)	std
1	1.01210	0.00050	1.01210	0.00050	1.01270	0.00040	1.01260	0.00038
2	1.01250	0.00050	1.01250	0.00050	1.01230	0.00040	1.01234	0.00045
3	1.01290	0.00060	1.01290	0.00060	1.01310	0.00040	1.01314	0.00041
4	1.01170	0.00060	1.01170	0.00060	1.01230	0.00050	1.01214	0.00056
5	1.01230	0.00040	1.01230	0.00040	1.01220	0.00040	1.01222	0.00037
6	1.01250	0.00050	1.01260	0.00050	1.01230	0.00040	1.01241	0.00038
7	1.01260	0.00060	1.01260	0.00060	1.01280	0.00040	1.01281	0.00049
8	1.01290	0.00050	1.01290	0.00050	1.01230	0.00040	1.01242	0.00035
9	1.01150	0.00060	1.01150	0.00060	1.01200	0.00050	1.01191	0.00050
10	1.01230	0.00060	1.01230	0.00060	1.01250	0.00030	1.01255	0.00031
11	1.01280	0.00050	1.01290	0.00050	1.01270	0.00040	1.01272	0.00039
12	1.01290	0.00050	1.01280	0.00050	1.01290	0.00050	1.01289	0.00046
13	1.01200	0.00040	1.01200	0.00040	1.01250	0.00030	1.01231	0.00029
14	1.01210	0.00060	1.01210	0.00060	1.01280	0.00040	1.01279	0.00042
15	1.01330	0.00060	1.01330	0.00060	1.01270	0.00040	1.01274	0.00040
16	1.01180	0.00050	1.01180	0.00050	1.01210	0.00040	1.01203	0.00044
17	1.01250	0.00050	1.01250	0.00050	1.01250	0.00030	1.01252	0.00032
18	1.01190	0.00050	1.01190	0.00050	1.01230	0.00040	1.01215	0.00038
19	1.01240	0.00040	1.01240	0.00040	1.01260	0.00030	1.01257	0.00033
20	1.01230	0.00050	1.01230	0.00050	1.01290	0.00040	1.01285	0.00039
21	1.01220	0.00060	1.01210	0.00060	1.01220	0.00040	1.01224	0.00047
22	1.01280	0.00060	1.01280	0.00060	1.01250	0.00040	1.01241	0.00043
23	1.01200	0.00050	1.01200	0.00050	1.01210	0.00040	1.01208	0.00039
24	1.01330	0.00050	1.01330	0.00050	1.01290	0.00040	1.01294	0.00050
25	1.01310	0.00040	1.01310	0.00040	1.01310	0.00030	1.01307	0.00028
26	1.01230	0.00050	1.01230	0.00050	1.01220	0.00040	1.01223	0.00039
27	1.01280	0.00050	1.01280	0.00050	1.01270	0.00040	1.01271	0.00039
28	1.01260	0.00040	1.01260	0.00040	1.01300	0.00040	1.01284	0.00039
29	1.01250	0.00050	1.01250	0.00050	1.01240	0.00050	1.01240	0.00042
30	1.01280	0.00050	1.01290	0.00050	1.01270	0.00040	1.01272	0.00038
31	1.01170	0.00050	1.01170	0.00050	1.01180	0.00040	1.01183	0.00043
32	1.01360	0.00050	1.01360	0.00050	1.01310	0.00040	1.01314	0.00040
33	1.01360	0.00040	1.01360	0.00040	1.01300	0.00040	1.01332	0.00035
34	1.01200	0.00030	1.01200	0.00030	1.01270	0.00040	1.01235	0.00035
35	1.01280	0.00050	1.01270	0.00050	1.01290	0.00030	1.01305	0.00034
36	1.01300	0.00050	1.01300	0.00050	1.01270	0.00040	1.01273	0.00037
37	1.01270	0.00050	1.01270	0.00050	1.01270	0.00040	1.01279	0.00042
38	1.01310	0.00040	1.01300	0.00040	1.01250	0.00030	1.01265	0.00036
39	1.01230	0.00050	1.01230	0.00050	1.01240	0.00040	1.01242	0.00034
40	1.01210	0.00050	1.01210	0.00050	1.01240	0.00040	1.01241	0.00037
41	1.01310	0.00050	1.01310	0.00050	1.01270	0.00040	1.01274	0.00041
42	1.01210	0.00040	1.01210	0.00040	1.01230	0.00050	1.01221	0.00042
43	1.01160	0.00060	1.01160	0.00060	1.01190	0.00030	1.01202	0.00035
44	1.01230	0.00040	1.01230	0.00040	1.01200	0.00040	1.01219	0.00038
45	1.01290	0.00060	1.01290	0.00060	1.01270	0.00040	1.01268	0.00043
46	1.01270	0.00050	1.01270	0.00050	1.01280	0.00030	1.01281	0.00038
47	1.01260	0.00060	1.01260	0.00060	1.01260	0.00040	1.01265	0.00044
48	1.01300	0.00050	1.01300	0.00050	1.01280	0.00030	1.01291	0.00033
49	1.01320	0.00040	1.01320	0.00040	1.01270	0.00040	1.01290	0.00036
50	1.01200	0.00050	1.01200	0.00050	1.01250	0.00040	1.01236	0.00039
51	1.01230	0.00060	1.01230	0.00060	1.01270	0.00040	1.01280	0.00033
52	1.01310	0.00060	1.01310	0.00060	1.01300	0.00040	1.01300	0.00045
53	1.01200	0.00050	1.01200	0.00050	1.01240	0.00030	1.01237	0.00040
54	1.01310	0.00050	1.01310	0.00050	1.01290	0.00040	1.01296	0.00042
55	1.01290	0.00040	1.01290	0.00040	1.01240	0.00030	1.01258	0.00030
56	1.01230	0.00050	1.01230	0.00050	1.01200	0.00040	1.01216	0.00039
57	1.01350	0.00050	1.01350	0.00050	1.01280	0.00030	1.01283	0.00040
58	1.01220	0.00060	1.01220	0.00060	1.01300	0.00050	1.01279	0.00058
59	1.01270	0.00050	1.01270	0.00050	1.01230	0.00040	1.01230	0.00037
60	1.01200	0.00050	1.01190	0.00050	1.01270	0.00050	1.01248	0.00053
61	1.01240	0.00050	1.01240	0.00050	1.01230	0.00040	1.01237	0.00039
62	1.01240	0.00050	1.01240	0.00050	1.01270	0.00040	1.01273	0.00048
63	1.01230	0.00040	1.01220	0.00040	1.01220	0.00040	1.01230	0.00043

64	1.01360	0.00060	1.01360	0.00060	1.01340	0.00040	1.01344	0.00042
65	1.01290	0.00060	1.01290	0.00060	1.01280	0.00040	1.01283	0.00045
66	1.01240	0.00050	1.01240	0.00050	1.01260	0.00040	1.01258	0.00040
67	1.01340	0.00050	1.01340	0.00050	1.01310	0.00040	1.01320	0.00038
68	1.01220	0.00040	1.01220	0.00040	1.01190	0.00040	1.01197	0.00037
69	1.01200	0.00040	1.01200	0.00040	1.01280	0.00040	1.01255	0.00043
70	1.01190	0.00060	1.01190	0.00060	1.01200	0.00040	1.01204	0.00042
71	1.01400	0.00040	1.01400	0.00040	1.01270	0.00030	1.01294	0.00037
72	1.01190	0.00050	1.01190	0.00050	1.01250	0.00040	1.01234	0.00050
73	1.01270	0.00050	1.01270	0.00050	1.01220	0.00040	1.01211	0.00043
74	1.01230	0.00050	1.01230	0.00050	1.01230	0.00040	1.01222	0.00036
75	1.01240	0.00060	1.01240	0.00060	1.01230	0.00040	1.01228	0.00043
76	1.01160	0.00050	1.01160	0.00050	1.01190	0.00040	1.01174	0.00037
77	1.01150	0.00050	1.01150	0.00050	1.01190	0.00040	1.01179	0.00037
78	1.01250	0.00050	1.01240	0.00050	1.01290	0.00040	1.01285	0.00046
79	1.01210	0.00060	1.01210	0.00060	1.01260	0.00050	1.01253	0.00049
80	1.01240	0.00050	1.01240	0.00050	1.01240	0.00040	1.01246	0.00040
81	1.01240	0.00050	1.01240	0.00050	1.01210	0.00040	1.01216	0.00043
82	1.01310	0.00060	1.01310	0.00060	1.01270	0.00040	1.01274	0.00038
83	1.01220	0.00050	1.01220	0.00050	1.01220	0.00040	1.01218	0.00034
84	1.01220	0.00050	1.01220	0.00050	1.01210	0.00050	1.01216	0.00045
85	1.01290	0.00050	1.01290	0.00050	1.01310	0.00040	1.01298	0.00038
86	1.01320	0.00040	1.01320	0.00040	1.01300	0.00030	1.01307	0.00029
87	1.01140	0.00050	1.01140	0.00050	1.01230	0.00040	1.01219	0.00041
88	1.01270	0.00050	1.01280	0.00050	1.01260	0.00040	1.01275	0.00041
89	1.01180	0.00050	1.01170	0.00050	1.01210	0.00040	1.01199	0.00038
90	1.01280	0.00050	1.01280	0.00050	1.01230	0.00030	1.01237	0.00036
91	1.01300	0.00050	1.01300	0.00050	1.01320	0.00040	1.01323	0.00041
92	1.01310	0.00050	1.01310	0.00050	1.01320	0.00040	1.01312	0.00037
93	1.01250	0.00050	1.01250	0.00050	1.01260	0.00040	1.01259	0.00037
94	1.01110	0.00040	1.01110	0.00040	1.01160	0.00040	1.01146	0.00035
95	1.01220	0.00050	1.01220	0.00050	1.01230	0.00040	1.01232	0.00034
96	1.01200	0.00060	1.01200	0.00060	1.01190	0.00040	1.01181	0.00040
97	1.01180	0.00050	1.01180	0.00050	1.01220	0.00040	1.01218	0.00037
98	1.01220	0.00050	1.01210	0.00050	1.01240	0.00040	1.01236	0.00040
99	1.01260	0.00050	1.01260	0.00050	1.01230	0.00040	1.01226	0.00040
100	1.01280	0.00040	1.01280	0.00040	1.01310	0.00030	1.01291	0.00033
mean	1.01249	0.00050	1.01249	0.00050	1.01252	0.00039	1.01252	0.00040
sigma	0.00055	0.00007	0.00055	0.00007	0.00037	0.00005	0.00039	0.00005
std of std	0.00009		0.00009		0.00008		0.00010	
difference in variance	-0.4822E-07		-0.5244E-07		0.1642E-07		0.7276E-08	
difference in stnd dev	-0.4592E-04		-0.4977E-04		0.2153E-04		0.9256E-05	

the results of the w test for normality applied to the collision, absorption, track-length, and combined keff values are:

the k(collision) values appear normally distributed at the 95 percent confidence level
the k(absorption) values appear normally distributed at the 95 percent confidence level
the k(trk length) values appear normally distributed at the 95 percent confidence level
the k(co/abs/trl) values appear normally distributed at the 95 percent confidence level

For 100 values of the collision estimator with average 1.01249 the data were:

confidence level	% of the time
0.680	63.0000
0.950	93.0000
0.990	97.0000
Largest deviation =	3.77268

For 100 values of the absorption estimator with average 1.01249 the data were:

confidence level	% of the time
0.680	62.0000
0.950	94.0000
0.990	97.0000

Largest deviation = 3.78519

For 100 values of the trk length estimator with average 1.01252 the data were:

confidence level	% of the time
0.680	71.0000
0.950	97.0000
0.990	100.0000

Largest deviation = 2.31236

For 100 values of the 3-combined estimator with average 1.01252 the data were:

confidence level	% of the time
0.680	70.0000
0.950	95.0000
0.990	99.0000

Largest deviation = 3.03643

XV. APPENDIX H: MCNP INPUT DECKS

A. U-233/Water Sphere, Implicit Capture

```
U-233 mixture
1    1 .099791850  -1
2    2 .100087941   1 -2
3    0               2

1    so 10.868779  $  aa = hh/2
2    so 26.068779  $  bb = aa + 15.2

imp:n  1 1 0
kcode 2000 1 10 110
ksrc  0 0 0
m1   1001.50c .066355625  8016.50c .033177812  92233.50c .000258413
mt1  lwtr.01t
m2   1001.50c .066725294  8016.50c .033362647
mt2  lwtr.01t
print
```

B. U-233/Water Sphere, Analog Capture

Add the following card to the implicit input after the mt2 card:

```
phys:n   20. 20.
```

C. U-233/Water Mixture in Infinite Medium, Implicit Capture

```
k-infinity for u-233 mixture
1    1 .1  -1
2    0      1

*1    so 1.e7

imp:n 1 0
kcode 2000 1 10 110
ksrc  0 0 0
m1    1001 .0666  8016 .0333  92233 .00003
mt1   lwtr.01t
dbcn  7j 3e6
print
```

D. U-233/Water Mixture in Infinite Medium, Analog Capture

This also contains a track length flux tally.

```
k-infinity for u-233 mixture
1    1 .1  -1
2    0      1

*1    so 1.e7

imp:n 1 0
kcode 2000 1 10 110
ksrc  0 0 0
m1    1001 .0666  8016 .0333  92233 .00003
mt1   lwtr.01t
dbcn  7j 1
phys:n   20 6.25-7
f4:n   1
sd4    1.
fm4    -1 1 -6 -7
e4     1-8 1-7 6.25-7 1-6 1-5 1-4 1-3 1-2 .1 1. 5. 20.
print
```

E. Godiva, Implicit Capture

```
godiva1
1    1  -18.74  -1
2    0           1

1    so 8.741

kcode 1000 1.0 10 110
ksrc  0. 0. 0.
imp:n 1 0
m1    92235 -93.71  92238 -5.27  92234 -1.02
dbcn  7j 1
```

F. Godiva, Analog Capture

Add the following card to the end of the implicit input file:

```
phys:n  20. 20.
```

G. Jezebel, Implicit Capture

```
nominal jezebel
1    1 -15.61 -1
2    0         1

1    so 6.384928
```

```
kcode 2000 1.0 10 60
ksrc   0. 0. 0.
m1     94239 1.
imp:n  1 0
```

H. Jezebel, Analog Capture

Add the following card to the end of the implicit input file:

```
phys:n  20. 20.
```

I. Two-Component System: Jezebel and Godiva

```
"jezebel" sphere & godiva sphere, 80 cm center-center
1    2 -18.74 -10
2    1 -15.61 -20
21   0         10 20 -21
22   0         21

10   sx  40.000 8.741
20   sx  -40.000 6.384928
21   so  49.0

kcode 5000 1.0 20 820
ksrc   40.000 0. 0.   -40.0 0. 0.   38. 0. 0.
       -42.0 0. 0.  -38. 0. 0.   42. 0. 0.
m1     94239 1.
m2     92235 -93.71  92238 -5.27  92234 -1.02
imp:n  1 1 1 0
dbcn  7j                 118900001
print
```

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