

# MONTE CARLO EIGENFUNCTION STRATEGIES AND UNCERTAINTIES

R. C. Gast and N. R. Candelore

Bettis Atomic Power Laboratory  
West Mifflin, Pennsylvania 15122, U.S.A.

## ABSTRACT

Comparisons of convergence rates for several possible eigenfunction source strategies led to the selection of the "straight" analog of the analytic power method as the source strategy for Monte Carlo eigenfunction calculations. To insure a fair game strategy, the number of histories per iteration increases with increasing iteration number. The estimate of eigenfunction uncertainty is obtained from a modification of a proposal by D. B. MacMillan and involves only estimates of the usual purely statistical component of uncertainty and a serial correlation coefficient of lag one.

## I. INTRODUCTION

It is convenient to consider each possible Monte Carlo eigenfunction strategy as composed of two basic parts. The first part is the totality of the Monte Carlo procedures that would be involved in a fixed source calculation. The second part is the eigenfunction source shape strategy that connects successive generations.

The construction of an efficient overall eigenfunction strategy requires that the fixed source procedures, and the method of connecting successive generations, each be made efficient. Methods for improving the efficiency, i.e. reducing the standard deviation per unit machine time, in fixed source procedures have been frequently investigated and developed. In contrast, methods for reducing the variance arising from the source shape strategy have received relatively little attention; even the basic requirements for a "fair game" strategy appear to have been little understood.

All source shape strategies considered in this report are required by the authors to be "fair game" strategies. Thus, the first subsection of Section II is a discussion of "fair game" requirements. This subsection also includes a description of a "reference" strategy which is used to provide a comparison of relative convergence rates of all other strategies. The remainder of Section II describes various source shape strategies considered; they include strategies using Green's function, strategies using

extrapolation factors, and strategies using importance sampling. The final subsection of Section II discusses the details of the source strategy selected.

Having selected a definite strategy, Section III of the report then describes the approach that led to the means of assigning eigenfunction uncertainties. The resulting uncertainty formula is partly empirical, and for that reason it required extensive numerical testing. The results of these tests are also presented in Section III.

## II. EIGENFUNCTION SOURCE STRATEGY

The investigation that led to the selected source shape strategy is described in this section. First, however, the "fair game" requirements for a general eigenfunction strategy are discussed and a reference strategy is defined.

### a. Requirements for Fair Game and a Reference Strategy

The presentation in this subsection will summarize some results given in detail in Ref. [1].

First, we introduce for convenience the term "limit in probability" denoted by the symbol "PLim." Thus  $\text{PLim}_{N \rightarrow \infty} X_N = X$  means that for the sequence of random variables  $X_N$ , and for some parameter  $X$ , the condition  $\text{Lim} [P\{|X_N - X| < \epsilon\}] = 1$  is met for any arbitrarily chosen positive  $\epsilon$ . In this case we say that the sequence of random variables,  $X_N$ , converges in probability to  $X$ . The concept of repeatability involved in determining  $P\{|X_N - X| < \epsilon\}$  for a given value of  $N = N_0$ , where  $X_N$  is a sequence of dependent random variables, is to repeatedly return to the calculation beginning with new sets of random numbers and obtain a sequence of values for  $X_{N_0}$ . The fraction of such values for which  $|X_{N_0} - X| < \epsilon$  is an estimate of the desired probability.

We may write any overall Monte Carlo eigenfunction strategy using a neutron production Green's function as

$$\psi_i^{n+1} = \sum_j G_{ij}^n K^n(S_j^n).$$

The three random variables in this equation are defined as follows:

1)  $G_{ij}^n$  is an estimate of the fission neutron production rate in elementary volume  $i$  due to a unit fission source in elementary volume  $j$  in the  $n^{\text{th}}$  iteration. Possible values of this random variable are determined by starting one or more neutrons in elementary volume  $j$  and determining the neutron production rate per start neutron in elementary volume  $i$  by Monte Carlo tracking. Consequently, the number of neutron histories in a value of  $G_{ij}^n$  will be the number of starting neutrons in elementary volume  $j$  in the

$n^{\text{th}}$  iteration. If the number of histories in a value of  $G_{ij}^n$  approaches infinity, then the limit in probability of  $G_{ij}^n$  is  $G_{ij}$  where  $G_{ij}$  is the analytic Green's function over elementary volumes.

2)  $\psi_i^{n+1}$  is an estimate of the fission neutron production rate in elementary volume  $i$  at the  $n^{\text{th}}$  iteration of the iteration process used. As implied by the above equation,  $\psi_i^{n+1}$  is a dependent random variable.

3)  $K^n(S_j^n)$  is another estimate of the fission neutron production rate in elementary volume  $j$  at the  $n^{\text{th}}$  iteration, but in general, is only relative to other elementary volumes.  $S_j^n$  alone is another estimate of the fission neutron production rate in elementary volume  $j$  at the  $n^{\text{th}}$  iteration, and is obtained in some manner, yet to be specified, from previous iteration results. One possible means of doing this is the analog of the analytic power method, i.e. set  $S_j^n = \psi_j^n$ . The symbol  $K^n(S_j^n)$  denotes an operator  $K^n$  acting on  $S_j^n$ . In general, the operator  $K^n$  involves a sampling process and a normalization process, although one or both of these processes may be absent. The sampling operator  $K^n$  in the Monte Carlo eigenfunction iteration process defines the means by which neutron starting sites and weights are determined in the  $n^{\text{th}}$  iteration. For example, a possible definition of the operator  $K^n$  which involves both sampling and normalization processes is as follows:

First a finite number of neutron starting sites are distributed among the elementary volumes using  $\frac{S_j^n}{\sum S_j^n}$  as the frequency distribution function and

using a set of random numbers designated by the index  $n$ . Second, the sum of neutron weights (say unity per site) over the starting sites are normalized to unity. If we let  $N^n$  be the number of neutron histories in iteration  $n$ , and if we let  $S_j$  be a source strength per elementary volume  $j$  that is independent of  $n$  (i.e. a fixed source), then we may write

$$\text{PLim}_{n \rightarrow \infty} \left( \frac{\sum_{n=1}^n N^n K^n(S_j)}{\sum_{n=1}^n N^n} \right) = \bar{S}_j,$$

where  $\bar{S}_j$  are normalized values of  $S_j$ , i.e.  $\sum_j \bar{S}_j = 1$ .

The only sampling operator used in this report is that given above as an example. In the discussion of this particular operator, we did not identify the precise means by which starting sites are selected using

$\frac{S_j^n}{\sum_j S_j^n}$  as the frequency distribution function. For example, a purely

random sampling could be used, or one that is purely systematic, or some combination of both (semi-systematic). We do not need to be concerned with these details, since all that is required to demonstrate a fair game is that the above PLim equation is satisfied; that is, the sampling operator will properly treat a fixed source.

We will now exhibit the condition to be met for a fair game in a Monte Carlo eigenfunction strategy. Let  $\psi_i$  be the fundamental mode eigenfunction neutron production rate over elementary volume  $i$  from analytic transport theory. Thus,  $\psi_i$  satisfies the equation

$$\psi_i = \sum_j G_{ij} \bar{\psi}_j,$$

where  $G_{ij}$  is the analytic Green's function over elementary volumes, and where  $\bar{\psi}_j = \frac{\psi_j}{\sum_j \psi_j}$ . Here the eigenvalue,  $\lambda$ , is a normalization factor, i.e.

$\lambda = \sum_j \psi_j$ . Using PLimits, the condition to be met for a fair game in an

eigenfunction strategy where iteration results are accumulated with weights equal to number of histories per iteration,  $N^n$ , is given by

$$\text{PLim}_{n \rightarrow \infty} \left( \frac{\sum_{n=1}^n N^n \psi_1^n}{\sum_{n=1}^n N^n} \right) = \psi_1.$$

As discussed previously,  $\psi_1^n$  satisfies an equation of the form

$$\psi_1^{n+1} = \sum_j G_{ij}^n K^n(S_j^n).$$

It may be observed at this point that it will generally be desirable to accumulate iteration results with weights equal to number of histories per iteration, since this will result in minimum variance in a fixed source

calculation.

The simplest Monte Carlo eigenfunction strategy is the analog of the analytic power method, i.e. set  $S_j^n = \psi_j^n$ . This strategy will be taken as the reference strategy, i.e. all other strategies will be compared to the power method to judge relative convergence rates. As shown in Ref. [1], this power method strategy is not a fair game if the number of histories per iteration,  $N^n$ , is a constant independent of  $n$ . (The appendix of this report gives a weighting scheme for neutron starting weights such that a fair game is obtained in this case). A sufficient set of conditions to insure a fair game in the power method strategy are:

- (1)  $\lim_{n \rightarrow \infty} N^n = \infty$ .
- (2) The sampling operator properly treats a fixed source. Since the number of histories per iteration becomes large as  $n$  increases (condition 1), we must have  $\text{PLim}_{n \rightarrow \infty} K^n(S_j) = \bar{S}_j$ .
- (3) Because the strategy is a Markov process, we must require that all iterations used in the calculation produce progeny. This is easily done with the device that should an iteration not produce progeny, then the first prior iteration with progeny is used to continue the process.
- (4) The physical problem under consideration must be one for which the analytic neutron transport equation has a unique fundamental mode eigenfunction. That is, certain sufficient "connectivity" conditions among the elementary volumes are met which insure such a unique eigenfunction. These connectivity conditions will be met for all reactor problems of practical interest.

With these conditions, it follows essentially by definition that the resulting "power method" strategy is a fair game. This is easily seen by considering the representation of the  $n^{\text{th}}$  iteration of the Monte Carlo calculation, i.e.

$$\psi_1^{n+1} = \sum_j G_{1j}^n K^n(\psi_j^n).$$

Because of conditions (3) and (4), we know that the  $\text{PLim}_{n \rightarrow \infty} \psi_1^n$  does exist. Let its value be  $\bar{\psi}_1$ . Taking  $\text{PLimits}$  of both sides of the above equation, we immediately obtain

$$\bar{\psi}_1 = \sum_j G_{1j} \bar{\psi}_j.$$

This is the analytic neutron transport equation over elementary volumes. Since negative neutrons are not permitted to be born at fission sites, and since the trivial zero solution is not possible because of condition (3),

then the above  $\Psi_1$  must be the fundamental mode eigenfunction. Thus the general condition for a fair game is met, i.e.

$$\text{PLim}_{n \rightarrow \infty} \left( \frac{\sum_{n=1}^n N^n \Psi_1^n}{\sum_{n=1}^n N^n} \right) = \Psi_1,$$

where  $\Psi_1$  is the fundamental mode eigenfunction over elementary volumes from analytic transport theory.

All of the source shape strategies considered in the remainder of this section are made fair games by the same approach used for the power method described above. That is, the number of histories per iteration will increase with increasing iteration number.

The subsequent subsections will describe the new eigenfunction strategies that were considered and the results of comparing their convergence rates to the reference strategy. In order to make these comparisons more meaningful, a source guess accuracy requirement was adopted. However, there is another obvious reason for adopting such a requirement. That is, in any conceivable eigenfunction strategy, one cannot permit an arbitrarily poor source guess in a large core and obtain satisfactory convergence in reasonable computing times. Thus in all strategies considered, we will require that the eigenfunction guess be within about 2 P.E.'s of the true eigenfunction, where the P.E. is computed for the number of histories in the 1st iteration. This condition can be easily met, since such a guess is not highly accurate. A workable method of verifying that the source guess is of this accuracy for practical size cores is to compare the eigenfunction estimate at the end of the problem with the guess. Should this comparison reveal that the guess was not within 2 P.E.'s, then a sequence of initial iterations should be omitted until the source accuracy condition is met. This procedure will be carried out in all subsequent testing of eigenfunction strategies.

#### b. Source Strategies Using Green's Function

An accumulated neutron production Green's function in an eigenfunction Monte Carlo calculation, say  $G_{jj}^n$ , is defined as the estimate of the fission neutron production rate in region  $j$  due to a unit fission source in region  $j'$ . This matrix is the result of normalizing an accumulative matrix formed by adding to a corresponding matrix element the fission neutron production as each neutron collision occurs. The normalization is performed by row; the normalization factor for the  $j'$  row being the reciprocal of the total number of neutrons born in region  $j'$ . The index  $n$  indicates the total number of iterations contributing to the accumulation. Thus if the Monte Carlo eigenfunction calculation is a fair game, i.e. capable of converging to the true transport theory solution, then at any stage of such a calculation an estimate of the region integrated eigenfunction, say  $P_j$ , and an

estimate of the eigenvalue, say  $\hat{\lambda}$ , may be made using the above Green's function. Of course these estimates would be in addition to those already available directly from the Monte Carlo calculation. The relative merits of these two types of estimates will be discussed later.

Knowing  $\hat{G}_{jj}^{n-1}$ , at the end of iteration  $n-1$ , we may obtain the estimated, i.e. projected, eigenvector  $\hat{P}_j$  and the projected eigenvalue  $\hat{\lambda}$  by the analytic power method. That is, we define  $\hat{P}_j^l$  as,

$$\hat{P}_j^l = \sum_{j'} \hat{G}_{jj'}^{n-1} \bar{P}_{j'}^{l-1}, \text{ where}$$

$$\bar{P}_j^l = \frac{\hat{P}_j^l}{\sum_j \hat{P}_j^l}.$$

The above iterative process is carried out by starting with some eigenvector guess and continuing until some convergence criterion for the eigenvector is met. Let  $L$  be the total number of iterations so performed. Then  $\hat{P}_j^L$  is the projected eigenvector and

$$\sum_j \hat{P}_j^L \text{ is the projected eigenvalue.}$$

Using the representation of a general Monte Carlo eigenfunction strategy from subsection (a), i.e.

$$\psi_i^{n+1} = \sum_j G_{ij}^n K^n(S_j^n),$$

we may hopefully define an accelerated strategy by setting the source for the  $n^{\text{th}}$  iteration as

$$S_j^n = \hat{P}_j^L.$$

Of course, this could be done with some chosen regularity during the course of the calculation rather than every iteration.

Use has been made of the projected eigenvalue, and the quantity  $L$  in conjunction with the O5R Monte Carlo program. For example, G. W. Morrison, J. T. Mihalcz, and D. C. Irving [2] use the quantity  $L$  to decide how many initial Monte Carlo iterations do not have a sufficiently converged source in order that they may be excluded from the eigenfunction accumulation. Of

course, in this application, the eigenvector guess, by region  $j$ , would be taken as the original source guess in the Monte Carlo calculation.

The projected, i.e. matrix, eigenvalue has been used in connection with O5R criticality calculations. This estimated eigenvalue is of interest since it is a separate estimate from that obtainable directly from the Monte Carlo calculation, i.e. the ratio of total neutron production to total source. Of course these two estimates are not independent. Mihalcz, in his O5R calculations of delayed-critical assemblies [3], found that the matrix eigenvalue was always within a standard deviation of that computed from the ratio of total neutron production to total source. A similar conclusion was arrived at by M. R. Mendelson in his Monte Carlo criticality calculations using the KAPL version of O5R [4]. Mendelson found that if a reasonable source guess was used, then the matrix eigenvalue does not appear to be any better than that obtained from a ratio.

The idea of using a Green's function in Monte Carlo eigenfunction calculations to obtain better estimates of the eigenfunction and eigenvalue has been frequently discussed by Monte Carlo workers. It appears to have originated with K. W. Morton [5] and was further developed by E. L. Kaplan [6]; however, it also appears that their work was purely theoretical. This idea is especially appealing if one views it as follows: Consider a reactor broken up into a finite number of gross regions over which a Green's function matrix is tabulated. In applying the analytic analog of the power method to such a problem, the eigenfunction error would consist principally of the first overtone component.

It intuitively seems that the matrix eigenfunction should enable rapid removal of the lower overtone modes, since they would be easily sensed over gross regions. After local normalization, deviations from the eigenfunction interior to a gross region would be more dependent on the higher overtones, which die out rapidly. Thus it would seem that if the projected eigenfunction over gross regions at iteration  $n$  were used to determine the source for iteration  $n+1$ , then a considerable gain in convergence rate would be obtained. This differs from the approach used with O5R calculations, since knowledge of the projected eigenfunction was not used to determine the source for the subsequent iteration.

This idea has been more recently discussed by L. L. Carter and N. J. McCormick [7]. Again, however, it was not actually tried in a Monte Carlo calculation. Instead, they constructed what was believed to be a reasonable analytic representation of the Monte Carlo procedure using diffusion theory. In their analysis of convergence rates with this model, they considered the straight power method, the use of the Green's function as in O5R, and the use of the Green's function at iteration  $n$  to determine the source shape over gross regions for iteration  $n+1$ . They found that the O5R approach gave faster convergence than the power method and that the last approach gave much faster convergence than the power method. It should be noted that the first part of their conclusion is in conflict with actual Monte Carlo calculations as performed by Mihalcz [3] and Mendelson [4].

Because of the intuitive appeal of using the Green's function at iteration  $n$  to determine source shape over gross regions for iteration  $n+1$ , the technique was tried. The projected eigenfunction as described earlier was



used to determine the source shape over gross regions in the power method. Semi-systematic sampling of actual sites within a gross region was used to accurately obtain the desired source strength by gross region. Also, the projected eigenfunction was made with a variety of periods, that is every iteration, every 2nd iteration, every 5th iteration, every 10th iteration.

In all cases that were tested, which covered a variety of core sizes, no gain in eigenfunction convergence rates could be detected relative to the straight power method. Since this Green's function procedure was more elaborate than the corresponding procedure used for O5R by Mihalczko and Mendelson, then by inference we have verified their conclusion of no gain in convergence rates with the simpler procedure. We must also conclude that the analytic modeling of Monte Carlo by Carter and McCormick was much too crude to permit reasonable estimates of gains in convergence rates using Green's functions.

In view of the complete failure of the Green's function approach, one might ask what is wrong with the intuitive argument that was given to support it. The best way to answer this is to state a proper view of the Green's function approach which is as follows: Within the straight Monte Carlo analog of the power method, the eigenfunction by gross region may be estimated by either the total cumulated source or the total cumulated fission neutron production. Since in the power method, the neutron production for the  $n^{\text{th}}$  iteration becomes, within statistics resulting from the semi-systematic sampling, the source for the  $n+1^{\text{st}}$  iteration, then it follows that the total cumulated source at the  $n^{\text{th}}$  iteration will be very close in shape to the cumulated fission neutron production. This will occur even for  $n$  small if a reasonable source guess is made. The Green's function matrix elements are formed from the same neutron histories that contribute to the cumulated neutron production. The eigenvector from this matrix, by definition, is a source that will yield a neutron production of the same shape. But based on the information content of the matrix, i.e. all histories, this is already nearly the case since the cumulated source is very close in shape to the cumulated neutron production. Thus the eigenvector from the matrix will always be close to that obtained by the power method after very few iterations. That is, the Green's function approach cannot provide a worthwhile improvement in convergence rate relative to the power method in Monte Carlo.

### c. Source Strategies Using Extrapolation Factors

The success of extrapolation factors in accelerating eigenfunction convergence in analytic diffusion theory calculations is well known; this suggests the application of such factors in Monte Carlo eigenfunction calculations.

First we will consider the use of a single linear extrapolation factor in the reference strategy, that is, a straight analog of the analytic power method. This will be done by obtaining the form of this factor for the analytic power method and applying it directly in a series of Monte Carlo test calculations. Making use of the neutron production Green's function,  $G_{ij}$ , as in subsection (a), we may write the analytic power method for the fundamental mode, using matrix notation and using subscripts for region indices, as

$$\lambda_0^{\ell} \bar{\psi}_i^{\ell} = G_{ij} \bar{\psi}_j^{\ell-1} \text{ for the } \ell-1^{\text{st}} \text{ iteration,}$$

where  $\lambda_0^l$  is the multiplication factor for the  $l^{\text{th}}$  iteration, i.e.  $\lambda_0^l = \sum \psi_i^l$ , and where bars denote normalization, e.g.  $\bar{\psi}_i^l = \frac{\psi_i^l}{\sum \psi_i^l}$ . When a single linear

extrapolation factor,  $\omega$ , is used in the power method to obtain the fundamental mode eigenfunction, then the above procedure is altered as follows. After obtaining  $G_{ij}\psi_j^{l-1}$  from the  $(l-1)^{\text{st}}$  iteration, we normalize it by dividing by the multiplication factor,  $\lambda_0^l$ , and define

$$\begin{aligned}\psi^l &= \bar{\psi}^{l-1} + \omega \left( \frac{G_{ij}\bar{\psi}_j^{l-1}}{\lambda_0^l} - \bar{\psi}^{l-1} \right), \\ &= \bar{\psi}^{l-1}(1-\omega) + \omega \frac{G_{ij}\bar{\psi}_j^{l-1}}{\lambda_0^l}.\end{aligned}$$

This  $\psi_i^l$  is then used on the right hand side of the equation for the  $l^{\text{th}}$  iteration, i.e.

$$\lambda_0^{l+1} \psi_i^{l+1} = G_{ij} \bar{\psi}_j^l.$$

For the Monte Carlo eigenfunction calculation, a corresponding procedure may be defined as follows. First write a general eigenfunction strategy as in subsection (a), i.e.

$$\psi_i^{n+1} = \sum_j G_{ij}^n K^n(S_j^n).$$

After obtaining  $\psi_i^n$  from the  $(n-1)^{\text{st}}$  iteration, we define

$S_i^n$  for the  $n^{\text{th}}$  iteration as,

$$S_i^n = \bar{\psi}_i^{n-1} + \omega (\bar{\psi}_i^n - \bar{\psi}_i^{n-1}).$$

The value of the extrapolation factor,  $\omega$ , in the analytic calculation is defined by the following considerations. Let  $\Psi_i$  be a general eigenfunction of  $\lambda \Psi_i = G_{ij} \Psi_j$ . When the extrapolation procedure is used, the corresponding eigenfunction equation with eigenvalues  $\mu$  is,

$$\mu_i = \psi_i(1-\omega) + \omega \frac{G_{ij}\psi_j}{\lambda_0},$$

where  $\lambda_0$  is the fundamental mode eigenvalue, i.e.  $\lambda_0 = \lim_{\ell \rightarrow \infty} \lambda_0^\ell$ .

We may rewrite this equation as

$$\left( \frac{\mu-1+\omega}{\omega/\lambda_0} \right) \psi_i = G_{ij}\psi_j.$$

That is, the eigenfunction is the same but the eigenvalues  $\mu$  have undergone a linear transformation,

$$\mu = \omega \frac{\lambda}{\lambda_0} + 1-\omega.$$

Let  $\lambda_n$  be the eigenvalue associated with the  $n^{\text{th}}$  mode eigenfunction of  $\lambda \psi_i = G_{ij}\psi_j$ . We know that  $\lambda_0 > \lambda_1 > \lambda_2 > \dots > \lambda_n > \dots > 0$  and for large  $n$ ,  $\lambda_n \rightarrow 0$  (this is known from physical considerations; not mathematical ones). Since the fundamental mode eigenfunction error for  $\omega = 1$  and large  $\ell$  is proportional to  $\left( \frac{\lambda_1}{\lambda_0} \right)^\ell$  then we may make use of the linear transformation to reduce the size of this quantity. If  $n$  can take on large values then the optimum transformation occurs when  $\mu_1 = -\mu_n$  for  $n$  large, since in this case we will have the minimum value of  $\text{Max} \left( \frac{\mu_n}{\mu_0}, n=1,2,\dots \right)$ . The value of  $\omega$  to achieve this transformation is obtained as follows. For  $n$  large  $\mu_n \rightarrow 1-\omega(\omega > 1)$ .

Also we know that  $\mu_1 = \omega \frac{\lambda_1}{\lambda_0} + 1-\omega$ . Thus the desired  $\omega$  is given by  $\omega-1 =$

$$\omega \frac{\lambda_1}{\lambda_0} + 1-\omega \text{ or } \omega = \frac{2}{2 - \frac{\lambda_1}{\lambda_0}} \left( \frac{\lambda_1}{\lambda_0} \text{ is called the dominance ratio} \right).$$

The fundamental mode eigenfunction error for large  $\ell$  in the analytic procedure is now proportional to  $\left( \frac{\mu_1}{\mu_0} \right)^\ell = (\omega-1)^\ell = \left( \frac{\frac{\lambda_1}{\lambda_0}}{2 - \frac{\lambda_1}{\lambda_0}} \right)^\ell$  instead of  $\left( \frac{\lambda_1}{\lambda_0} \right)^\ell$ .

A series of test problems were carried out using the single linear extrapolation factor. The indices  $i$  and  $j$  refer to different fuel compositions. The values of  $\omega$  used were set by the dominance ratio as described

above and the  $w$  was applied every iteration. The test problems demonstrated that no gain in convergence rates could be obtained relative to the reference strategy. This failure occurs because the difference required in the extrapolation,  $(\bar{\Psi}_i^n - \bar{\Psi}_i^{n-1})$ , is dominated by statistical fluctuations; this happens even when only a few gross regions (i.e. compositions) are used and with as many as 2000 histories per iteration. In all tests, the source accuracy conditions were met as described in subsection (a).

In spite of the failure of the use of a single linear extrapolation factor in the reference strategy, the question still remains as to whether a more elaborate extrapolation scheme could provide a gain in Monte Carlo eigenfunction convergence rates. One of the more elaborate extrapolation schemes involves the use of multiple linear extrapolation factors, i.e. the Chebyshev polynomial scheme such as that applied in diffusion theory calculations [8]. In this scheme the above extrapolation equation,

$$\Psi_i^l = \bar{\Psi}_i^{l-1} + w \left( \frac{G_{ij} \bar{\Psi}_j^{l-1}}{\lambda_0^l} - \bar{\Psi}_i^{l-1} \right)$$

is replaced by,

$$\Psi_i^l = \bar{\Psi}_i^{l-1} + \alpha_l \left( \frac{G_{ij} \bar{\Psi}_j^{l-1}}{\lambda_0^l} - \bar{\Psi}_i^{l-1} \right) + \beta_l (\bar{\Psi}_i^{l-1} - \bar{\Psi}_i^{l-2}).$$

Here  $\alpha_l$  and  $\beta_l$  are functions of the iteration number  $l$  and of the dominance ratio  $\frac{\lambda_1}{\lambda_0}$ .

The expressions for  $\alpha_l$  and  $\beta_l$  are

$$\alpha = \frac{2}{2 - \frac{\lambda_1}{\lambda_0}}, \quad \beta_1 = 0,$$

$$\alpha_l = \frac{4}{\left(\frac{\lambda_1}{\lambda_0}\right)} \left[ \frac{\cosh [(l-1)\gamma]}{\cosh [l\gamma]} \right], \quad \beta_l = \frac{\cosh [(l-2)\gamma]}{\cosh [l\gamma]}; \quad l \geq 2,$$

where  $\gamma = \cosh^{-1} \left( \frac{2}{\left(\frac{\lambda_1}{\lambda_0}\right)} - 1 \right)$ .

Thus, if repeated applications of Chebyshev polynomials of degree one are made then the scheme is identical to the previous one with a single extrapolation factor. In general applications  $\alpha_l$  and  $\beta_l$  would approach values given by

$$\lim_{l \rightarrow \infty} \alpha_l = \frac{4}{\left( \frac{\lambda_1}{\lambda_0} \right)}, \quad \lim_{l \rightarrow \infty} \beta_l = 1. \quad \text{It is now clear that if the use of}$$

the single extrapolation factor fails because of statistical fluctuations in the difference

$$\left( \frac{G_{ij} \psi_j^{l-1}}{\lambda_0^l} - \psi_i^{l-1} \right),$$

then the Chebyshev polynomial approach must fail also (it will fail all the more because  $\alpha_l > 0$ ).

In rejecting both of the above extrapolation schemes for Monte Carlo calculations, we have rejected successful schemes for analytic calculations. One still might raise the question as to whether an extrapolation scheme could be devised for Monte Carlo that could overcome the difficulties caused by statistical fluctuations. In attempting to answer this question, it is convenient to use some concepts from information theory. First, however, let us recall that the Chebyshev polynomial scheme originated by asking the following question: Is it possible when forming  $\psi^l$  for the  $l^{\text{th}}$  iteration to take as the value of  $\psi^l$  a linear combination of  $\psi^l$  and all previous  $\psi$ 's and thereby accelerate convergence? That is, if we write

$$\psi^l = \sum_{n=0}^l a_{ln} \psi^n, \quad \text{then can we choose constants } a_{ln}, \text{ independent of source}$$

guess, such that this  $\psi^l$  is closer to the fundamental mode eigenfunction? The answer is yes, and although the  $a_{ln}$  are not obtained explicitly, the resulting procedure is the three-term Chebyshev polynomial extrapolation described above.

There is an analogous question we may ask when considering a Monte Carlo eigenfunction procedure, and as stated earlier it can be developed using some notation from information theory. Let the eigenfunction estimate from the  $l^{\text{th}}$  iteration be written as,  $\psi^l = S^l + N^l$ , where  $S^l$  represents a wanted signal from the  $l^{\text{th}}$  iteration and  $N^l$  is a random noise. Consider now a prediction of the eigenfunction at iteration  $l+n$ , say  $\hat{S}^{l+n}$ , written as a linear combination of  $\psi^m$ ,  $m=1, \dots, l$ . That is:

$$\hat{S}^{l+n} = \sum_{m=1}^l h_m \psi^{l-m+1},$$

where the constants  $h_m$  are to be chosen such that  $\hat{S}^{l+n}$  is closer in some sense to the fundamental mode eigenfunction. Here the  $h_m$  are called a linear filter. The problem of finding an optimum linear filter has been considered by N. Wiener [9]. In particular, he solves for  $h_m$  which will minimize

$$E \left\{ [S^{\ell+n} - \hat{S}^{\ell+n}]^2 \right\},$$

where  $E$  denotes expected value. What is required then, is an extension of the linear filter approach which will have the property that if the noise approaches zero (i.e. number of histories per iteration becomes large), then the  $h_m$ 's become similar to those that are obtained from the Chebyshev polynomial approach. If the signal is constant (i.e. a fixed source problem), then clearly minimum variance will occur for  $\hat{S}^{\ell+n}$  if the  $h_m$ 's are proportional to the number of histories in  $\psi^{\ell-m+1}$ .

Initial iterations, with on the order of 500 histories each, will be closer to the latter case than to the former. That is, the initial iterations will be more like constant signal with random noise than like variable signal with zero noise. But the reference strategy already weighs iteration results by the number of histories per iteration. Of course, the noise to signal ratio does diminish with increasing iteration number because of the increasing number of histories per iteration.

If the above extension of linear filter theory were obtained, its use might not result in large gains in Monte Carlo eigenfunction convergence rates; nevertheless this approach has some promise [10], but is outside the scope of this study.

#### d. Source Strategies Using Importance Sampling

Importance sampling offers a general means of reducing the Monte Carlo uncertainty in a specified neutron reaction rate. For example, if an approximate solution of the adjoint transport equation is known, where the adjoint source is the space-energy dependent cross section for the desired reaction rate, then one may alter the frequency distribution functions in the normal Monte Carlo process (and introduce weights to retain a fair game) in such a way that the standard deviation for the desired reaction rate is decreased per history. As the approximate adjoint solution approaches the true adjoint solution, this standard deviation per history approaches zero; if the approximate solution becomes too crude, the standard deviation can become larger than that from a normal Monte Carlo calculation.

In addition to the difficulty of obtaining a sufficiently accurate approximate solution of the adjoint transport equation, the importance sampling approach described above has another serious drawback. Namely, one may choose only one neutron reaction rate per calculation to be obtained with small standard deviation. In general, importance sampling may be viewed as a process where the reduction of variance for a reaction of interest is obtained at the cost of increasing the variance for other reactions. Thus, such a process would not be generally acceptable when attempting to obtain the eigenfunction shape by Monte Carlo.

However, one may still raise the question as to whether there are importance sampling techniques that could significantly improve the definition of the overall eigenfunction shape by reducing the ratio of the source shape uncertainty to the statistical uncertainty and by reducing the total

uncertainty. A definitive answer to this question is outside the scope of this study, but the answer is conjectured to be no. For example, consider the following limited form of importance sampling, a form that may be called "source" importance sampling. Start with the observation that neutrons from the high energy part of the fission spectrum are more important in determining overall eigenfunction shape than those from the low energy part. Thus, source importance sampling that would start more neutrons at high energy (with adjusted weights to retain the proper source spectrum) could result in some reduction of source shape uncertainty, but would increase statistical uncertainty because of the non-constant starting weights. Intuitively, we feel that such a process could not result in a significant reduction of total eigenfunction uncertainty.

More generally, several specialized forms of importance sampling are frequently available for fixed source problems that could be used in eigenfunction calculations. These are available in splitting and Russian Roulette. Such forms of importance sampling have not been used in test calculations because again we intuitively believed that significant reductions in total eigenfunction uncertainty would not occur. An exception, which is used routinely in eigenfunction calculation, is Russian Roulette in the thermal group in large water reflectors.

### 3. A Reference Strategy

In the preceding subsections, we have discussed several possible source strategies including a reference strategy, ie. the straight analog of the analytic power method with an increasing number of histories per iteration. The strategies discussed include: 1) those using a Green's function approach, 2) those using extrapolation factors, and 3) those using importance sampling. The test calculations performed in this study did not reveal any strategy superior to a reference strategy, which will be described. Also from this study, the approach that has been deemed most likely to offer some improvement in Monte Carlo eigenfunction convergence rates relative to the reference strategy is the extension of linear filter theory discussed in subsection (c); but, as stated earlier, this is beyond the scope of this work.

Some important operational details of the reference strategy are as follows: Because all neutrons in a given iteration are processed through an energy group before proceeding to the next energy group, then the calculational time per history becomes shorter if the problem has fewer iterations with more histories per iteration. On the other hand, it is desirable in an eigenfunction calculation to have as many iterations as possible. Thus, reducing the number of histories as far as possible without losing too much machine efficiency in initial iterations led the authors to adopt 500 as the minimum number of histories per iteration. Because of correlated sampling, it is desirable that all eigenfunction problems have the same number of histories per iteration.

The reference strategy uses an increase of 10 histories per iteration in successive iterations. Thus in the  $N^{\text{th}}$  iteration, the number of histories per iteration would be  $500 + 10N$  and the total number of histories through the  $N^{\text{th}}$  iteration would be  $500N + 5N(N+1)$ .

The rate of increase of 10 histories per iteration was arrived at as follows: From the work of Lieberoth [11], it is known that the eigenfunction error that results from an infinite number of power iterations, each with a constant number of histories per iteration, decreases as  $\frac{1}{N}$ . Thus, the desire to keep the total number of iterations as large as possible for a fixed total number of histories, and at the same time to insure a reasonable removal rate for the eigenfunction error that would result from a fixed number of histories, led the authors to adopt the rate increase of 10 histories per iteration. From the discussion of this error removal in Ref. [1], it is evident that this error will tend to cause the approach to the eigenfunction to be on the side in which there is some power shift toward regions of low  $k_{\infty}$ , and that the eigenvalue will tend to converge from below rather than above. However, calculations for realistic types of reactors have not shown such a discernible trend. This suggests, for realistic calculations, that in general such a component of the source shape uncertainty is small relative to the statistical uncertainty.

There is one final important operational detail connected with the eigenfunction strategy adopted; the procedure to be used to obtain an estimate of the total eigenfunction uncertainty. The remainder of this report will deal with arriving at such a procedure.

### III. EIGENFUNCTION UNCERTAINTY

This section presents the arguments that led to a formula for total eigenfunction uncertainty for the strategy adopted. As in previous sections, it will again be convenient to consider the overall strategy as composed of the same two parts. That is, the first part is the totality of the Monte Carlo procedures that would be involved in a fixed source calculation; the uncertainties in this part are called statistical. The second part is the eigenfunction source strategy that connects successive generations; the uncertainties in this part are called source shape uncertainties. It is obvious that in any eigenfunction calculation, the uncertainties from these two parts are connected. However, this breakdown is convenient here simply because uncertainties that arise from fixed source calculations are very easily obtained and are an integral part of all fixed source Monte Carlo calculations. Some insights as to the nature of the source shape uncertainties can be obtained by considering some properties of the statistical uncertainties. This is done in subsection (a). Subsection (b) formalizes these observations through use of serial correlation coefficients and arrives at a formula for total eigenfunction uncertainty by a modification of an approach proposed by D. B. MacMillan. Because the overall formula for eigenfunction uncertainty is partly empirical, subsection (c) then gives some results of its verification by numerical testing.

#### a. Some Properties of the Statistical Uncertainties

There are two commonly used methods in Monte Carlo to provide estimates of statistical uncertainties. The first is a variance calculation based on a history by history basis; i.e. each experiment is taken to be one history. This estimate is an accurate estimate of the purely statistical uncertainty, since it yields the identical result that one would obtain from a



hypothetical fixed source problem where the total sampling from the fixed source yields the total set of source sites from all iterations in the eigenfunction calculation.

The second estimate of statistical uncertainty that is commonly used appears superficially to be a correct combination of source shape uncertainty and statistical uncertainty. This estimate is that obtained from a variance calculation on an iteration by iteration basis. This estimate appears to include the source shape uncertainty, because within the power method the iteration source change is by iteration. However, test calculations which compare these two estimates of uncertainty have shown that their magnitudes are reasonably close to each other. Since the first estimate is without question the purely statistical uncertainty, then we must consider the second estimate the same uncertainty as the first.

The above observations suggest the following argument. Since the uncertainty calculation on an iteration by iteration basis does sense the changing source shape, this uncertainty could be of the same magnitude as the statistical uncertainty only if there exists a correlation among iteration source shapes such that there is almost a cancellation of the source shape component of uncertainty. But the existence of such a correlation suggests that asymptotically (i.e. after a large number of iterations) the source shape uncertainty is some constant times the statistical uncertainty. Stated differently, after a large number of iterations we can visualize that the sampling of possible source shapes lags behind the sampling of possible neutron production shapes based on these source shapes, and that the ratio of sampling rates tends to some constant.

Of course, the above argument, which suggests that the ratio of source shape and statistical uncertainties tends to a constant for a large number of iterations, is of little value unless the magnitude of this constant can be estimated. This ratio strongly depends on the type of quantity being edited in the Monte Carlo calculation; for example, let us consider the region dependence of the ratio for neutron production rates. If the region size starts to approach the whole reactor, then because the neutron production shape error will most likely consist of the lower overtones which will roughly integrate to zero, the ratio of source shape and statistical uncertainty decreases. Stated differently, there are negative correlations among neutron production rates over some large subregions of a reactor. At the other extreme of a region size becoming small, it is obvious that again the ratio of source shape and statistical uncertainties decreases. Thus, one concludes that the ratio becomes a maximum for some intermediate sized region.

An early approach taken by the authors for obtaining the asymptotic source shape uncertainty was to obtain a maximum ratio of source shape and statistical uncertainties from test calculations and use this constant universally [12]. Thus, in practice we computed the usual statistical uncertainty, and applied a constant multiplicative factor to obtain the source shape uncertainty. When continuing calculations revealed that this factor was greater than 10 for some edit quantities, this approach was dropped since it would force unreasonable conservatism in the uncertainties for most edit quantities.

b. Eigenfunction Uncertainty Using Serial Correlation

The conjecture of the previous subsection, that in the asymptotic range the source shape uncertainty is some constant times the statistical uncertainty, may be formalized as follows: Let  $x_n$  be an estimate of some neutron reaction rate from iteration  $n$  in an eigenfunction calculation. Accumulating iteration results for  $N$  iterations yields the Monte Carlo estimate of this reaction rate, say  $R_N$ , where

$$R_N = \sum_{n=1}^N a_n x_n,$$

where  $a_n = \frac{N_n}{\sum_{n=1}^N N_n}$ , and  $N_n$  is the number of neutron histories in iteration  $n$ .

As discussed in Section II, the eigenfunction strategy insures that  $\text{PLim}_{N \rightarrow \infty} R_N$  is the transport theory value of the reaction rate. Following a well-known derivation using expected value notation, we may write

$$\sigma^2(R_N) = E [R_N - E(R_N)]^2.$$

Let  $\mu_n = E(x_n)$ , then we have

$$\begin{aligned} \sigma^2(R_N) &= E [a_1(x_1 - \mu_1) + \dots + a_N(x_N - \mu_N)]^2 \\ &= \sum_{n=1}^N (a_n^2 E(x_n - \mu_n)^2) + 2 \sum_{n < m} a_n a_m E[(x_n - \mu_n)(x_m - \mu_m)]. \end{aligned}$$

But  $\sigma^2(x_n) = E(x_n - \mu_n)^2$ , and the correlation coefficient between  $x_n$  and  $x_m$ , say  $\rho_{nm}$ , is defined by,

$$\rho_{nm} \sigma(x_n) \sigma(x_m) = E[(x_n - \mu_n)(x_m - \mu_m)],$$

Thus we may write,

$$\sigma^2(R_N) = \sum_{n=1}^N \left( a_n^2 \sigma^2(x_n) + 2 \sum_{n < m} a_n a_m \rho_{nm} \sigma(x_n) \sigma(x_m) \right).$$

Let  $\sigma_S^2(R_N)$  be the purely statistical component of variance for  $R_N$ , after  $N$  iterations; then in the asymptotic range we must have

$$\sigma^2(x_n) = \frac{1}{a_n} \sigma_s^2(R_N).$$

We may write

$$\sigma^2(R_N) = \sigma_s^2(R_N) \left[ 1 + 2 \sum_{n=1}^N \sum_{n < m} \sqrt{a_n} \sqrt{a_m} \rho_{nm} \right].$$

Now if the source shape uncertainty is some constant times the statistical uncertainty, then this only implies that

$$\text{PLim}_{N \rightarrow \infty} \left[ \sum_{n=1}^N \sum_{n < m} \sqrt{a_n} \sqrt{a_m} \rho_{nm} \right] \text{ exists. However, if the}$$

number of histories per iteration were a constant, that is,  $a_n = a_m = \frac{1}{N}$ , then it is also obvious that in the asymptotic range the correlation coefficient,  $\rho_{nm}$ , is a function only of the difference in  $n$  and  $m$ . The expectation that this should be true even when the number of histories per iteration increases with iteration number has been verified by test calculations. Thus, if we set  $k = n - m$ , then we may write

$$\rho_{nm} = \rho_k,$$

where  $\rho_k$  is called the serial correlation coefficient of lag  $k$ .

The expression for  $\sigma^2(R_N)$  now becomes

$$\sigma^2(R_N) = \sigma_s^2(R_N) \left[ 1 + 2 \sum_{k=1}^{N-1} \left( \sum_{n=1}^{N-k} \sqrt{a_n} \sqrt{a_{n+k}} \rho_k \right) \right].$$

Let us define

$$A = \sum_{k=1}^{N-1} \left( \sum_{n=1}^{N-k} \sqrt{a_n} \sqrt{a_{n+k}} \rho_k \right).$$

We may note in passing, that if we assume that the purely statistical uncertainty and source shape uncertainty are independent, then  $\sqrt{2A} \sigma_s(R_N)$  is the magnitude of the source shape uncertainty.

Attempts by the authors to use the above expression for  $\sigma^2(R_N)$  in test eigenfunction calculations did not prove to be workable. For example, for some edit quantities the series that defines  $A$  was slowly converging, and the  $\rho_k$  involved appeared erratic for larger values of  $k$  even after a few hundred iterations. Also, there are practical difficulties in this approach because of the machine storage requirements in obtaining a large number of serial

correlation coefficients for every edit quantity.

A workable alternative to this approach was proposed by D. B. MacMillan [13]. He proposed that only the serial correlation coefficient of lag 1 be calculated explicitly and that those of higher lags be inferred. He argues on a physical basis that an upper bound on the value of  $\rho_k$  may be obtained by writing

$$\rho_k = \rho_1 \left( \frac{\lambda_1}{\lambda_0} \right)^{k-1},$$

where  $\frac{\lambda_1}{\lambda_0}$  is the dominance ratio.

Test calculations by MacMillan as well as subsequent tests by the authors have shown that this argument is sound. Thus with MacMillan's approach we have upper estimates for all  $\rho_k$  once we have estimated  $\rho_1$  and supplied a value of  $\frac{\lambda_1}{\lambda_0}$ . We will now consider Lim A with values of  $\rho_k$  obtained from

MacMillan's conjecture. Because of the fixed increase in number of histories per iteration, we may write

$$\lim_{N \rightarrow \infty} \sum_{n=1}^{N-k} \sqrt{a_n} \sqrt{a_{n+k}} = 1$$

for any value of  $k$ . Thus we have

$$\lim_{N \rightarrow \infty} A = \sum_{k=1}^{\infty} \rho_k = \rho_1 \sum_{k=1}^{\infty} \left( \frac{\lambda_1}{\lambda_0} \right)^{k-1} = \frac{\rho_1}{1 - \left( \frac{\lambda_1}{\lambda_0} \right)}$$

MacMillan's formula for total eigenfunction uncertainty in reaction rate  $R_N$  becomes

$$\sigma(R_N) = \sigma_s(R_N) \sqrt{1 + \frac{2\rho_1}{1 - \left( \frac{\lambda_1}{\lambda_0} \right)}}.$$

A modification of this approach for estimating  $\sigma(R_N)$  was developed by the authors for two reasons. First, the above approach requires supplying the dominance ratio, which is not always easy to obtain. Second, test calculations reveal that the estimated  $\sigma(R_N)$  is conservative if  $\rho_1$  is small in a core with large  $\frac{\lambda_1}{\lambda_0}$ . Recall from the discussion in subsection (a) that we

can expect, for a core with a given dominance ratio, there will be reaction rates for which the ratio of source shape and statistical uncertainties will be a maximum and hence  $\rho_1$  will be a maximum. Further, this maximum value of

$\rho_1$  will increase as  $\frac{\lambda_1}{\lambda_0}$  increases. The authors concluded by test calculations that MacMillan's formula is not overly conservative in its estimate of  $\sigma(R_N)$  for reaction rates for which  $\rho_1$  is a maximum. These same test calculations have revealed that for reaction rates for which  $\rho_1$  is much less than its maximum value, the values of  $\rho_k$  decline with increasing  $k$  more like  $\rho_1^{k-1}$  than like  $\left(\frac{\lambda_1}{\lambda_0}\right)^{k-1}$ . That is,

$$\rho_k = \rho_1(\rho_1)^{k-1} \text{ (for small } \rho_1 \text{).}$$

This would lead to

$$\lim_{N \rightarrow \infty} A \approx \frac{\rho_1}{1 - \rho_1} \text{ (for small } \rho_1 \text{).}$$

But since the maximum value of  $\rho_1$  depends on  $\frac{\lambda_1}{\lambda_0}$ , we may hopefully scale this expression such that we obtain a reasonable value of  $\lim_{N \rightarrow \infty} A$  for the maximum value of  $\rho_1$ . This scale factor was empirically determined to be about 5. Thus we have

$$\lim_{N \rightarrow \infty} A \approx \frac{5\rho_1}{1 - \rho_1} \text{ (for maximum } \rho_1 \text{).}$$

We may now linearly connect the values of  $\lim_{N \rightarrow \infty} A$  for maximum  $\rho_1$  and for small  $\rho_1$  at the values  $\rho_1 = 1$  and  $\rho_1 = 0.2$  by writing

$$\lim_{N \rightarrow \infty} A \approx \frac{5\rho_1^2}{1 - \rho_1}.$$

This gives an alternate formula for  $\sigma(R_N)$ , i.e.

$$\sigma(R_N) = \sigma_S(R_N) \sqrt{1 + \frac{10\rho_1^2}{1 - \rho_1}}.$$

As a result of test calculations which will be described in the next subsection, this formula for  $\sigma(R_N)$  was adopted.

### c. Numerical Testing of Formula for Total Eigenfunction Uncertainty

The formula for total eigenfunction uncertainty in a reaction rate  $R_N$  is given in the previous subsection as

$$\sigma(R_N) = \sigma_S(R_N) \sqrt{1 + \frac{10\rho_1^2}{1 - \rho_1}},$$

where  $\sigma_s(R_N)$  is the purely statistical standard deviation, and  $\rho_1$  is the serial correlation coefficient of lag 1. Some details of the calculational steps are as follows: If the estimate of the reaction rate  $R_N$  is given by

$$R_N = \sum_{n=1}^N a_n x_n,$$

then the purely statistical variance  $\sigma_s^2(R_N)$  is given by

$$\sigma_s^2(R_N) = \frac{1}{N} \sum_{n=1}^N a_n (x_n - R_N)^2.$$

Since for convenience we desire to use the above  $R_N$  and  $\sigma_s^2(R_N)$  in obtaining  $\rho_1$ , we may introduce the number of histories per iteration,  $N_n$ , as weights in the definition of  $\rho_1$  as follows:

$$\rho_1 = \frac{1}{N\sigma_s^2(R_N)} \sum_{n=2}^N \sqrt{a_{n-1}'} \sqrt{a_n''} (x_{n-1} - R_N')(x_n - R_N'')$$

$$\text{where } a_{n-1}' = \frac{N_{n-1}}{\sum_{n=2}^N N_{n-1}}, \quad a_n'' = \frac{N_n}{\sum_{n=2}^N N_n}$$

$$R_N' = \sum_{n=2}^N a_{n-1}' x_{n-1},$$

$$R_N'' = \sum_{n=2}^N a_n'' x_n.$$

By making use of the approximations

$$R_N' \approx \sum_{n=2}^N \sqrt{a_{n-1}'} \sqrt{a_n''} x_{n-1} \left( \frac{1}{\sum_{n=2}^N \sqrt{a_{n-1}'} \sqrt{a_n''}} \right),$$

$$\text{and } R_N'' \approx \sum_{n=2}^N \sqrt{a_{n-1}'} \sqrt{a_n''} x_n \left( \frac{1}{\sum_{n=2}^N \sqrt{a_{n-1}'} \sqrt{a_n''}} \right),$$

we obtain the expression used, that is

$$\rho_1 = \frac{1}{N\sigma_S^2(R_N)} \left[ \left( \sum_{n=2}^N \sqrt{a_{n-1}'} \sqrt{a_n''} x_{n-1} x_n \right) - \left( R_N' R_N'' \sum_{n=2}^N \sqrt{a_{n-1}'} \sqrt{a_n''} \right) \right].$$

The eigenfunction test calculations may be described as follows: The cross sections and fixed source procedures are such that a zero variance results in an infinite medium calculation. In particular, the cross sections are energy independent and purely absorbing. The Monte Carlo eigenfunction calculations were performed for a series of eight slab cores with dominance ratios ranging from 0.36 to 0.995. Although the dominance ratio,

$\frac{\lambda_1}{\lambda_0}$ , is not required in the uncertainty formula adopted, it is estimated

for each of the slab cores in the following manner: The neutron flux distribution, say  $\varphi(x)$ , due to a plane unit source at  $x=0$  in an infinite purely absorbing medium with constant cross section is given by  $\varphi(x) = \frac{1}{2} E_1(\Sigma|x|)$ .

The neutron flux age,  $J$ , is then  $\frac{1}{3\Sigma^2}$ .

Using well known results from two-group diffusion theory, we may write the  $n^{\text{th}}$  mode eigenvalue as proportional to  $\frac{1}{1+JB_n^2}$ , where  $B_n^2$  is the geometric buckling for the  $n^{\text{th}}$  mode eigenfunctions. For a slab reactor,  $B_0^2 = \left(\frac{\pi}{H}\right)^2$  and  $B_1^2 = \left(\frac{2\pi}{H}\right)^2$ , where  $H$  is the effective slab width, given as the actual slab width plus twice the extrapolation distance. The extrapolation distance may be taken as  $\frac{2}{3\Sigma}$ . Thus the dominance ratio may be estimated as

$$\frac{\lambda_1}{\lambda_0} = \frac{1 + \frac{1}{3} \left(\frac{\pi}{H\Sigma}\right)^2}{1 + \frac{1}{3} \left(\frac{2\pi}{H\Sigma}\right)^2}.$$

For each slab core calculated, 17 different region edits of the neutron production rate were obtained and compared to accurate production rates. The 17 regions are: 2 symmetrically placed slab regions of volume fraction 0.01 each, 10 uniform slabs of volume fraction 0.1 each, 2 symmetrically placed slab regions of volume fraction 0.3 each, 2 symmetrically placed slab regions of volume fraction 0.3 each, 2 symmetrically placed slab regions of volume

fraction 0.5 each, and the whole core. The accurate production rates were obtained by averaging results in symmetrically placed regions after 400 iterations and a total of  $10^6$  histories. In all calculations, the source guess accuracy requirement was met as discussed in subsection (b) of Part II.

The eigenfunction uncertainties for the five different sizes of regions, in each of the eight cores, are tabulated at multiples of 50 iterations up to 250 iterations in Table I. The eigenfunction uncertainties are tabulated using naively the purely statistical standard deviation as well as using the standard deviation obtained with the formula. The method of uncertainty tabulation is by use of a figure of merit,  $f_m$ . For example, the figure of merit for the regions of size 0.1 is the number of the ten regions with a neutron production rate error greater than one probable error, plus the number of the ten regions with an error greater than two probable errors, etc. to an infinite sum. Thus, in this case the expected figure of merit,  $\bar{f}_m$ , is 7.58. A value much greater than this indicates that the uncertainty estimates are too small, and a smaller value indicates a conservative estimate. Shown in Table I is the expected figure of merit plus  $2\sigma$ . An acceptable means of estimating eigenfunction uncertainties is defined to be one with a figure of merit less than this.

Table I shows that for a very small core,  $\frac{\lambda_1}{\lambda_0} = .36$ , an acceptable estimate of uncertainties is provided by the purely statistical standard deviation, and that the formula gives only a slightly more conservative result. As the cores become larger, we see that the purely statistical estimate of uncertainty becomes, in general, unacceptable, whereas the formula gives acceptable results. We may note that in the special case of the neutron production over the whole core, i.e. the eigenvalue, the purely statistical standard deviation for all cores is acceptable and that the formula gives essentially the same standard deviation. For the case of the largest core,  $\frac{\lambda_1}{\lambda_0} = .995$ , the unacceptable results from the formula when the number of iterations is 50 or 100 is because the magnitude of the serial correlation coefficient,  $\rho_1$ , is not reasonably estimated for a large core unless more than 100 iterations are performed. Although more than 100 iterations appears to be necessary to obtain acceptable eigenfunction shape uncertainties, this is not required if only an acceptable eigenvalue uncertainty is desired.

One final observation will be made concerning the approach of an estimated Monte Carlo eigenfunction shape to the true eigenfunction shape. When viewing an accumulation by iteration of a neutron reaction rate, one almost naturally looks for an oscillation about the true reaction rate as the number of iterations increases. Of course this tendency also exists when viewing a fixed source calculation. The properties of accumulated results by iteration in a fixed source calculation are those of the classical random walk problem. W. Feller [14] points out that in such a problem, the most probable number of times that the estimated reaction rate crosses the true reaction rate is zero, and that zero times is more probable than one time, etc. Further, the mean number of iterations between crossings approaches infinity as the number of iterations increases.

These same properties exist in a somewhat more severe form in a Monte Carlo eigenfunction calculation even though the number of histories increases



with increasing iteration number. This is because of the positive correlation between successive iteration reaction rates. Thus, if the neutron source shape at one iteration tends to make a single iteration reaction rate too high, then more likely than not the source shape of the next iteration will tend to make the next single iteration reaction rate too high. In contrast, for a fixed source calculation, each single iteration result, assuming a symmetrical frequency distribution function, is equally likely to be above or below the true reaction rate. By analogy to the classical random walk problem, we conclude for the eigenfunction calculation that the mean number of iterations between crossings of the estimated and true reaction rates approaches infinity as the number of iterations increases.

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APPENDIX

As discussed in Section II, the strategy adopted is an analog of the analytic power method, with an increasing number of histories per iteration. A question that naturally arises is whether neutron weights could be introduced in an analog of the power method with a fixed number of histories per iteration so as to make it a fair game. This appendix gives a procedure for doing this and a proof that the result is a fair game.

We know from Section II.a that the equation describing the analog of the power method with an increasing number of histories per iteration, i.e.

$$\psi_i^{n+1} = \sum_j G_{ij}^n K^n (\psi_j^n)$$

results in the analytic transport equation,

$$\psi_i = \sum_j G_{ij} \bar{\psi}_j,$$

upon taking the P Lim as  $n \rightarrow \infty$ .

Suppose now we have a system that is supercritical and follow all progeny such that the number of histories increases with iteration number (continuation of the Markov process must be assured as discussed in Section II.a. This process may be represented in a power method analog with a fixed number of histories per iteration by the use of weights as follows: Let  $k_n$  be the multiplication factor for the  $n^{\text{th}}$  iteration, i.e. the total neutron production divided by the total starting weight in the  $n^{\text{th}}$  iteration. Then the supercritical process could be represented by having the weight for iteration  $n$ , say  $W_n$  determined by  $W_0 = 1$ ,  $W_n = \prod_{i=0}^{n-1} k_i$ . Suppose for the moment there are no statistical fluctuations in the multiplication factor  $k_n$ , then asymptotically ( $n$  large)  $k_n$  becomes a constant, say  $\bar{k}$ . In this case the weight  $W_n$  will have an exponential increase, i.e., we may write  $W_{n+1} = \bar{k}^n = e^{\alpha n}$  where  $\alpha = \ln \bar{k}$ . With such a weighting, the effective number of histories contributing to any estimated reaction rate remains finite as  $n$  increases and hence the process cannot be a fair game. This is easily seen by observing that the effective number of histories contributing to a reaction rate is proportional to the mean value of  $n$  for a fixed number of histories per iteration; that is the mean value of  $n$ , say  $\bar{n}$ , over previous iterations up to iteration  $N$ . But,

$$\bar{n} = \int_0^N e^{\alpha(N-n)} (N-n) dn = \frac{1}{\alpha^2} [1 - e^{-\alpha N}(\alpha N + 1)],$$

and

$$\lim_{N \rightarrow \infty} \bar{n} = \frac{1}{\alpha^2};$$

hence the effective number of histories contributing to a reaction rate is finite as  $N \rightarrow \infty$  (of course the same occurs in a subcritical reactor).

If we did not have statistical fluctuations in the asymptotic multiplication factor  $\bar{k}$ , then a scaling of  $\nu$  (neutrons per fission) such that  $\bar{k} = 1$  and hence  $\alpha = 0$  will produce the basic requirement that the effective number of histories contributing to a reaction rate approaches  $\infty$  as  $N \rightarrow \infty$ . In this case the weight  $W_n$  would be,

$$W_n = \frac{\prod_{i=0}^{n-1} k_i}{(\bar{k})^{n-1}}.$$

Because of the statistical fluctuations in  $k_i$ , the estimated multiplication factor for iteration  $i$ , caused by a finite number of histories in the Monte Carlo calculation, a reactor that is just critical as defined by the analytic transport equation is subcritical in reality and the neutron density will approach zero as the iterations approach  $\infty$  (this also occurs in a real reactor). This may be easily seen as follows: A reactor that is just critical mathematically (i.e. continuous neutron density in the linear transport equation) will meet the condition:

$$\text{Plim}_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N k_i = 1.$$

We may write  $k_i = 1 - \Delta_i$  where  $\Delta_i$  are the statistical fluctuations and assume without loss of generality

$$\sum_{i=1}^N \Delta_i = 0.$$

The amplitude of the spatially integrated neutron density after  $N$  iterations is then proportional to

$$\prod_{i=1}^N k_i.$$

We may write

$$\prod_{i=1}^N (1-\Delta_i) = 1 - \sum_{i=1}^N \Delta_i + \Delta_1 \left( \sum_{i=2}^N \Delta_i \right) + \Delta_2 \left( \sum_{i=3}^N \Delta_i \right) + \dots + O(\Delta^3).$$

Making use of

$$(\Delta_1 + \Delta_2 + \dots + \Delta_N)^2 = \Delta_1^2 + \Delta_2^2 + \dots + \Delta_N^2 + 2\Delta_1 \left( \sum_{i=2}^N \Delta_i \right) + 2\Delta_2 \left( \sum_{i=3}^N \Delta_i \right) + \dots,$$

we may write

$$\prod_{i=1}^N (1-\Delta_i) = 1 - \frac{1}{2} \left[ \sum_{i=1}^N \Delta_i^2 \right] + O(\Delta^3) < 1.$$

Hence it is clear that the expected neutron density amplitude will approach zero as  $N \rightarrow \infty$ . The degree of supercriticality required to keep the expected neutron density amplitude at a constant for a large number of generations,  $N$ , in a reactor with finite neutron density, is obtained by scaling  $\nu$  by

$$\frac{1}{\left( \prod_{i=1}^N k_i \right)^{\frac{1}{N}}}.$$

Thus the desired neutron weight at iteration  $n$  in a problem with a total of  $N$  iterations is given by

$$W_n(N) = \frac{\prod_{i=1}^{n-1} k_i}{K^{n-1}}, \text{ where } K = \left( \prod_{i=1}^N k_i \right)^{\frac{1}{N}}.$$

(This weighting was first suggested by D. B. MacMillan, private communication).

The proof that the use of the above weight,  $W_n(N)$ , in the Monte Carlo process produces a fair game may be summarized as follows: Using the definitions of Section II.a, we may write the Monte Carlo process as

$$\psi_i^{n+1} = \sum_j G_{ij}^n W_n(N) K^n (\psi_j^n).$$

Summing both sides of this equation over  $n$ , we have

$$\frac{1}{N} \sum_{n=1}^N \psi_i^{n-1} = \sum_j \left[ \frac{\sum_{n=1}^N G_{ij}^n W_n(N) K^n(\psi_j^n)}{\sum_{n=1}^N W_n(N) K^n(\psi_j^n)} \right] \frac{1}{N} \sum_{n=1}^N W_n(N) K^n(\psi_j^n).$$

The quantity in the parenthesis above is simply a weighted average of the estimated neutron production in elementary volume  $i$  due to a neutron born in elementary volume  $j$ ; hence, its PLim as  $N \rightarrow \infty$  is the analytic neutron production Green's function  $G_{ij}$ . All that is additionally required to show that the above equation reduces to the analytic transport equation,

$$\psi_i = \frac{1}{\lambda} \sum_j G_{ij} \psi_j, \text{ where } \psi_i = \text{PLim}_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \psi_i^{n+1}$$

is to show that

$$\text{PLim}_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N W_n(N) K^n(\psi_j^n) = \text{PLim}_{N \rightarrow \infty} \frac{1}{\lambda} \frac{1}{N} \sum_{n=1}^N \psi_j^{n+1},$$

where

$$\lambda = \frac{\text{PLim}_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \sum_i \psi_i^{n+1}}{\text{PLim}_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N W_n(N)}.$$

The desired result is immediately obtained by recognizing that the product,  $W_n(N)$  times the sampling operator  $K^n$ , defines simply a Russian Roulette operator.

The weights  $W_n(N)$  and a fixed number of histories per iteration were not used, since the weight for the  $n^{\text{th}}$  iteration continually changes as the total number of iterations increases, thereby destroying the ability to use accumulative counters for internal editing of reaction rates (this difficulty would not exist for post editing).

TABLE I

## Slab Core Eigenfunction Uncertainties

Values of $f_m$ for $\frac{\lambda_1}{\lambda_0} = .36$													
Region Data		No. of Iterations										$\bar{f}_m$	$\bar{f}_m + 2\sigma$
No.	Fract. Size	50		100		150		200		250			
		Stat.	For	Stat.	For	Stat.	For	Stat.	For	Stat.	For		
2	.01	1	1	1	1	2	2	3	3	1	1	1.51	4.44
10	.1	10	9	9	8	12	12	5	5	10	10	7.58	14.12
2	.3	1	1	2	2	3	3	0	0	1	1	1.51	4.44
2	.5	0	0	2	2	3	3	1	1	1	1	1.51	4.44
1	1.0	0	0	1	1	1	1	1	1	1	1	.76	2.82

  

Values of $f_m$ for $\frac{\lambda_1}{\lambda_0} = .68$													
Region Data		No. of Iterations										$\bar{f}_m$	$\bar{f}_m + 2\sigma$
No.	Fract. Size	50		100		150		200		250			
		Stat.	For	Stat.	For	Stat.	For	Stat.	For	Stat.	For		
2	.01	1	1	0	0	2	2	2	2	3	3	1.51	4.44
10	.1	10	4	10	6	16	9	15	9	13	7	7.58	14.12
2	.3	2	0	2	0	4	1	5	2	5	2	1.51	4.44
2	.5	1	0	0	0	1	0	1	0	5	2	1.51	4.44
1	1.0	1	1	1	1	0	0	0	0	0	0	.76	2.82

  

Values of $f_m$ for $\frac{\lambda_1}{\lambda_0} = .84$													
Region Data		No. of Iterations										$\bar{f}_m$	$\bar{f}_m + 2\sigma$
No.	Fract. Size	50		100		150		200		250			
		Stat.	For	Stat.	For	Stat.	For	Stat.	For	Stat.	For		
2	.01	2	0	0	0	1	1	0	0	1	1	1.51	4.44
10	.1	13	6	19	7	17	6	13	6	17	8	7.58	14.12
2	.3	3	0	4	1	6	1	3	1	6	1	1.51	4.44
2	.5	0	0	6	0	1	0	0	0	1	0	1.51	4.44
1	1.0	0	0	1	1	2	2	1	1	1	1	.76	2.82

TABLE I - (Cont'd)

Values of $f_m$ for $\frac{\lambda_1}{\lambda_0} = .92$													
Region Data		No. of Iterations										$\bar{f}_m$	$\bar{f}_m + 2\sigma$
No.	Fract. Size	50		100		150		200		250			
		Stat.	For	Stat.	For	Stat.	For	Stat.	For	Stat.	For		
2	.01	4	3	7	6	4	3	4	4	5	4	1.51	4.44
10	.1	16	6	28	13	27	11	38	14	33	10	7.58	14.12
2	.3	12	3	19	6	21	6	25	7	10	1	1.51	4.44
2	.5	9	2	16	4	11	2	23	4	8	0	1.51	4.44
1	1.0	0	0	1	0	1	1	1	1	1	1	.76	2.82

  

Values of $f_m$ for $\frac{\lambda_1}{\lambda_0} = .96$													
Region Data		No. of Iterations										$\bar{f}_m$	$\bar{f}_m + 2\sigma$
No.	Fract. Size	50		100		150		200		250			
		Stat.	For	Stat.	For	Stat.	For	Stat.	For	Stat.	For		
2	.01	2	2	2	2	1	1	3	3	4	3	1.51	4.44
10	.1	36	6	43	9	41	8	41	9	36	9	7.58	14.12
2	.3	12	1	13	1	4	0	1	0	5	0	1.51	4.44
2	.5	18	0	28	2	18	1	19	2	26	2	1.51	4.44
1	1.0	1	1	1	1	0	0	0	0	1	1	.76	2.82

  

Values of $f_m$ for $\frac{\lambda_1}{\lambda_0} = .98$													
Region Data		No. of Iterations										$\bar{f}_m$	$\bar{f}_m + 2\sigma$
No.	Fract. Size	50		100		150		200		250			
		Stat.	For	Stat.	For	Stat.	For	Stat.	For	Stat.	For		
2	.01	1	1	2	2	3	2	3	2	3	2	1.51	4.44
10	.1	61	16	53	12	45	8	26	6	40	10	7.58	14.12
2	.3	33	7	19	2	14	1	12	1	18	2	1.51	4.44
2	.5	36	13	24	4	12	0	2	0	0	0	1.51	4.44
1	1.0	1	1	1	1	0	0	0	0	0	0	.76	2.82



TABLE I - (Cont'd)

Values of $f_m$ for $\frac{\lambda_1}{\lambda_0} = .99$														
Region		No. of Iterations										$\bar{f}_m$	$\bar{f}_m + 2\sigma$	
Date	Fract. Size	5		100		150		200		250				
No.	Fract. Size	Stat.	For	Stat.	For	Stat.	For	Stat.	For	Stat.	For	$\bar{f}_m$	$\bar{f}_m + 2\sigma$	
2	.01	5	2	1	0	3	1	4	2	6	3	1.51	4.44	
10	.1	50	20	38	3	42	5	42	4	56	8	7.58	14.12	
2	.1	24	2	2	0	8	0	14	1	17	2	1.51	4.44	
2	.1	20	2	0	0	10	0	17	0	24	2	1.51	4.44	
1	1.0	0	0	0	0	0	0	0	0	0	0	.76	2.82	
Values of $f_m$ for $\frac{\lambda_1}{\lambda_0} = .995$														
Region		No. of Iterations										$\bar{f}_m$	$\bar{f}_m + 2\sigma$	
Date	Fract. Size	5		100		150		200		250				
No.	Fract. Size	Stat.	For	Stat.	For	Stat.	For	Stat.	For	Stat.	For	$\bar{f}_m$	$\bar{f}_m + 2\sigma$	
2	.01	5	3	5	3	7	1	6	4	7	3	1.51	4.44	
10	.1	81	23	124	26	90	13	95	13	69	10	7.58	14.12	
2	.1	46	0	20	3	13	1	8	0	16	1	1.51	4.44	
2	.1	38	0	18	2	6	1	25	2	24	2	1.51	4.44	
1	1.0	0	0	1	1	1	1	1	1	1	0	.76	2.82	

## DISCUSSION

*Gelbard:* You say that in one case run at Knolls Atomic Power Laboratory (KAPL) it was observed that there was a tenth of a percent bias in the eigenvalue. How many histories were run per generation in that case?

*Gast:* Five hundred. The 0.1% bias was not considered acceptable by people at KAPL. Their approach was simply to go to approximately 2000 histories per iteration on the assumption that the bias would then drop to 0.025%.

*Gelbard:* Did they have other information about other problems? For example, was this 0.1% particularly large or was it typical of the problems they ran?

*Gast:* Their conclusion was that it could be typical.

*Kalos:* I was there at the time. They were trying to compute  $k$ 's to about 0.1% and they wanted their errors to be small compared with that.

*Gelbard:* Any questions or comments?

*Kalos:* I have a great many comments, because I think that this was a very stimulating, careful, and interesting paper. First of all, once you have decided for various reasons that you must make your simulated system supercritical, why insist on any restrictions on the number of histories in successive generations, or on the number of fissions? Why not simply let these numbers vary freely and prepare yourself to contend with the mild programming problem of handling lists of variable length. The lists will probably go out on discs anyway, and you totally remove the bias. The bias associated with increasing  $n$  is removed from the problem, and the game is fairer still. It seems to me that the use of an increasing  $n$  presents complications in understanding and analyzing errors. As I remarked to you before, a scheme for analyzing errors that I find seems to work in situations of this kind is to do the following. Assume that I am going to do 120 iterations, of which the first twenty are to be ignored. I then divide the remaining 100 into groups of 20, and I calculate a mean for each group. This, of course, is a biased mean, and the bias is different from the bias of the grand ensemble mean. Then I compute the standard deviation of the individual means, estimate serial correlation coefficients between each group, and infer a statistical error for the whole problem. It is a rather simple strategy.

*Gelbard:* Let me comment on one of the suggestions that Kalos was making. The suggestion seems to be essentially that, when you average over generations, you do this without normalizing the eigenvectors per generation. You then end up with an arbitrarily normalized eigenvector which you may normalize, of course, after you are finished. Suppose that is what you do. Now that you have normalized you will introduce a bias again, because the bias comes from the fluctuation in the denominator when you normalize. That is the conclusion that comes out of the analysis that we are going to talk about in our next paper. The bias comes from nonlinear terms in the iteration equations, the nonlinear terms being introduced by the denominator in the normalization process. So, if the bias is to be decreased by the process that you described, the amplitude of the fluctuations in the denominator must be decreased. Now, you might expect that they would be decreased because the denominator now

comes, not from one generation, but from a sum over all of the generations which are being averaged. In other words, if you take as your estimate of the eigenfunction a sum over, let us say 100 generations, then to normalize, you divide by the volume integral of this sum. You might expect that the denominator, being a mean over many generations, might not fluctuate much. Mal, do you disagree?

*Kalos:* I disagree with the whole argument. There is no fundamental normalization here for the eigenfunction anyway.

*Gelbard:* That's the real question. What I am asserting is that when you go to use the eigenvector, you always find yourself forced to normalize it in some way. You may want to estimate ratios between the eigenvector at one point and another, and when you find these ratios, you are adopting a particular normalization procedure. The simplest normalization to adopt, in principle, is the one where you normalize the final average to one.

*Kalos:* But in estimating ratios my procedure introduces no bias.

*Gelbard:* That is where I disagree. I disagree because any estimate you make eventually is based on a normalized eigenvector.

*Kalos:* But the normalization drops out.

*Gelbard:* Why does it drop out? You divide the vector you are getting by an integral of that vector.

*Kalos:* Suppose I decided to divide the eigenvector by 73.

*Gelbard:* If you always divided it by 73 you would again have an unnormalized eigenfunction.

*Kalos:* Right!

*Gelbard:* And you could not compare the value at one point with the value at another point. To make a comparison of values at one point with values at another point, you always must, in one way or another, introduce a normalization.

*Kalos:* I am afraid I don't understand that remark at all.

*Gelbard:* What I am saying is that you cannot get away from normalizing the eigenvector that comes out of a Monte Carlo code calculation. I am saying that the value of the eigenvector at a point, unnormalized, is not useable, is not what you are after. You are after a value at a point normalized in some way, or else the value at one point divided by the value at another point.

*Kalos:* Well, if it is the value at one point divided by value at another point, then obviously the normalization is irrelevant.

*Gelbard:* Well, I would say that the normalization then is the normalization to the value at the point at which you are getting the ratio. But another way of doing the same thing, of comparing different eigenvectors, or eigenvectors at different points, is to normalize the eigenvector so that its

integral is one. This is the most convenient way of normalizing; and once you normalize in this way, you are taking the eigenfunction and dividing it by a fluctuating denominator, and you have a bias again. So I think that the elimination of the bias in this way, although it sounds attractive at first glance, is really an illusion. I think that you must normalize the eigenvector, eventually, when you use it for any practical purpose, and when you do, you will again introduce a bias. The question is whether you have diminished the bias by normalizing in this modified way.

*Coveyou:* Are you talking about taking the value of the eigenfunction at two different points and comparing them?

*Gelbard:* I say that that is what you usually do when you compute the eigenvector.

*Cashwell:* Isn't it clear then that, when you take the ratio, normalization cancels out?

*Kalos:* Therefore, the bias that comes from the denominator is totally irrelevant, and if you bring it into the analysis of variance you are making a mistake?

*Gelbard:* Let me then define an alternative way of normalizing. I will take one point in the problem and normalize to one. That is another way of normalizing. I also say that it is a biased way of normalizing.

*Kalos:* All ways of normalizing are biased.

*Gelbard:* So, I am saying that you cannot get away from a normalization procedure of one kind or another and when you introduce a normalization procedure, whether you like it or not, you will come back with a bias.

*Kalos:* It is true that the ratio of the two estimates of the eigenfunction, being a ratio, is very likely to be a biased quantity. But, one must deal with the bias in that ratio directly, and in fact the bias introduced by another normalization factor, is totally irrelevant.

*Gelbard:* What I am saying is that some sort of normalization of the eigenvector is inescapable when you go to use or exhibit your results; and whatever normalization you use will introduce bias. Every time that you introduce a normalization procedure, you introduce the bias again. The question is: How large is the bias for different normalization procedures? Suppose you normalize in the way I described, namely you get the sum over many many unnormalized generations, then divide by that sum. You now have an alternate way of normalizing. Now, you may ask, how is this mean biased, compared to the other mean? I think that is a question that you have to look at if you are going to propose this procedure. I think you have to recognize that the end result is going to be normalized; the most convenient way to normalize is to divide by the integral. You can ask: what kind of bias you have once that normalization is carried out. Is it smaller than the bias you would get by normalizing each eigenvector and averaging? This I think is a question one ought to be able to answer.

*Cashwell:* Yes, but still, the question is: What is biased? The estimate of the normalized eigenfunction is biased, each estimate separately. The ratio of two of the values of the eigenfunction is biased also. But, the second is not biased because the first one is biased. The ratio is biased because it is a ratio.

*Gelbard:* Normalizing to a value at one point is one way of normalizing. I am saying a more common, and also perfectly satisfactory way, is to normalize so that the integral is one. In any case you must normalize to exhibit your results, and to use them, and then you come back with a bias. The question that you should ask is whether one of these approaches gives you less bias in the normalized result than the other. My suspicion is that the bias in this alternative procedure, which does sound attractive when you think about it first, is not really smaller than the bias in the conventional normalization.

*Gast:* I would like to make one point about normalization. In our RECAP program the eigenfunction can be represented, either by the accumulated neutron source which is input at the beginning of each iteration, or by the accumulated output of an iteration, the neutron production. You can visualize normalizing either end of the generation. We always normalize the input. To normalize the input one keeps the total starting weight of all neutrons the same in each generation. If you want to normalize the output, the neutron production (and I am not sure whether you were referring to this), the process becomes much more complex.

*Gelbard:* Another way of avoiding bias in the eigenvector is to keep a fixed number of histories per generation but, when you average, to assign each generation a weight — the weight being equal to the eigenvalue coming from that generation. I think this approach is very closely related to what is in one of Lieberoth's papers. But I suspect, again, that when you try to use the eigenfunction you are forced to normalize it. And, when you normalize it, you are again forced to divide by a fluctuating denominator, and again I think that you will get a bias when you finally do normalize. It is just hard to see what you can do with the unnormalized shape: every time you try to use it you are forced to normalize in one way or another. Well, anymore comments?

*Kalos:* Yes. I would like to comment on the subject of importance sampling. You conjecture that there is no other form of importance sampling which would have direct application to the reduction of variance of the eigenfunction or, in general, to the acceleration of the iterative process. This is false. There is such a form of importance sampling, at least, in theory. Work on this sort of importance sampling originally goes back to Goad and Johnson. A variant of their method was published by me in a paper presented at the ANS Topical Meeting in Kiamesha Lake. There I pointed out that if you solve the adjoint transport equation, and if you use the fundamental mode of the power distribution as an importance function then, in the limit where ordinary importance sampling is carried out exactly, you get zero variance estimates for the flux at any point you care to choose to start the history. This process converges in one generation and, therefore, you have an acceleration and zero variance technique at the same time. The estimates you need to bias with are the value of the power. Thus you have the possibility of starting with an approximation and, perhaps, doing a multi-stage sampling in which improvements in your guess are fed back. I have no idea how this would work out in practice but at least, in theory, there is an importance sampling method

which reduces variance and accelerates convergence. It is of the same general character as those you have looked at, but the point of view is quite different.

*Gast:* Our feeling was that because we need the flux or the power over many edit regions, that in trying to get a shape we would be confronted with a sequence of adjoints, and we ....

*Kalos:* No, it is one adjoint only — there is a single adjoint. There is a single adjoint which gives the flux at any point in the reactor with zero variance.

*Gast:* At a prechosen point. Then you have to do many points.

*Kalos:* Yes, yes.

*Gast:* It is our intuitive feeling (though we intend to look into this in more detail, by the way) that we could probably not gain very much relative to a normal forward run.

*Gelbard:* Because of the number of points you are interested in?

*Gast:* Yes, but I am very interested in your feelings as to what the gain could be.

*Kalos:* I wish I had feelings as to what the gain could be.

*Cashwell:* My experience has been mainly with shielding problems, not criticality problems, but my guess is that almost any method of getting an approximate adjoint function will help a lot. Whether that is true for the reactor, for the criticality problem, I do not know, but I see no reason why it would not be true.

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