MONTE CARLO WORK AT ARGONNE NATIONAL LABORATORY*

E. M. Gelbard and R. E. Prael

Argonne National Laboratory
Argonne, Illinois 60439, U.S.A.

* * *

Presented by E. M. Gelbard

*Work supported by the U.S. Energy Research and Development Administration.

Distribution Category:
LMFBR Physics (UC-79d)

ANL-75-2
NEACRP-L-118

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

PROCEEDINGS OF THE NEACRP MEETING OF A MONTE CARLO STUDY GROUP

July 1-3, 1974
Argonne, Illinois, U.S.A.

Sponsored by

The Nuclear Energy Agency Committee on Reactor Physics

Hosted by

Argonne National Laboratory

Chairman

Ely M. Gelbard

Compiled by

Cyrilla Hytry

Arrangements

Cyrilla Hytry
Miriam Holden
Joyce Stejskal

MONTE CARLO WORK AT ARGONNE NATIONAL LABORATORY

E. M. Gelbard and R. E. Prael

Argonne National Laboratory
Argonne, Illinois 60439, U.S.A.

ABSTRACT

This paper is divided into three parts. In Part I we describe a simple model of the Monte Carlo process and develop a (nonlinear) recursion relation between fission sources in successive generations. From the linearized form of these recursion relations, it is possible to derive expressions for the mean square coefficients of error modes in the iterates and for correlation coefficients between fluctuations in successive generations. In a simple test problem, we find that MacMillan's prescription for computing variances in means in fairly accurate.

Part II deals with first-order nonlinear terms in the recursion relation. From these nonlinear terms an expression for the bias in the eigenvalue estimator is derived, and prescriptions for measuring the bias are formulated.

In Part III we outline plans for the development of the VIM code, and describe briefly the proposed treatment of small sample perturbations in VIM.

Part I

THEORETICAL STUDY OF THE MONTE CARLO EIGENVALUE COMPUTATION, LINEARIZED EQUATIONS

A. Basic Features of the Mathematical Model

Although the mathematical principle underlying the Monte Carlo method in fixed-source computations are well understood, the Monte Carlo methods used in eigenvalue calculations have generally been based primarily on intuition. It is known that many of the methods in use today are biased [1,2]. It is known that correlations between generations tend to complicate the statistical estimation process [3]; but one finds very little theoretical work in the technical literature on the magnitude of the bias, or on the nature of these correlations. We propose here a mathematical model of the Monte Carlo process, a model from which perhaps some of the mathematical properties of the Monte Carlo process can be deduced. For convenience we deal with a $K \times K$ matrix eigenvalue equation rather than an integral equation.

Suppose that, in the Monte Carlo process, we treat precisely N sample particles per generation. One is to imagine that these particles execute a random walk among K boxes. Let $T_{\mu\nu}$ be the probability that a particle in the ν-*th* box will step, next, into the μ-*th*. Suppose, further, that the μ-*th* box has a fixed weight, W_μ ($\mu = 1, 2, \ldots, K$), attached to it. Define a diagonal matrix, W, such that its $\mu\mu$-*th* element is equal to the weight, W_μ. Let $WT = H$. Then our matrix analogue of the reactor eigenvalue equation is the matrix equation

$$H \underline{W}_n = \lambda_n \underline{W}_n \, . \tag{1}$$

It should be understood that each box in our model represents an elementary volume of phase-space in the reactor. We are interested in estimating the largest eigenvalue, λ_1, the corresponding eigenvector $\underline{W}_1$ and, perhaps integrals of $\underline{W}_1$ over specified regions in the reactor configuration.

Assume that, at the end of the i-1"*st* generation, N_μ^i particles have terminated their histories in the μ-*th* box. Here, of course,

$$\sum_{\mu=1}^{K} N_\mu^i = N \, ,$$

where K, again, is the order of the matrix, H.

To begin the next generation we form the probability distribution

$$p_\mu^i \equiv v_\mu^i \Big/ \left[\sum_{\nu=1}^{K} v_\nu^i\right] , \qquad v_\mu^i \equiv N_\mu^i W_\mu \, , \tag{2}$$

and select N starters for the i-*th* generation from this distribution. In vector notation

$$\underline{v}^i = \left(v_1^i, v_1^i, \ldots v_\mu^i, \ldots, v_k^i\right)^T . \tag{3}$$

Note that in our model, each particle of the i-1"*st* generation produces one, and only one, potential fission site for the i-*th*. Thus, our analysis will not apply to a process in which the site of each collision is a potential fission site or, generally, to any process in which the number of fission sites generated, per history, is a random variable. Note that every box in which a history terminates is, in our terminology, a "potential fission site", even if the weight assigned to that box is zero. This peculiarity in terminology is of no importance here, since in order to avoid substantial theoretical complications, we shall assume that all the weights are positive. Although we do not allow any weights to vanish, the W_μ may be arbitrarily small, and it seems reasonable to assume that a Monte Carlo process in which some weights are very small will be practically indistinguishable from a process in which those weights are set to zero.

Define a K-dimensional vector $\underline{\tau}^T = (1, 1, \ldots, 1)$. Clearly $p_\mu^i = v_\mu^i/(\underline{\tau}^T \cdot \underline{v}^i)$. The vectors $\underline{v}^i$ and $\underline{v}^{i+1}$ are connected by the recursion

relation

$$\underline{V}^{i+1} = N \frac{H \underline{V}^i}{\underline{\tau}^T \cdot \underline{V}^i} + \underline{\varepsilon}^i , \tag{4}$$

$$\underline{V}^{i+1} = \left(1/\lambda^i\right) H \underline{V}^i + \underline{\varepsilon}^i , \qquad \lambda^i \equiv \left(\underline{\tau}^T \cdot \underline{V}^i\right) \Big/ N . \tag{5}$$

Here λ^i is a familiar i-1'*st* generation estimate of the dominant eigenvalue while $\underline{V}^i$ is an estimate of the corresponding eigenvector. In Eq. (5), $\underline{\varepsilon}^i$ is the net statistical error committed during the i-*th* generation in transferring particles from their starting locations into the μ-*th* box. More precisely

$$\varepsilon_k^i \equiv V_k^{i+1} - E\left\{V_k^{i+1} \middle| V^i\right\} = V_k^{i+1} - \bar{V}_k^{i+1} . \tag{6}$$

It will be seen that $\bar{V}_k^{i+1}$ is the conditional mean of V_k^{i+1}, given V^i. From Eq. (6),

$$E\left\{\varepsilon_k^i\right\} = E\left\{E\left\{\varepsilon_k^i \middle| \underline{V}^i\right\}\right\} = E\left\{E\left\{V_k^{i+1} - \bar{V}_k^{i+1} \middle| \underline{V}^i\right\}\right\}$$
$$= E\left\{\bar{V}_k^{i+1} - \bar{V}_k^{i+1}\right\} = 0 . \tag{7}$$

Of course $\underline{V}^i$ and $\underline{V}^{i-1}$ are not independent, so that $\underline{\varepsilon}^i$ and $\underline{\varepsilon}^{i-1}$ cannot be independent either. But

$$E\left\{\varepsilon_k^i \varepsilon_\ell^{i-1}\right\} \equiv \int P\left(\underline{V}^i, \underline{V}^{i-1}\right) d\underline{V}^i \, d\underline{V}^{i-1} \left[V_k^i - E\left\{V_k^i \middle| \underline{V}^{i-1}\right\}\right]$$
$$\times \int P\left(\underline{V}^{i+1} \middle| \underline{V}^i\right) d\underline{V}^{i+1} \left[V_\ell^{i+1} - E\left\{V_\ell^{i+1} \middle| \underline{V}^i\right\}\right] .$$

Here $P(\underline{V}^i, \underline{V}^{i-1})$ is the joint probability distribution function of $\underline{V}^i$ and $\underline{V}^{i-1}$, while $P(\underline{V}^{i+1} | \underline{V}^i)$ is the conditional distribution function of $\underline{V}^{i+1}$ given $\underline{V}^i$. By definition

$$\int P\left(\underline{V}^{i+1} \middle| \underline{V}^i\right) d\underline{V}^{i+1} \left[V_\ell^{i+1} - E\left\{V_\ell^{i+1} \middle| \underline{V}^i\right\}\right] = 0 ,$$

and it follows that

$$E\left\{\varepsilon_k^i \varepsilon_\ell^{i-1}\right\} = 0 .$$

Thus, although $\underline{\varepsilon}^i$ and $\underline{\varepsilon}^{i-1}$ are not independent, they are, in the technical sense, uncorrelated. It will be necessary, later, to examine the properties of the statistical errors, $\underline{\varepsilon}^i$, more closely, but we need say no more about them at this point. Note that it follows from Eq. (7) that

$$E\left\{\underline{V}^{i+1}\right\} = H\, E\left\{\underline{V}^i/\lambda^i\right\} . \tag{8}$$

Define

$$\underline{V}^i = N\,\underline{U}_1 + \underline{\delta}^i , \tag{9}$$

$\underline{U}_1$ being the main mode eigenvector normalized so that $\underline{\tau}^T \cdot \underline{U}_1 = \lambda_1$. From Eqs. (5) and (9) we see that

$$N\,\underline{U}_1 + \underline{\delta}^{i+1} = N\,\frac{H\left(N\,\underline{U}_1 + \underline{\delta}^i\right)}{\underline{\tau}^T \cdot \left(N\,\underline{U}_1 + \underline{\delta}^i\right)} + \underline{\varepsilon}^i . \tag{10}$$

Equation (10) is clearly nonlinear in $\underline{\delta}^i$. In our analysis it will be convenient to treat separately those effects which can be deduced from the linearized form of Eq. (10), and those whose study requires retention of higher terms. Intergeneration correlations fall into the first category, biases into the second.

B. The Linearized Iteration Equation and Correlations

Retaining only linear terms in Eq. (10), we get

$$\underline{\delta}^{i+1} \approx \underline{\tilde{\delta}}^{i+1} \equiv \lambda_1^{-1}\left[H - \underline{U}_1\underline{\tau}^T\right]\underline{\tilde{\delta}}^i + \underline{\varepsilon}^i . \tag{11}$$

Taking expectation values of both sides, it is easy to show that $E\left\{\underline{\tilde{\delta}}^i\right\} \to 0$ as $i \to \infty$, so that to first order in $\underline{\varepsilon}$ the bias vanishes. In all the work which follows, we will assume that H has a complete set of eigenvectors and that all eigenvalues are real and nonnegative. It is our hope that, even when these assumptions fail, our analysis will still give us some valid insight into the character of the Monte Carlo iterative process. At any rate, assuming completeness, we write

$$\underline{\tilde{\delta}}^i = \sum_n \tilde{\delta}^i_n \underline{U}_n , \tag{12}$$

where, as in Eq. (1), the $\underline{U}_n$ are the eigenvectors of H. We have already specified that $\underline{\tau}^T \cdot \underline{U}_1 = \lambda_1$. It will be convenient to normalize the other eigenvectors similarly if possible. If $\underline{\tau}^T \cdot \underline{U}_n \neq \lambda_n$, let $\underline{\tau}^T \cdot \underline{U}_n = \lambda_n$; otherwise the normalization of $\underline{U}_n$ will remain unspecified. Clearly

$$\underline{\tau}^T \cdot \tilde{\delta}^i = \sum_N{}' \lambda_n \tilde{\delta}^i_n , \tag{13}$$

where the primed summation runs over all n such that $\underline{\tau}^T \cdot \underline{U}_n \neq 0$.

Write Eq. (11) in the form

$$\tilde{\underline{\delta}}^{i+1} = A\tilde{\underline{\delta}}^i + \underline{\varepsilon}^i , \qquad A \equiv \hat{H} - \underline{U}_1 \hat{\underline{\tau}}^T ,$$

$$\hat{H} \equiv H/\lambda_1 , \qquad \hat{\underline{\tau}} \equiv \underline{\tau}/\lambda_1 . \tag{14}$$

Assume that the iterative process has been in progress for an infinite number of generations. It is easy to show, given our assumptions on H, that $||A|| < 1$. It follows then, from Eq. (14), that

$$\tilde{\underline{\delta}}^{i+1} = \sum_{n=0}^{\infty} A^n \underline{\varepsilon}^{i-n} , \tag{15}$$

where, of course, the superscript on $\underline{\varepsilon}$ is an iteration index, not an exponent.

The reader can verify that

$$A^n = \hat{H}^n - \underline{U}_1 \hat{\underline{\tau}}^T \hat{H}^{n-1} , \qquad n \geq 1 . \tag{16}$$

Putting Eq. (16) into Eq. (15), we see that

$$\tilde{\underline{\delta}}^{i+1} = \underline{\varepsilon}^i + \sum_{n=1}^{\infty} \sum_{k=1}^{K} \rho_k^n \underline{U}_k - \underline{U}_1 \sum_{k=1}^{K}{}' \rho_k^n \varepsilon_k^{i-n}$$

$$= \underline{\varepsilon}^i + \sum_{n=1}^{\infty} \sum_{k=2}^{K} \rho_k^n \underline{U}_k - \underline{U}_1 \sum_{k=2}^{K}{}' \rho_k^n \varepsilon_k^{i-n} . \tag{17}$$

Here $\rho_k \equiv \lambda_k/\lambda_1$, while ε_k^i is the coefficient of the k-*th* eigenvector in the eigenfunction expansion for $\underline{\varepsilon}^i$:

$$\underline{\varepsilon}^i = \sum_{k=1}^{K} \varepsilon_k^i \underline{U}_k . \tag{18}$$

It follows from Eq. (17) that

$$\tilde{\delta}_1^{i+1} = \varepsilon_1^i - \sum_{k=2}^{K}{}' \sum_{n=1}^{\infty} \rho_k^n \varepsilon_k^{i-n} ,$$

$$\tilde{\delta}_k^{i+1} = \sum_{n=0}^{\infty} \rho_k^n \varepsilon_k^{i-n} , \qquad k > 1 . \tag{19}$$

To compute the mean-square coefficients of the error modes, we write

$$\left(\tilde{\delta}_k^{i+1}\right)^2 = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \rho_k^n \rho_k^m \varepsilon_k^{i-n} \varepsilon_k^{i-m} , \qquad k \neq 1 . \tag{20}$$

Defining $r_{k\ell} = E\left\{\delta_k^{i+1} \delta_\ell^{i+1}\right\}$, we see from Eq. (20) that

$$r_{kk} = \frac{\varepsilon_{kk}}{1 - \rho_k^2} , \qquad k \neq 1 . \tag{21}$$

For later use, we also cite, here, expressions for the other $r_{k\ell}$'s:

$$r_{11} = \varepsilon_{11} + \sum_{k=2}^{K'}\sum_{\ell=2}^{K'} \frac{\rho_k \rho_\ell}{\left(1 - \rho_k \rho_\ell\right)} \varepsilon_{k\ell} ,$$

$$r_{1\ell} = r_{\ell 1} = \varepsilon_{1\ell} - \sum_{k=2}^{K'} \frac{\rho_k \rho_\ell}{\left(1 - \rho_k \rho_\ell\right)} \varepsilon_{k\ell} , \qquad \ell \neq 1 ,$$

$$r_{k\ell} = \frac{\varepsilon_{k\ell}}{\left(1 - \rho_k \rho_\ell\right)} , \qquad k \neq 1 , \qquad \ell \neq 1 . \tag{22}$$

Above, and in all the work which follows,

$$\varepsilon_{k\ell} \equiv E\left\{\varepsilon_k^i \varepsilon_\ell^i\right\} . \tag{23}$$

Note that we are assuming that the right-hand side of Eq. (23) is independent of i.

The quantity r_{kk} is the mean-square coefficient of the k-*th* eigenvector in an expansion of the "asymptotic" fission source (i.e., the fission source in any single generation preceded by infinitely many iterations). At this point we want to derive a corresponding expression for r_{kk} in a fission source averaged over M successive generations. Define

$$\tilde{\delta}_{k,M}^{i+1} = \frac{1}{M} \sum_{n=1}^{M} \tilde{\delta}_k^{i+2-n} , \tag{24}$$

and

$$r_{kk,M} = E\left\{\left(\tilde{\delta}^{i}_{k,M}\right)^2\right\}, \tag{25}$$

$$r_{kk,M} = \frac{1}{M^2}\sum_{n=1}^{M}\sum_{m=1}^{M} E\left\{\tilde{\delta}^{i+2-n}_{k}\tilde{\delta}^{i+2-m}_{k}\right\}. \tag{26}$$

We consider, for the sake of simplicity, only the variance in the amplitudes of contaminating modes, modes for which $k > 1$. For such modes

$$E\left\{\tilde{\delta}^{i+1-n}_{k}\tilde{\delta}^{i+1-m}_{k}\right\} = \sum_{j=0}^{\infty}\sum_{\ell=0}^{\infty}\rho_k^j\rho_k^\ell E\left\{\varepsilon^{i-n-j}_{k}\varepsilon^{i-m-\ell}_{k}\right\}, \qquad k > 1. \tag{27}$$

If $n \geq m$, then

$$E\left\{\tilde{\delta}^{i+1-n}_{k}\tilde{\delta}^{i+1-m}_{k}\right\} = \sum_{j=0}^{\infty}\rho_k^j\rho_k^{n-m+j}\varepsilon_{kk}, \qquad k > 1. \tag{28}$$

$$E\left\{\tilde{\delta}^{i+1-n}_{k}\tilde{\delta}^{i+1-m}_{k}\right\} = \frac{\rho_k^{n-m}}{\left(1-\rho_k^2\right)}\varepsilon_{kk}, \qquad k > 1. \tag{29}$$

Putting Eq. (29) into Eq. (26), we find after some manipulation that

$$r_{kk,M} = \frac{1}{M}\frac{\varepsilon_{kk}}{\left(1-\rho_k^2\right)}\left[1 + 2h_M\left(\rho_k\right)\right], \qquad k > 1, \tag{30}$$

where

$$h_M\left(\rho_k\right) \equiv \frac{\rho_k}{\left(1-\rho_k\right)}\left[1 - \frac{1}{M}\frac{\left(1-\rho_k^M\right)}{\left(1-\rho_k\right)}\right]. \tag{31}$$

Obviously $h_M(\rho) \to \rho/(1-\rho)$ as $M \to \infty$. It is easy to show in addition that $h_M(\rho) \approx (M-1)/2$ if $\rho^M \approx 1$. Thus

$$r_{kk,M} \approx \frac{\varepsilon_{kk}}{\left(1-\rho_k^2\right)}, \qquad \text{if } M << -\left(\ell n\ \rho_k\right)^{-1}, \qquad k > 1, \tag{32}$$

and

$$r_{kk,M} \approx \frac{1}{M}\frac{\varepsilon_{kk}}{\left(1-\rho_k^2\right)}\left[1+\frac{2\rho_k}{\left(1-\rho_k\right)}\right] = \frac{1}{M}\frac{\varepsilon_{kk}}{\left(1-\rho_k\right)^2},$$

$$\text{if } M >> -\left(\ell n\ \rho_k\right)^{-1}, \qquad k > 1 . \tag{33}$$

Note that if successive generations were uncorrelated, one would find that

$$r_{kk,M} = \frac{1}{M}\frac{\varepsilon_{kk}}{\left(1-\rho_k^2\right)} \quad \text{(without correlation)} . \tag{34}$$

Thus we see that the factor $1 + \left[2\rho_k/(1-\rho_k)\right]$ in Eq. (33) is an amplification factor embodying effects due to intergeneration correlations. A closely related amplification factor is introduced by MacMillan in Ref. 3.

In order to make any use of the expressions derived above, it will be necessary to evaluate the covariances ε_{kk}. We discuss this problem next.

C. Computation of $\varepsilon_{k\ell}$

The quantity $\underline{\varepsilon}^i$ in Eq. (5) is a vector whose spatial components have the form

$$\varepsilon_\nu^i = W_\nu \Delta_\nu^{i+1}, \qquad \Delta_\nu^{i+1} \equiv N_\nu^{i+1} - E\left\{N_\nu^{i+1} \middle| \underline{V}^i\right\} . \tag{35}$$

Expanding $\underline{\varepsilon}^i$ into eigenvectors of H, we find that

$$\varepsilon_k^i = \sum_{\nu=1}^{K} U_{k\nu}^* W_\nu \Delta_\nu^{i+1} . \tag{36}$$

Here $U_{k\nu}^*$ is the ν-*th* components of the adjoint eigenvector $\underline{U}_k^*$. Thus

$$\varepsilon_{k\ell} = \sum_{\nu=1}^{K}\sum_{\mu=1}^{K} U_{k\nu}^* U_{\ell\mu}^* W_\nu W_\mu E\left\{\Delta_\nu^{i+1}\Delta_\mu^{i+1}\right\} . \tag{37}$$

To evaluate $\varepsilon_{k\ell}$, we must now compute the expectation value which appears on the right-hand side of Eq. (37).

Neglecting any bias, we shall assume that the expected number of particles in the ν-*th* box is $\bar{N}_\nu$, where

$$W_\nu \bar{N}_\nu = N\, U_{1\nu} . \tag{38}$$

Further, we suppose that in each generation the probability that a typical particle will be assigned to the ν-th box is equal to $\bar{N}_\nu/N$. Under these assumptions one can show that

$$E\left\{\Delta_\nu^{i+1}\Delta_\nu^{i+1}\right\} = \bar{N}_\nu\left(1 - \bar{N}_\nu/N\right) , \tag{39}$$

$$E\left\{\Delta_\nu^{i+1}\Delta_\mu^{i+1}\right\} = -\bar{N}_\nu\bar{N}_\mu/N , \qquad \nu \neq \mu . \tag{40}$$

Putting Eqs. (39) and (40) into Eq. (37), we find that

$$\epsilon_{k\ell} = \sum_{\nu=1}^{K} U_{k\nu}^* U_{\ell\nu} W_\nu^2 \bar{N}_\nu\left(1 - \bar{N}_\nu/N\right)$$

$$- \sum_{\nu=1}^{K}\sum_{\mu=1}^{K} \left(U_{k\nu}^* U_{\ell\mu}^* W_\nu W_\mu \bar{N}_\nu \bar{N}_\mu\right)/N$$

$$+ \sum_{\nu=1}^{K} \left(U_{k\nu}^* U_{\ell\nu}^* W_\nu^2 \bar{N}_\nu\right)/N , \tag{41}$$

$$\epsilon_{k\ell} = \sum_{\nu=1}^{K} U_{k\nu}^* U_{\ell\nu}^* W_\nu^2 \bar{N}_\nu$$

$$- \sum_{\nu=1}^{K}\sum_{\mu=1}^{K} \left(U_{k\nu}^* U_{\ell\mu}^* W_\nu W_\mu \bar{N}_\nu \bar{N}_\mu\right)/N . \tag{42}$$

Because of the biorthogonality of eigenvectors and adjoints, the second term on the right-hand side of Eq. (42) vanishes unless $k = \ell = 1$:

$$\epsilon_{k\ell} = \sum_{\nu=1}^{K} U_{k\nu}^* U_{\ell\nu}^* W_\nu^2 \bar{N}_\nu , \qquad k \neq 1 \text{ or } \ell \neq 1 . \tag{43}$$

Again using biorthogonality, one finds that

$$\varepsilon_{11} = \sum_{w=1}^{K} \left(\mathbb{U}^{*}_{1w} W_w\right)^2 N_w - N \,. \tag{44}$$

It is interesting to note that the vector

$$\underline{I}_k = W \underline{\mathbb{U}}^{*}_{k} \,,$$

((where W is the weight matrix, defined in Section A)) is the importance function for absorption. From Eq. ((42)), it is easy to show that, in general,

$$\varepsilon_{k\ell} = N \sum_{w=1}^{K} \left(I_{kw} - \bar{I}_k\right)\left(I_{\ell w} - \bar{I}_\ell\right) \mathbb{I}_w \,, \tag{46}$$

where

$$\bar{I}_k \equiv \sum_{w=1}^{K} I_{kw} \mathbb{I}_w \,,$$

$$\mathbb{I}_w = \bar{N}_w / N \,.$$

Clearly $\mathbb{I}_w$ is the fundamental-mode absorption probability in the w-*th* box. Thus the quantity $\left(\varepsilon_{k\ell}/N\right)$ can be interpreted as the covariance of the importance functions, I_k and I_ℓ, with respect to the absorption probability distribution function.

D. Qualitative Features of the Monte Carlo Estimates

Note that we have, so far, been discussing the fluctuations in the net fission source produced in a typical generation by N sample particles. The amplitude of such a fission source would, of course, be proportional to N. It is, however, somewhat more interesting to consider the behavior of a fission source whose normalization is independent of N. Define

$$\underline{v}^{i+1} = \underline{W}^{i+1}/N \,. \tag{47}$$

It will be seen that $\underline{v}^{i}$ is an estimate of the fission source density produced at the end of the i-*th* generation, by one fission neutron born at the beginning of the i-*th* generation. Correspondingly, we define

$$\underline{Y}^{i+1} = \underline{\Theta}^{*i+1}/N \,,$$

$$\bar{\varepsilon}_{k\ell} = \frac{1}{N^2} \varepsilon_{k\ell} \,,$$

and

$$\bar{r}_{k\ell} = \frac{1}{N^2} r_{k\ell} \triangleq E\left\{\tilde{\gamma}_k^{i+1}\tilde{\gamma}_\ell^{i+1}\right\}. \tag{48}$$

In terms of the newly defined quantities, we may write

$$\bar{r}_{k\ell} = \frac{\bar{\varepsilon}_{k\ell}}{\left(1 - \rho_k\rho_\ell\right)}, \qquad k \neq 1, \qquad \ell \neq 1, \tag{49}$$

$$\bar{r}_{11} = \bar{\varepsilon}_{11} + \sum_{k=2}^{K}{}' \sum_{\ell=1}^{K}{}' \frac{\rho_k\rho_\ell}{\left(1 - \rho_k\rho_\ell\right)} \bar{\varepsilon}_{k\ell}, \tag{50}$$

$$\bar{r}_{1\ell} = \bar{\varepsilon}_{1\ell} - \sum_{k=2}^{K}{}' \frac{\rho_k\rho_\ell}{\left(1 - \rho_k\rho_\ell\right)} \bar{\varepsilon}_{k\ell} = \bar{r}_{\ell 1}, \qquad \ell \neq 1, \tag{51}$$

$$\bar{r}_{kk,M} = \frac{1}{M^2} \frac{\varepsilon_{kk}}{\left(1 - \rho_k^2\right)} \left[1 + 2h_M\left(\rho_k\right)\right], \qquad k \neq 1, \tag{52}$$

$$\bar{r}_{kk,M} \approx \frac{\bar{\varepsilon}_{kk}}{\left(1 - \rho_k^2\right)}, \qquad M >> -\left(\ell n\, \rho_k^{-1}\right), \qquad k \neq 1, \tag{54}$$

$$\bar{\varepsilon}_{11} = \frac{1}{N} \sum_{\nu=1}^{K} \left(U_{1\nu}^* W_\nu\right)^2 \Pi_\nu - 1, \tag{55}$$

$$\bar{\varepsilon}_{k\ell} = \frac{1}{N} \sum_{\nu=1}^{K} U_{k\nu}^* U_{\ell\nu} W_\nu^2 \Pi_\nu, \qquad k,\ell \neq 1. \tag{56}$$

We see from Eqs. (49)-(51) that the asymptotic fission source contains an "equilibrium" distribution of modes. Although the amplitude of all error modes tends to vanish like 1/N (since the $\bar{\varepsilon}_{k\ell}$ vanish like 1/N), the spectrum of error modes is independent of N.

Generally one would expect that the $\bar{\varepsilon}_{kk}$ would decrease with k, since the number of zeros in U_k^* increases with k. On the other hand there seem to be no reason to suppose that $\bar{\varepsilon}_{kk}$ is very sensitive to k and we shall assume that variations in $\bar{\varepsilon}_{kk}$ are not very important. Certainly this is true in the model problems discussed in Section E. Neglecting variations in $\bar{\varepsilon}_{kk}$, and assuming that $\rho_k \approx 1$, $\rho_\ell \approx 1$, we find that

$$\bar{r}_{kk} \Big/ \bar{r}_{\ell\ell} \approx \left(1 - \rho_\ell\right) \Big/ \left(1 - \rho_k\right) . \tag{57}$$

Clearly it is not safe to assume (as one does in a deterministic eigenvalue calculation) that only a single error mode survives after many iterations.

Averaging over many generations, we find that

$$\bar{r}_{kk,M} \Big/ \bar{r}_{\ell\ell,M} \approx \left(1 - \rho_\ell\right)^2 \Big/ \left(1 - \rho_k\right)^2 . \tag{58}$$

It will be seen that when M is sufficiently large the spectrum of error modes, which is always independent of N, becomes independent of M as well. In the averaged fission source the importance of error modes with large ρ is considerably enhanced though higher-order error modes persist.

To compute the variance of the eigenvalue estimate, we recall that

$$\lambda^i = \left(\underline{\tau}^T \cdot \underline{V}^i\right) N \approx \lambda_1 + \underline{\tau}^T \cdot \underline{\tilde{\gamma}}^i , \tag{59}$$

$$\Delta\lambda^i \equiv \lambda^i - \lambda_1 \approx \underline{\tau}^T \cdot \underline{\tilde{\gamma}}^i = \sum_{k=1}^{K} \lambda_k \tilde{\gamma}_k^i , \tag{60}$$

$$\left(\Delta\lambda^i/\lambda_1\right) = \sum_{k=1}^{K'} \rho_k \tilde{\gamma}_k^i . \tag{61}$$

From Eq. (19) we see that

$$\sum_{k=1}^{K'} \rho_k \tilde{\gamma}_k^i = \frac{1}{N} \left[\varepsilon_1^i - \sum_{k=2}^{K'} \sum_{n=1}^{\infty} \rho_k^n \varepsilon_k^{i-n} + \sum_{n=0}^{\infty} \sum_{k=2}^{\infty} \rho_k^{n+1} \varepsilon_k^{i-n} \right] , \tag{62}$$

$$\sum_{k=1}^{K'} = \frac{1}{N} \left[\sum_{k=1}^{K'} \rho_k \varepsilon_k^i - \sum_{k=2}^{K} \sum_{n=1}^{\infty} \rho_k^n \left(1 - \rho_k\right) \varepsilon_k^i \right] , \tag{63}$$

From Eqs. (61) and (63), it follows that

$$\alpha \equiv E\left\{\left(\Delta\lambda^i/\lambda_1\right)^2\right\} = \sum_{k=1}^{K'} \sum_{\ell=1}^{K'} \rho_k \rho_\ell \bar{\varepsilon}_{k\ell}$$

$$+ \sum_{k=1}^{K'} \sum_{\ell=1}^{K'} \frac{\rho_k \rho_\ell \left(1 - \rho_k\right)\left(1 - \rho_\ell\right)}{\left(1 - \rho_k \rho_\ell\right)} \bar{\varepsilon}_{k\ell} . \tag{64}$$

Define

$$\alpha_0 = \sum_{k=1}^{K}\sum_{\ell=1}^{K} \rho_k \rho_\ell \varepsilon_{k\ell} = \frac{1}{N^2} E\left\{\left(\underline{\tau}^T \cdot \underline{\varepsilon}^i\right)^2\right\} . \tag{65}$$

After a little manipulation, one finds that

$$\alpha_0 = \frac{1}{N}\sum_{\nu=1}^{K}\left(W_\nu - \bar{W}\right)^2 \Pi_\nu , \qquad \bar{W} \equiv \sum_{\nu=1}^{K} W_\nu \Pi_\nu , \qquad \Pi_\nu \equiv \frac{\bar{N}_\nu}{N} . \tag{66}$$

This α_0 is equal to 1/N times the variance of the weights. It can be shown that α_0 has, in addition, the following significance. Suppose one were to draw N fission source sites from the main mode fission source distribution, starting one sample particle from each site. Each sample particle is to be followed for <u>one generation</u>. Let N_ν be the number of sample particles which end their histories in box ν, and define

$$\lambda = \sum_{\nu=1}^{K} N_\nu W_\nu . \tag{67}$$

Then α_0 is the variance in (λ/λ_1). The second term on the right of Eq. (66) is, then, the additional variance induced by the iterative process. This second term may be written in the form

$$\alpha_1 = \sum_{n=1}\sum_{k=2}^{K'}\sum_{\ell=2}^{K'} \rho_k^n \rho_\ell^n \left(1 - \rho_n\right)\left(1 - \rho_\ell\right) \bar{\varepsilon}_{k\ell} . \tag{68}$$

Since the $\bar{\varepsilon}_{k\ell}$ are elements of a covariance matrix, and such a matrix must be non-negative definite, α_1 is a sum of non-negative quadratic forms. It is, therefore, non-negative. The iterative process will tend to increase (and will certainly not decrease) the variance of the eigenvalue estimator.

We have seen that in the asymptotic mixture of modes, the modes with $\rho \approx 1$ ("low-order" modes) occur with relatively large mean-square amplitudes. On the other hand, because of the factor $(1 - \rho_k)(1 - \rho_\ell)$, such modes do not play a particularly important role in amplifying the variance of the eigenvalue estimator. In fact, the fluctuations in amplitude of low-order modes has little effect on the eigenvalue estimates precisely because the eigenvalues of such modes are almost the same as the main mode eigenvalue. Because the contributions of low-order modes are suppressed in α_1, one would expect the net amplification in the variance of the eigenvalue to be small.

Suppose, now, that we are interested in estimating the fission rate in a volume, k, within a reactor configuration, From Eq. (48)

$$\underline{v}^i \approx \underline{U}_1 + \tilde{\underline{\gamma}}^i , \qquad \underline{v}^i - \underline{U}_1 = \sum_{k=1}^{K} \tilde{\gamma}_k^i \underline{U}_k , \tag{69}$$

$$\underline{r}_R^i \equiv \int_R \left(\underline{v}^i - \underline{U}_1\right) dV = \sum_{k=1}^{K} C_k \tilde{\gamma}_k^i , \qquad C_k \equiv \int_R \underline{U}_k dV , \tag{70}$$

$$\sigma_R^2 \equiv E\left\{\left(r_R^i\right)^2\right\} = \sum_{k=1}^{K}\sum_{\ell=1}^{K} C_k C_\ell \bar{r}_{k\ell} . \tag{71}$$

Define

$$\sigma_{R,M}^2 = E\left\{\left(\frac{1}{M}\sum_{i=1}^{M} \underline{r}_R^i\right)^2\right\} , \tag{72}$$

and

$$\bar{r}_{k\ell}^{i,i+j} \equiv E\left\{\tilde{\gamma}_k^i \tilde{\gamma}_\ell^{i+j}\right\} . \tag{73}$$

By straightforward computation, we find that

$$\bar{r}_{11}^{i,i+j} = -\sum_{\ell=1}^{K} \varepsilon_{1\ell}\rho_\ell^j + \sum_{k=2}^{K}\sum_{\ell=2}^{K} \rho_\ell^j \frac{\rho_k\rho_\ell}{\left(1-\rho_k\rho_\ell\right)} \varepsilon_{k\ell} , \tag{74}$$

$$\bar{r}_{1k}^{i,i+j} = -\bar{\varepsilon}_{1k}\rho_k^j + \sum_{\ell=2}^{K} \rho_k^j \frac{\rho_k\rho_\ell}{\left(1-\rho_k\rho_\ell\right)} \bar{\varepsilon}_{k\ell} , \qquad k \neq 1 , \tag{75}$$

$$\bar{r}_{k1}^{i,i+j} = -\sum_{\ell=2}^{K} \rho_\ell^j \frac{\rho_k\rho_\ell}{\left(1-\rho_k\rho_\ell\right)} \bar{\varepsilon}_{k\ell} , \qquad k \neq 1 , \tag{76}$$

and

$$\bar{r}_{k\ell}^{i,i+j} = \rho_\ell^j \frac{\rho_k\rho_\ell}{\left(1-\rho_k\rho_\ell\right)} \bar{\varepsilon}_{k\ell} , \qquad k \neq 1, \qquad \ell = 1 . \tag{77}$$

Making use of the above expressions we find that

$$E\left\{r_R^i r_R^{i+j}\right\} = \sum_{k=2}^{K} \alpha_k \rho_k^{j-1} , \qquad j \geq 1 , \tag{78}$$

where the α_k are complicated functions of all the ρ's and all the $\bar{\varepsilon}$'s. Using MacMillan's approach, we write

$$\sigma^2_{R,M} = \frac{1}{M}\sigma_R^2 + \frac{2\sum_{i=2}^{M} E\left\{r_R^i r_R^{i-1}\right\} + 2\sum_{i=3}^{M} E\left\{r_R^i r_R^{i-2}\right\} + \cdots}{M^2} , \tag{79}$$

so thus, for large M

$$\sigma^2_{R,M} \approx \frac{1}{M}\left[\sigma_R^2 + 2\sum_{k=1}^{K} \frac{\alpha_k}{\left(1 - \rho_k\right)}\right] . \tag{80}$$

Equation (80) is a generalization of the equation for σ on page 74 of Ref. 3, and is identical with MacMillan's expression if only one ρ_k is different from zero. It is possible that one could use Eq. (80) assuming, perhaps, that only two of the ρ_k (ρ_2 and ρ_3 for example) are different from zero. The four parmeters α_2, α_3, ρ_2, and ρ_3 could, then, be fitted to match observed correlation coefficients of lag 1, 2, 3, and 4. Whether or not such a procedure would be practical is not clear at present.

E. Analysis of Model Problems

In our analysis of the Monte Carlo process we have dealt with a random walk in a discretized phase space, i.e., a random walk among K distinct boxes. It is easy, however, to adapt this analysis to a continuous random walk by letting K go to infinity, while replacing sums over ν by integrals over space and energy. The model problems discussed in this section are problems in which the position and energy variables are regarded as continuous.

We consider, as our model problem configuration, a homogeneous cube of thickness T. Suppose that the scalar flux vanishes on all faces of the cube, and that T is large enough so that diffusion theory is valid. In one group the eigenvectors are, then, given by the expression

$$U_{k\ell m} = C_{k\ell m} \sin B_k X \sin B_\ell Y \sin B_m Z , \qquad B_k \equiv kB ,$$
$$B \equiv \pi/T , \qquad k,\ell,m = 1, 2, \ldots , \tag{81}$$

where the $C_{k\ell m}$ are normalization constants. The adjoints take the form

$$U^*_{k\ell m} = \left(8/T^3 C_{k\ell m}\right) \sin B_k X \sin B_\ell Y \sin B_m Z . \tag{82}$$

$$\bar{\varepsilon}_{k\ell m,k\ell m} = \frac{1}{N}\left(8/T^3C_{k\ell m}\right)^2\left(C_{111}/B^3\right)\alpha_k\alpha_\ell\alpha_m \tag{83}$$

for k, ℓ, and m are not all equal to one, and

$$\alpha_k \equiv 1 + 1/(4k^2 - 1) .$$

Our normalization condition requires that

$$C_{111} = \lambda_{111}(B/2)^3 ,$$

so that we may write

$$\bar{\varepsilon}_{k\ell m,k\ell m} = \frac{1}{N}\left[8\lambda_{111}\Big/\left(T^3C_{k\ell m}\right)^2\right]\alpha_k\alpha_\ell\alpha_m . \tag{84}$$

In the proposed model problem

$$\lambda_{k\ell m} = \left[1 + \tau B^2(k^2 + \ell^2 + m^2)\right]^{-1} . \tag{85}$$

Consequently

$$\rho_{k\ell m} \approx 1 - \tau B^2(k^2 + \ell^2 + m^2 - 3)/\lambda_{111} . \tag{86}$$

and, to first order in B^2,

$$1 - \rho^2_{k\ell m} = 2\tau B^2(k^2 + \ell^2 + m^2 - 3)/\lambda_{111} . \tag{87}$$

Approximately, then

$$\bar{r}_{k\ell m,k\ell m} = \frac{1}{N}\frac{4\lambda^2_{111}\alpha_k\alpha_\ell\alpha_m}{\left(T\,C_{k\ell m}\right)^2\left(k^2 + \ell^2 + m^2 - 3\right)} . \tag{88}$$

Thus the root-mean-square coefficient of the kℓm-*th* mode is

$$C_{k\ell m}\sqrt{\frac{4\lambda_{111}^{2}\alpha_k\alpha_\ell\alpha_m}{N\pi B^2\left[T^3C_{k\ell m}\right]^2\left(k^2+m^2+\ell^2-3\right)}} = \sqrt{\frac{4\lambda_{111}^{2}\alpha_k\alpha_\ell\alpha_m}{N\pi B^2\pi^6\left(k^2+\ell^2+m^2-3\right)}} \,. \qquad (89)$$

On the other hand, the expected fission source density produced, at the end of the i-*th* generation, by a single fission neutron of the $i-1^{st}$ generation has the form

$$\varepsilon = \lambda_{111}(B/2)^3 \sin BX \sin BY \sin BZ$$

$$= \lambda_{111}(\pi/2T)^3 \sin BX \sin BY \sin BZ \,. \qquad (90)$$

Therefore the ratio, $f_{k\ell m}$, of the root-mean-square coefficient of the $k\ell m$-*th* error mode, to the expected coefficient of the main mode, is given by the expression

$$f_{k\ell m} = \sqrt{\frac{256\,\alpha_k\alpha_\ell\alpha_m}{N\pi^6\tau B^2\left(k^2+\ell^2+m^2-3\right)}} \,. \qquad (91)$$

The quantity $f_{k\ell m}$ is a rough measure of the relative amplitude of the $k\ell m$-*th* error mode in the fission source distribution. If the main mode leakage probability is 30% (fairly typical for experimental fast reactors), then $\tau B^2 = 0.1$. In this case we find that roughly 15,000 histories would be required, per generation, to reduce contamination by each of the three principle error modes to 1%. On present computers it is generally unfeasible to work with such a large number of histories per generation.

Averaging over M generations we get

$$f_{k\ell m,M} = \sqrt{\frac{512\,\alpha_k\alpha_\ell\alpha_m\lambda_{111}}{N M\pi^6(\tau B^2)^2\left(k^2+\ell^2+m^2-3\right)^2}} \,, \qquad (92)$$

assuming that M is sufficiently large so that Eq. (54) is valid. Now we find that 100,000 histories would be required (i.e. $NM = 100{,}000$), after settling to reduce contaminations by each of the three principle error modes to 1%. This is a rather large number of histories, but a Monte Carlo problem with 100,000 histories can be run in roughly three hours, generally, on the latest IBM or CDC computers.

This simple analysis may give us some idea of the nature of the modal spectrum in the asymptotic fission source, and of the dependence of the spectrum on the number of histories. On the other hand, it tells us very little about fluctuations in the source, or in reaction rates, in specified

subregions of the problem configuration. Certainly it would be possible to study local fluctuations in this first model problem. However, to shorten our computations, we turn now to a model problem which is similar to the first, but still simpler. The second problem configuration is again a cube of thickness T, but with reflecting boundary conditions imposed on each face. It will be convenient, in this case, to designate the main mode with subscripts 000, in place of the subscripts 111. In this modified notation

$$U_{k\ell m} = \sum_{k\ell m} h_k(x)h_\ell(y)h_m(z) \ . \tag{93}$$

Here the $\alpha_{k\ell m}$ are normalization constants; further

$$\begin{aligned} h_k(x) &\equiv 1 , \qquad k = 0 , \\ h_k(x) &\equiv \cos kBx , \qquad k \neq 0 , \end{aligned} \tag{94}$$

where $B \equiv \pi/T$. As for the adjoints

$$\begin{aligned} U^*_{k\ell m} &= \left(1/\alpha_{k\ell m}\right)\left[\beta_k h_k(x)\beta_\ell h_\ell(y)\beta_m h_m(z)\right] , \\ \beta_k &\equiv (2/T) , \qquad k \neq 0 , \\ \beta_k &= (1/T) , \qquad k = 0 . \end{aligned} \tag{95}$$

From Eqs. (93) and (95) we see that

$$\bar{\varepsilon}_{k\ell m,k\ell m} = \frac{\alpha_{000}}{N}\frac{\beta_k\beta_\ell\beta_m}{\alpha^2_{k\ell m}} \quad \text{unless } k = \ell = m = 0 \ . \tag{96}$$

Further it is clear that

$$\varepsilon_{000,000} = 0 , \tag{97}$$

and that

$$\varepsilon_{k\ell m,k'\ell'm'} = 0 \quad \text{unless } k = k',\ \ell = \ell',\ m = m' \ . \tag{98}$$

As in Eq. (70) define

$$\underline{r}^i_R = \int_R \left(\underline{v}^i - \underline{U}_1\right) dV = \sum_{k,\ell,m} C_{k\ell m}\tilde{\gamma}_{k\ell m} , \tag{99}$$

$$C_{k\ell m} = \int_R U_{k\ell m}\, dV \ . \tag{99}$$

Let R be the cube bounded by the planes $x = 0$, $x = t$, $y = 0$, $y = t$, $z = 0$, and $z = t$ Then

$$C_{k\ell m} = \alpha_{k\ell m} f_k f_\ell f_m \ ,$$

$$f_k = (\sin kBt)/kB \ , \qquad k \neq 0 \ ,$$

$$f_k = t \ , \qquad k = 0 \ . \tag{100}$$

As in Eq. (71)

$$\sigma_R^2 = \sum_{k,\ell,m} \sum_{k',\ell',m} C_{k\ell m} C_{k'\ell'm'} \bar{r}_{k\ell m,k'\ell'm'} \ . \tag{101}$$

But one can show from Eqs. (50), (51), (97), and (98) that

$$r_{000,000} = 0 \ . \tag{102}$$

$$\bar{r}_{k\ell m,k'\ell'm'} = 0 \ , \quad \text{unless } k = k',\ \ell = \ell',\ m = m' \ . \tag{103}$$

Therefore

$$\sigma^2 = 3 \sum_{k=1}^{\infty} \sum_{\ell=0}^{\infty} \sum_{m=0}^{\infty} C_{k\ell m}^2 \bar{r}_{k\ell m,k\ell m} \ , \tag{104}$$

$$\sigma_R^2 = 3 \sum_{k=1}^{\infty} \sum_{\ell=0}^{\infty} \sum_{m=0}^{\infty} C_{k\ell m}^2 \frac{\bar{\varepsilon}_{k\ell m,k\ell m}}{1 - \rho_{k\ell m}^2} \ , \tag{105}$$

$$\sigma_R^2 = 3 \frac{\alpha_{000}}{N} \sum_{k,\ell,m} \frac{\beta_k f_k^2 \beta_\ell f_\ell^2 \beta_m f_m^2}{1 - \rho_{k\ell m}^2} \ , \tag{106}$$

$$\sigma_R^2 = \frac{3}{N} \sum_{k,\ell,m} \frac{\left[F_k F_\ell F_m\right]^2}{1 - \rho_{k\ell m}^2} \ , \tag{107}$$

since $\alpha_{000} = T^3$. Here

$$F_k \equiv \sqrt{(\beta_k/T)}\, f_k \ ,$$

$$= (t/T) \ , \qquad k = 0 \ ,$$

$$= (\sqrt{2}/\pi) \sin (kBt)/k \ , \qquad k \neq 0 \ . \tag{108}$$

Since high harmonics may contribute substantially to the variance, it seems worthwhile, in Eq. (107), to use a rigorous expression for $\rho_{k\ell m}$. For the sake of simplicity, we assume that the medium in the cube is a pure absorber. Then

$$\rho_{k\ell m} \equiv \lambda_{k\ell m}/\lambda_{000} , \tag{109}$$

$$\lambda_{k\ell m} = \frac{\Sigma_t}{B\sqrt{k^2 + \ell^2 + m^2}} \tan^{-1}\left(\frac{B\sqrt{k^2 + \ell^2 + m^2}}{\Sigma_t}\right) . \tag{110}$$

Via Eqs. (107), (108), and (110), it is possible to compute σ_R^2 numerically to any desired level of accuracy.

By methods now familiar, it can be shown that

$$E\left\{r_R^i r_R^{i-1}\right\} = \frac{3}{N} \sum_{k,\ell,m}^{\infty} \rho_{k\ell m} \frac{\left[F_k F_\ell F_m\right]^2}{1 - \rho_{k\ell m}^2} , \tag{111}$$

and that, for M sufficiently large

$$\sigma_{R,M}^2 = \frac{1}{NM} \sigma_R^2 \left\{1 + \frac{6 \sum_{k,\ell,m} \rho_{k\ell m}\left[F_k F_\ell F_m\right]^2 / \left(1 - \rho_{k\ell m}^2\right)\left(1 - \rho_{k\ell m}\right)}{\sigma_R^2}\right\} . \tag{112}$$

On the other hand, MacMillan's method gives

$$\sigma_{R,M}^2 \approx \sigma_{R,M}^2 \equiv \frac{1}{NM} \sigma_R^2 \left\{1 + \frac{6 \sum_{k,\ell,m} \rho_{k\ell m}\left[F_k F_\ell F_m\right]^2 / \left(1 - \rho_{k\ell m}^2\right)}{\sigma_R^2\left(1 - \rho_{100}\right)}\right\} . \tag{113}$$

We see, again, that MacMillan's approximation would be rigorous if all the eigenvalues were zero, except for λ_{000} and for $\lambda_{100} = \lambda_{010} = \lambda_{001}$.

In the absence of correlations we would have

$$\sigma_{R,M}^2 = \frac{1}{NM} \sigma_R^2 .$$

Thus, in Eqs. (112) and (113), the quantities in parentheses act as amplification factors embodying the correlation effects. Define

$$A = 1 + \frac{6 \sum_{k,\ell,m} \rho_{k\ell m} \left[F_k F_\ell F_m\right]^2 \Big/ \left(1 - \rho_{k\ell m}^2\right)\left(1 - \rho_{k\ell m}\right)}{\sigma_R^2}, \tag{114}$$

$$\hat{A} = 1 + \frac{6 \sum_{k,\ell,m} \rho_{k\ell m} \left[F_k F_\ell F_m\right]^2 \Big/ \left(1 - \rho_{k\ell m}^2\right)}{\sigma_R^2\left(1 - \rho_{100}\right)}. \tag{115}$$

Here A is the "true" amplification factor while $\hat{A}$ is the approximate "MacMillan amplification factor". It will be seen that A and $\hat{A}$ depend only on the absorption probability $p = (t/T)^3$, and on $\tau B^2 = B^2/3\Sigma_t^2$. The intergeneration correlation coefficient

$$C \equiv E\left\{r_R^i r_R^{i-1}\right\} \Big/ \sigma_R^2$$

is also determined by p and τB^2. Values of A, $\hat{A}$, and C are listed in Table I for various combinations of p and τB^2. In the last colume of Table I we have displayed the percentage errors in $\sqrt{\hat{A}}$ (in place of the errors in A) since $\sqrt{A}$ is a measure of the uncertainty in the fission rate within R. Note that when $\tau B^2 = 0.1$ the dominance ratio (ρ_{100}) is approximately equal to 0.9, and that this dominance ratio is not at all large for a thermal reactor. On the other hand, $\tau B^2 = 0.3$ corresponds to $\rho_{100} \approx 0.7$, a dominance ratio characteristic of a small fast reactor.

The entries in Table I display some fairly obvious regularities. First of all we see that:

(a) As one would expect, the amplification factors tend to be large when the dominance ratio is close to one. In fact it is clear from Eq. (114) that as $\rho_{100} \to 1$, $A \to \infty$.

(b) Secondly, A and C are large when p is large (i.e., when t/T is large), and both are small when p is small. For $k \ll (1/\pi)(T/t)$, we see that $F_k \approx p$: thus if p is small, F_k is almost constant for a wide range of k's. Many modes, including many for which $\rho_{k\ell m}$ is small, then contribute to the sums in Eqs. (111) and (112). The presence of $\rho_{k\ell m}$ as a factor in these sums then tends to make the correlation coefficient C, and the amplification factor, A, small. On the other hand, when p is large, F_k decreases as 1/k, enhancing the importance of modes near the main mode. A and C then become large.

Finally we see that when $\rho_{100} \approx 0.09$, the MacMillan method is reasonably accurate down to $p = 0.005$. In leakier reactors with $\rho_{100} \approx 0.07$, the MacMillan method is adequate for p's as low as 0.001. Eventually, as p becomes still smaller, C approaches zero and A approaches one. Significant errors in the MacMillan method do occur, but in a range where p is so small that the binomial estimator (the only absorptions estimator we can deal with here) starts to become ineffective.

TABLE I

Amplification Factors and Correlation Coefficients for Various Values of the Problem Parameters

τB^2	p	C	A	A	Error in $\sqrt{\hat{A}}$ (%)
0.1	0.25	0.86	18.1	18.2	0
0.1	0.1	0.84	16.5	17.8	4
0.1	0.01	0.69	8.9	14.8	29
0.1	0.005	0.62	7.0	13.4	38
0.1	0.001	0.45	3.8	10.0	160
0.3	0.1	0.67	6.4	7.7	10
0.3	0.01	0.49	3.7	5.9	26
0.3	0.001	0.28	2.0	3.8	38

On the other hand there are many other estimators which can be introduced in this range. Track length estimators, collision and line-of-sight estimators are often used, when p is small, to reduce the variance in reaction rate estimates. We cannot say what these estimators will do to correlation coefficients or amplification factors. It is possible, however, that such estimators reduce variance by suppressing the uncorrelated "noise" component of the statistical fluctuations, without strongly affecting correlated large-scale fluctuations. In this case, amplification factors would again become large and a more extended analysis of MacMillan's method would be necessary.

Part II

THEORETICAL STUDY OF THE MONTE CARLO EIGENVALUE COMPUTATION, BIASES

A. Calculation of the Eigenvalue Bias in the Mathematical Model

As discussed in Part I, the retention of terms nonlinear in statistical fluctuations when calculating deviations from the fundamental mode eigenvector will give rise to estimates of the bias in the calculated eigenvalue. Following the definitions of Section A of Part I, one obtains from Eq. (10)

$$\underline{\delta}^{i+1} = A\underline{\delta}^{i} - \frac{1}{N}\left(\hat{\underline{\tau}}^{T} \cdot \underline{\delta}^{i}\right) A\underline{\delta}^{i} + \underline{\varepsilon}^{i} , \tag{116}$$

where A and $\hat{\underline{\tau}}^{T}$ are defined by Eq. (14). The statistical error vector $\underline{\varepsilon}^{i}$ is defined in Eq. (6) and has the property $E\{\underline{\varepsilon}^{i}\} = 0$. However, due to the presence of nonlinear terms in Eq. (116), the expectation value of $\underline{\delta}^{i+1}$ does not generally vanish even in the limit $i \to \infty$. Since the deviation of the estimated eigenvalue of the i-*th* generation from the fundamental mode eigenvalue is given by

$$\Delta\lambda^i = \lambda^i - \lambda_1 = \frac{\lambda_1}{N} \hat{\underline{\tau}}^T \cdot \underline{\delta}^i , \tag{117}$$

the expected value of the bias may be obtained from

$$\Delta\lambda \equiv \lim_{i\to\infty} E\left\{\Delta\lambda^i\right\} = \frac{\lambda_1}{N} \lim_{i\to\infty} E\left\{\hat{\underline{\tau}}^t \cdot \underline{\delta}^i\right\}. \tag{118}$$

If we retain only terms quadratic in $\underline{\varepsilon}^i$ in Eq. (116), we have the equation

$$\underline{\delta}^{i+1} = A\underline{\delta}^i - \frac{1}{N}\left(\hat{\underline{\tau}}^T \cdot \tilde{\underline{\delta}}^i\right) A\tilde{\underline{\delta}}^i + \underline{\varepsilon}^i , \tag{119}$$

where

$$\tilde{\underline{\delta}}^{i+1} = \sum_{n=0}^{\infty} A^n \underline{\varepsilon}^{i-n} \tag{120}$$

was obtained in Eq. (15). Assuming again that an infinite number of generations have passed, Eq. (119) possesses the solution

$$\underline{\delta}^{i+1} = \tilde{\underline{\delta}}^{i+1} - \frac{1}{N}\sum_{n=0}^{\infty}\left(\hat{\underline{\tau}}^T \cdot \hat{\underline{\delta}}^{i-n}\right) A^{n+1}\tilde{\underline{\delta}}^{i-n} . \tag{121}$$

Defining

$$\alpha \equiv \Delta\lambda/\lambda_1$$

and noting that

$$E\left\{\tilde{\underline{\delta}}^{i+1}\right\} = 0 ,$$

we obtain

$$\alpha = -\frac{1}{N^2}\sum_{n=0}^{\infty} E\left\{\left(\hat{\underline{\tau}}^T \cdot \tilde{\underline{\delta}}^{i-n}\right)\left(\hat{\underline{\tau}}^T \cdot A^{n+1}\tilde{\underline{\delta}}^{i-n}\right)\right\} . \tag{122}$$

Upon substitution of Eq. (120),

$$\alpha = -\frac{1}{N^2}\sum_{n=0}^{\infty}\sum_{p=0}^{\infty}\sum_{q=0}^{\infty} E\left\{\left(\hat{\underline{\tau}}^T \cdot A^p \underline{\varepsilon}_{i-n-p-1}\right)\left(\hat{\underline{\tau}}^T \cdot A^{n+q+1} \underline{\varepsilon}_{i-n-q-1}\right)\right\}$$

or

$$\alpha = -\frac{1}{N^2}\sum_{n=0}^{\infty}\sum_{p=0}^{\infty} E\left\{\left(\hat{\underline{\tau}}^T \cdot A^p \underline{\varepsilon}_{i-n-p-1}\right)\left(\hat{\underline{\tau}}^T \cdot A^{n+p+1} \underline{\varepsilon}_{i-n-p-1}\right)\right\} , \qquad (123)$$

since the statistical fluctuations in different generations are uncorrelated. Using Eqs. (18) and (23), we obtain

$$\alpha = -\frac{1}{N^2}\sum_{n=0}^{\infty}\sum_{p=0}^{\infty}\sum_{k}\sum_{\ell}\left(\hat{\underline{\tau}}^T \cdot A^p \underline{U}_k\right)\left(\hat{\underline{\tau}}^T \cdot A^{n+p+1} \underline{U}_\ell\right) \varepsilon_{k\ell} .$$

From Eq. (16), we obtain

$$\hat{\underline{\tau}}^T \cdot A^p \underline{U}_k = \left(\rho_k - 1\right) \rho_k^p ,$$

for $p \geq 1$ and for all modes k such that $\hat{\underline{\tau}}^T \cdot \underline{U}_k \neq 0$. It then follows that

$$\alpha = +\frac{1}{N^2}\sum_{k=1}^{'}\sum_{\ell=2}^{'} \rho_k\rho_\ell\left(1 - \rho_\ell\right)\sum_{n=0}^{\infty} \rho_\ell^n \varepsilon_{k\ell}$$

$$-\frac{1}{N^2}\sum_{k'=2}^{'}\sum_{\ell=2}^{'}\sum_{p=1}^{\infty}\left(1 - \rho_k\right)\left(1 - \rho_\ell\right) \rho_k^p\rho_\ell^p \sum_{n=0}^{\infty} \rho_\ell^{n+1}\varepsilon_{k\ell} ,$$

which reduces to

$$\alpha = \frac{1}{N^2}\sum_{k=1}^{'}\sum_{\ell=2}^{'}\frac{\rho_k\rho_\ell\left(1 - \rho_\ell\right)}{1 - \rho_k\rho_\ell} \varepsilon_{k\ell} . \qquad (124)$$

As in Part I, $\rho_k = \lambda_k/\lambda_1$, and the summations designated with primes run over those modes with $\hat{\underline{\tau}}^T \cdot \underline{U}_k \neq 0$.

B. Approximations for Estimating the Eigenvalue Bias

Equation (124), for the fractional eigenvalue bias, may be written as

$$\alpha = \alpha_0 + \alpha_1 + \alpha_2 ,$$

where

$$\alpha_0 = \frac{1}{N^2} \sum_{\ell=2}' \rho_\ell \varepsilon_{\ell 1} , \tag{125}$$

$$\alpha_1 = \frac{1}{N^2} \sum_{k=2}' \sum_{\ell=2}' \rho_k \rho_\ell \left(1 - \rho_\ell\right) \varepsilon_{k\ell} , \tag{126}$$

$$\alpha_2 = \frac{1}{N^2} \sum_{k=2}' \sum_{\ell=2}' \frac{\left(\rho_k \rho_\ell\right)^2 \left(1 - \rho_\ell\right)}{1 - \rho_k \rho_\ell} \varepsilon_{k\ell} . \tag{127}$$

In the above partition, α_0 contains all contributions which are weighted by the fundamental mode and can be expected to contain a large contribution to the bias; α_1 is the leading term in the series expansion of that part of α which contains contributions only from higher-order modes. The expressions for α_0 and α_1 can be converted into sums over regions rather than over modes by utilizing the following relations:

$$\varepsilon_{k\ell} = \sum_{\mu,\nu} U^*_{k\mu} U^*_{\ell\nu} \varepsilon_{\mu\nu} ,$$

$$\varepsilon_{\mu\nu} = N\left[\delta_{\mu\nu} W_\nu U_{1\nu} - U_{1\mu} U_{i\nu}\right] ,$$

and

$$\sum_{k=1}' \rho_k \varepsilon_{k\ell} = \frac{1}{\lambda_1} \sum_{k=1}' \sum_{\sigma} \sum_{\mu} \sum_{\nu} U_{k\sigma} U^*_{k\mu} U^*_{\ell\nu} \varepsilon_{\mu\nu}$$

$$= \frac{1}{\lambda_1} \sum_{\sigma} \sum_{\mu} \sum_{\nu} \delta_{\sigma\mu} U^*_{\ell\nu} \varepsilon_{\mu\nu}$$

$$= \frac{1}{\lambda_1} \sum_{\mu} \sum_{\nu} U^*_{\ell\nu} \varepsilon_{\mu\nu} ,$$

where completeness has been assumed. Applying the above relationships to Eq. (125), we obtain

$$\alpha_0 = \frac{1}{N^2}\left[\frac{1}{\lambda_1}\sum_{\mu}\sum_{\nu} U^*_{1\nu}\varepsilon_{\mu\nu} - \sum_{\mu,\nu} U^*_{1\mu}U^*_{1\nu}\varepsilon_{\mu\nu}\right]$$

$$= \frac{1}{N}\sum_{\nu}\left(\frac{1}{\lambda_1} - U^*_{1\nu}\right) U^*_{1\nu}W_\nu U_{1\nu} \ . \qquad (128)$$

In Eq. (126), we obtain

$$\alpha_1 = \frac{1}{N^2}\left[\frac{1}{\lambda_1}\sum_{\ell=1}{}' \rho_\ell \left(1 - \rho_\ell\right) \sum_{\mu,\nu} U^*_{\ell\nu}\varepsilon_{\mu\nu}\right.$$

$$\left. - \sum_{\ell=1}{}' \rho_\ell\left(1 - \rho_\ell\right) \sum_{\mu,\nu} U^*_{1\mu}U^*_{\ell\nu}\varepsilon_{\mu\nu}\right] \ .$$

Noting that

$$\left(1 - \rho_\ell\right) U^*_{\ell\nu} = \sum_{\sigma} U^*_{\ell\sigma}\left[\delta_{\sigma\nu} - \hat{H}_{\sigma\nu}\right]$$

and

$$\sum_{\ell=1}{}' \rho_\ell U^*_{\ell\sigma} = \frac{1}{\lambda_1}\sum_{\ell=1}\sum_{\tau} U_{\ell\tau}U^*_{\ell\sigma} = \frac{1}{\lambda_1}\sum_{\tau}\delta_{\tau\sigma} = \frac{1}{\lambda_1} \ ,$$

we obtain

$$\alpha_1 = \frac{1}{N^2\lambda_1^2}\sum_{\sigma,\mu\nu}\left[\delta_{\sigma\nu} - \hat{H}_{\sigma\nu}\right]\varepsilon_{\mu\nu} - \frac{1}{N^2\lambda_1}\sum_{\sigma,\mu,\nu}\left[\delta_{\sigma\nu} - \hat{H}_{\sigma\nu}\right] U^*_{1\mu}\varepsilon_{\mu\nu} \ .$$

Inserting the expression for $\varepsilon_{\mu\nu}$ gives

$$\alpha_1 = \frac{1}{N\lambda_1}\sum_{\nu}\left(\frac{1}{\lambda_1} - U^*_{1\nu}\right)\left(1 - \sum_{\sigma}\hat{H}_{\sigma\nu}\right) W_\nu U_{1\nu} \ . \qquad (129)$$

Define the quantity G_ν by

$$G_\nu = \sum_\mu H_{\mu\nu} = \lambda_1 \sum_\mu \hat{H}_{\mu\nu} \cdot \tag{130}$$

Then

$$\alpha_1 = \frac{1}{N} \sum_\nu \left(\frac{1}{\lambda_1} - U^*_{1\nu} \right) \left(\frac{1}{\lambda_1} - \frac{G_\nu}{\lambda_1^2} \right) W_\nu U_{1\nu} \cdot$$

If we now estimate α with the approximation

$$\alpha \approx \alpha_0 + \alpha_1 ,$$

we obtain

$$\alpha \approx \frac{1}{N} \sum_\nu \left(\frac{1}{\lambda_1} - U^*_{1\nu} \right) \left(\frac{1}{\lambda_1} + U^*_{1\nu} - \frac{1}{\lambda_1^2} G_\nu \right) W_\nu U_{1\nu} \cdot \tag{131}$$

The approximation, Eq. (131), may be evaluated during a Monte Carlo run if the appropriately normalized importance function $U^*_{1\nu}$ is supplied. The other quantities appearing have the following interpretation: $U_{1\nu}/\lambda_1$ is the contribution of a unit source in region ν; W_ν is the weight of a site produced by the absorption of a unit-weight neutron in region ν; and G_ν is the weight of a site produced by a unit-weight neutron <u>born</u> in region ν.

Another approximation for the eigenvalue bias may be derived by noting that

$$\alpha_1 + \alpha_2 = \frac{1}{N^2} \sum_{k=2} \sum_{\ell=2} \sum_{n=0}^{\infty} \left(\underline{\hat{\tau}}^T \cdot \underline{U}_k \right) \left(\underline{\hat{\tau}}^T \cdot \underline{U}_\ell \right) \left(1 - \rho_\ell \right) \left(\rho_k \rho_\ell \right)^n \varepsilon_{k\ell}$$

$$= \frac{1}{N^2} \sum_{n=0}^{\infty} E \left\{ \left(\underline{\hat{\tau}}^T \cdot [I - \underline{U}_1 \underline{U}_1^*] \hat{H}^n \underline{\varepsilon}^{i-n-1} \right) \right.$$

$$\left. \times \left(\underline{\hat{\tau}}^T \cdot [I - \underline{U}_1 \underline{U}_1^*] [\hat{H}^n - \hat{H}^{n+1}] \, \underline{\varepsilon}^{i-n-1} \right) \right\} .$$

It follows that

$$\alpha_1 + \alpha_2 = \frac{1}{N^2} E\left\{\left[\underline{\hat{\tau}}^T \cdot \left(1 - \underline{U}_1\underline{U}_1^*\right) \underline{\tilde{\delta}}^i\right]\left[\underline{\hat{\tau}}^T \cdot \left(1 - \underline{U}_1\underline{U}_1\right)\left(\underline{\tilde{\delta}}^i - \underline{\tilde{\delta}}^{i+1}\right)\right]\right\} .$$

If, in the above equation, we make the approximation that

$$\underline{\tilde{\delta}}^i \approx \underline{\delta}^i \approx \underline{V}^i - \underline{V}_{ave} ,$$

then

$$\alpha_1 + \alpha_2 \approx \frac{1}{N^2} E\left\{\left[\left(\underline{\hat{\tau}}^T \cdot \left[\underline{V}^i - \underline{V}_{ave}\right]\right) - \left(\underline{U}_1^* \cdot \left[\underline{V}^i - \underline{V}_{ave}\right]\right)\right]\right.$$
$$\left. \times \left[\left(\underline{\hat{\tau}}^T \cdot \left[\underline{V}^i - \underline{V}^{i+1}\right]\right) - \left(\underline{U}_1^* \cdot \left[\underline{V}^i - \underline{V}^{i+1}\right]\right)\right]\right\} .$$

The approximation for $\alpha_1 + \alpha_2$ may be estimated from a Monte Carlo run if the importance functions are either supplied externally or generated by the run. When combined with α_0 from Eq. (128), an estimate of the eigenvalue bias will be obtained.

C. The Bias in the Eigenvector

The bias which occurs in the eigenvector is related to our previously defined quantities by

$$\Delta\underline{U} = \frac{1}{N} E\left\{\underline{\delta}^i\right\} , \tag{132}$$

where $\underline{\delta}^i$ is obtained from Eq. (116). The eigenvalue bias is related to $\Delta\underline{U}$ by

$$\alpha \equiv \frac{\Delta\lambda}{\lambda_1} = \underline{\hat{\tau}}^T \cdot \Delta\underline{U} .$$

By steps similar to those used in the derivation of Eq. (124), we obtain

$$\Delta\underline{U} = \frac{1}{N^2} \sum_{k=1} \sum_{\ell=2} \frac{\left(\underline{\hat{\tau}}^T \cdot \underline{U}_k\right) \varepsilon_{k\ell}}{1 - \rho_k\rho_\ell} \left[\left(\underline{\hat{\tau}}^T \cdot \underline{U}_\ell\right) \underline{U}_1 - \rho_\ell \underline{U}_\ell\right] . \tag{133}$$

By examination of Eq. (133), two features may be noticed. First, contributions from modes may be present which do not contribute at all to the eigenvalue bias (i.e., those with $\underline{\tau}^T \cdot \underline{U}_\ell = 0$). Second, modes with eigenvalues close to the fundamental, which contribute only slightly to the eigenvalue bias, are much

stronger contributors to the eigenvector bias. As a consequence, large local bias in source shape may be present even when eigenvalue bias is unimportant.

Some understanding of the potential difficulty may be gained by examining the leading term in Eq. (135) coming from the series expansion of $[1 - \rho_k \rho_\ell]^{-1}$:

$$\Delta \underline{U}^{(0)} = \frac{1}{N^2} \sum_{k=1} \sum_{\ell=2} \left(\hat{\tau}^T \cdot \underline{U}_k \right) \left[\left(\hat{\tau}^T \cdot \underline{U}_\ell \right) \underline{U}_1 - \rho_\ell \underline{U}_\ell \right] \varepsilon_{k\ell} \cdot$$

Using the relationships of the previous section, we obtain

$$\Delta \underline{U}^{(0)} = H \frac{1}{N\lambda_1^2} \sum_{\mu} W_\mu U_{1\mu} \left[\frac{1}{\lambda_1} \underline{U}_1 - \sum_{\ell=1} U^*_{\mu\ell} \underline{U}_\ell \right] . \tag{134}$$

By using the assumed completeness of the eigenvectors, Eq. (134) may be reduced to the form

$$\Delta \underline{U}^{(0)} = H \underline{S} , \tag{135}$$

where

$$\underline{S} = \frac{1}{N\lambda_1^2} \left[\bar{W} - W \right] \underline{U}_1 . \tag{136}$$

In Eq. (136), W is the diagonal matrix with elements $W_\mu \delta_{\mu\nu}$ and

$$\bar{W} = \left(\frac{\sum_\mu W_\mu U_{1\mu}}{\sum_\mu U_{1\mu}} \right) I . \tag{137}$$

The lowest-order estimate for the eigenvector bias may thus be obtained from a source vector constructed by weighting the fundamental mode eigenvector by the deviation of the weight from its average over the fundamental mode. Applying the appropriate operator to $\underline{S}$ as defined in Eq. (136) will produce corresponding results for the bias in reaction rate estimates.

D. A Note on Reducing the Bias

It has been suggested by Lieberoth [1] that the bias may be reduced by modifying the Monte Carlo procedure. The analog of his suggestion which applies to our mathematical model may be described as follows:

(1) define a maximum weight $W_{max} \geq W_\nu$ for all ν;

(2) at each absorption, accept a source site with probability W_ν/W_{max}; and

(3) if the site is accepted, assign the weight W_{max}.

The effect of the procedure is to do a Monte Carlo calculation with only constant or zero weights allowed. A correlation matrix analogous to $\varepsilon_{\mu\nu}$ may be derived which is given by

$$\varepsilon^*_{\mu\nu} = N\left\{\delta_{\mu\nu} W_{max} U_{1\mu} - U_{1\mu} U_{1\nu}\right\}$$

and

$$\varepsilon^*_{k\ell} = N\left\{W_{max} \sum_{\mu} U^*_{k\mu} U^*_{1\mu} U_{1\mu} - \delta_{k\ell}\delta_{\ell,1}\right\} . \qquad (138)$$

The effect may be seen in Eq. (134) by the replacement $W_\nu \to W_{max}$, causing the lowest-order estimate of the eigenvector bias to vanish identically: $\Delta\underline{U}^{(0)} \to 0$ when $W_\nu \to W_{max}$. The increase in the magnitude of the correlation matrix, Eq. (138), will increase the magnitude of the nonvanishing terms, partly offsetting the gain obtained by eliminating the first term. Variances in calculated quantities will be increased as well.

If the presence of the bias is considered to be a potential difficulty, then the simplest and most direct approach is to try to use as large a number N of neutrons per generation as is feasible after sufficient source settling and to take advantage of the 1/N dependence of the bias.

Part III

MONTE CARLO CODE DEVELOPMENT AT ARGONNE NATIONAL LABORATORY, VIM DEVELOPMENT

Monte Carlo work at Argonne has, as its main goal, the construction of a Monte Carlo code for use in the analysis of Argonne critical experiments. The code presently available at Argonne is the VIM code originally written by Levitt, et al, [4] at Atomics International. Responsibility for the maintenance of VIM, and for its future development, was transferred about a year ago from Atomics International to Argonne.

VIM is a continuous energy Monte Carlo code designed to treat a fast reactor lattice of rectangular subassemblies (or "drawers"). In the original VIM it was assumed that all interfaces within any drawer would be planar surfaces, and that each planar interface would be parallel to one of the three cartesian coordinate planes. Recently, however, combinatorial geometry routines written by MAGI [5] have been incorporated into VIM. The use of combinatorial geometry allows VIM calculations to be made in complex, irregular geometries as well as in lattice geometries. The combinatorial routines are being extended to the lattice environment to permit a full range of geometric options within repeating subassemblies. This capability is required for the

analysis of small-sample-worth experiments and for the analysis of pin-type fuel loadings, since small cylinders are used within the drawers.

The VIM cross-section library at present consists of 20 isotopes. Cross sections are specified pointwise from 10 eV to 10 MeV with different interpolation schemes possible in different energy ranges. ENDF/B data specifications are closely followed in the VIM library with respect to scattering angular distributions and individual isotopic fission spectra. Probability tables [6] are used for unresolved resonance cross sections. In the present library, all resonance data has been Doppler broadened to 300°K. Since the VIM cross-section library codes are now operational at Argonne, the number of isotopes in the library is being extended and it is now feasible to generate a multi-temperature library.

Among the modifications to VIM, which have been made at Argonne, has been the inclusion of variable dimensioning with dynamic allocation of storage. A small test problem may be executed in a total core requirement of about 60,000 words, with a realistic full-core eigenvalue problem requiring perhaps 400,000 words. The Monte Carlo calculation is completely core contained. The use of variable dimensioning has removed most limitations on problem complexity, with the exception of a temporary limit of 20 isotopes in a calculation; core size is the practical limitation on problem specification.

The computation of small sample worths is a primary goal in the VIM code development program. Such calculations are difficult simply because the samples are small. It is our intention, at present, to explore carrying out these calculations by a combination of three techniques, namely,

(1) roulette and splitting, to build up the density of particles around the sample;

(2) line-of-sight estimation, to make optimum use of collisions near the sample; and

(3) complete correlation.

By "complete correlation" we mean the simultaneous treatment of perturbed and unperturbed problems in a single random walk. The proposed computational method has the advantage that it is exact and that it does not require the simulation of the adjoint transport equation.

REFERENCES

1. J. LIEBEROTH, "A Monte Carlo Technique to Solve. The Static Eigenvalue Problem of the Boltzmann Transport Equation," *Nukleonik*, Bd. II, 213 (1968).

2. R. C. GAST, "Monte Carlo Eigenfunction Iteration Strategies That Are and Are Not Fair Game," WAPD-TM-878 (1969).

3. D. B. MAC MILLAN, "Monte Carlo Confidence Limits for Iterated-Source Calculations," *Nucl. Sci. Eng.*, 50, 73 (1973).

4. L. B. LEVITT and R. C. LEWIS, "VIM-1, A Nonmultigroup Monte Carlo Code for Analysis of Fast Critical Assemblies," AI-AEC-12951, Atomics International (1970).

5. M. O. COHEN et al, "SAM-CE: A Three-Dimensional Monte Carlo Code for the Solution of the Forward Neutron and Forward and Adjoint Gamma Ray Transport Equations," MR-7021, Mathematical Applications Group Inc. (1971).

6. L. B. LEVITT, "The Probabilty Table Method for Treating Unresolved Resonances in Monte Carlo Criticality Calculations," *Trans. Am. Nucl. Soc.*, 14, 648 (1974).