

On the Markov Chain Analysis of Source Iteration Monte Carlo Procedures for Criticality Problems: I

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Abstract—Monte Carlo techniques for the calculation of the effective multiplication factor K_{eff} of a nuclear reactor are discussed. A source iteration procedure based on a fixed number of fission points per generation is rigorously analyzed in the framework of the Markov chain corresponding to that procedure. It is shown that the estimated eigenvalue converges asymptotically to the correct eigenvalue of the transport equation and the bias in K_{eff} is bounded by an expression of the form $C \cdot N^{-1/2}$, where N is the number of fission points in each generation and C is a constant depending on the bulk properties of the reactor.

Sur l'analyse de l'itération de source à l'aide de la chaîne de Markoff — Techniques de Monte Carlo pour traiter les problèmes de criticité: I

Résumé—Sont discutées des techniques de Monte Carlo pour calculer le facteur effectif de multiplication K_{eff} d'un réacteur nucléaire. Un procédé d'itération de source reposant sur un nombre fixe de points de fission par génération est analysé rigoureusement à l'aide de la chaîne de Markoff correspondant à ce procédé. On montre que la valeur propre estimée converge de manière asymptotique vers la valeur propre correcte de l'équation de transport et que le biais en K_{eff} se trouve limité par une expression $C \cdot N^{-1/2}$, N étant le nombre des points de fission dans chaque génération et C étant une constante dépendant des propriétés principales du réacteur.

Zur Markow-Ketten-Analyse der Quelliteration — Monte-Carlo-Verfahren bei Kritikalitätsproblemen: I

Zusammenfassung—Es werden Monte-Carlo-Verfahren zur Berechnung des effektiven Multiplikationsfaktors K_{eff} eines Kernreaktors diskutiert. Ein auf einer festen Zahl von Spaltpunkten pro Generation beruhendes Quelliterationsverfahren wird im Rahmen der diesem Verfahren entsprechenden Markow-Kette unter Zugrundelegung strenger Maßstäbe analysiert. Es wird gezeigt, daß der geschätzte Eigenwert asymptotisch zum richtigen Eigenwert der Transportgleichung konvergiert und der systematische Fehler von K_{eff} durch einen Ausdruck der Form $C \cdot N^{-1/2}$ begrenzt wird. Dabei ist N die Anzahl der Spaltpunkte in jeder Generation und C eine von den Haupteigenschaften des Reaktors abhängige Konstante.

I. INTRODUCTION

Monte Carlo methods have become increasingly important in solving complicated eigenvalue problems of reactor physics. The reason is that the Monte Carlo

method can be applied with essentially no simplifying assumptions to the solution of the problems where more standard numerical techniques suffer from various degrees of approximation. The problem arising in any Monte Carlo simulation of a transport problem is

(a) to guarantee that the estimators used in the simulation be unbiased for the quantities to be estimated, and (b) to meet the requirement that the simulation procedure and estimator result in a Monte Carlo game with the lowest possible statistical error for a given computing time. For fixed-source problems the elaborated theory of unbiased estimators and variance reduction techniques are well developed. The relatively recent results in predicting statistical error of the Monte Carlo calculation permit at least in principle the solution of the second part of the problem, i.e., selecting a simulation procedure and an estimator most appropriate from the point of view of efficiency for the solution of the problem in question. Thus the mathematical principles underlying the Monte Carlo method for fixed-source calculations are well developed.

The status of the Monte Carlo development for the fixed-source problems is quite superior to that for Monte Carlo eigenvalue calculations, however. It is well known that Monte Carlo eigenvalue estimators are all biased.¹⁻⁷ Nevertheless, no methods are available to calculate the amount of this bias or to obtain some theoretical bounds for the value of the bias. The obvious cause for the bias is the use of ratio estimators. The following simple considerations suggest that a ratio used for K_{eff} estimation will be biased. Suppose that $\tilde{\lambda}_N^{(n)}$ and $\tilde{\lambda}_N^{(n+1)}$ are estimators of the neutron population in the n 'th and $(n+1)$ 'th generations^a based on finite samples of size N . Assume also that the equilibrium neutron distribution is attained, i.e., samples in the n 'th and $(n+1)$ 'th generations are obtained from the same probability density distribution. Thus, if $\langle \tilde{\lambda}_N^{(n)} \rangle = N_0$, then $\langle \tilde{\lambda}_N^{(n+1)} \rangle = K_{eff} N_0$ where the symbol $\langle \cdot \rangle$ stands for the average over the equilibrium neutron distribution. Then we may represent $\tilde{\lambda}_N^{(n)}$ and $\tilde{\lambda}_N^{(n+1)}$ in the following manner:

$$\tilde{\lambda}_N^{(n)} = N_0 [1 + \tilde{\epsilon}_N^{(n)}]$$

and

$$\tilde{\lambda}_N^{(n+1)} = K_{eff} N_0 [1 + \tilde{\epsilon}_N^{(n+1)}]$$

with $\langle \tilde{\epsilon}_N^{(n)} \rangle = \langle \tilde{\epsilon}_N^{(n+1)} \rangle = 0$. Consider the following ratio estimator for K_{eff} :

$$\tilde{K}_N^{(n)} = \frac{\tilde{\lambda}_N^{(n+1)}}{\tilde{\lambda}_N^{(n)}}. \quad (1)$$

^aWe will confine ourselves to consideration of the Monte Carlo eigenvalue calculations by means of sampling successive neutron generation, leaving as outside the scope of this paper the surface multiplication concept² and the method of fission matrix.¹ To our knowledge, these two methods were applied only occasionally for the solution of special classes of eigenvalue problems while different versions of K_{eff} estimation procedures based on sampling successive neutron generations are incorporated in any Monte Carlo criticality code.

The average of the estimator (1) does not equal K_{eff} , i.e., the estimator (1) is biased. It is convenient to define the value of the bias as follows:

$$B = \left| \left\langle \frac{\tilde{\lambda}_N^{(n+1)}}{\tilde{\lambda}_N^{(n)}} \right\rangle - K_{eff} \right| = K_{eff} \left| \left\langle \frac{\tilde{\epsilon}_N^{(n+1)} - \tilde{\epsilon}_N^{(n)}}{1 + \tilde{\epsilon}_N^{(n)}} \right\rangle \right|.$$

After a simple algebraic transformation, we obtain

$$B = K_{eff} \left| \left\langle \frac{[\tilde{\epsilon}_N^{(n)}]^2 - \tilde{\epsilon}_N^{(n+1)} \cdot \tilde{\epsilon}_N^{(n)}}{1 + \tilde{\epsilon}_N^{(n)}} \right\rangle \right|.$$

Assuming the sample size N to be sufficiently large so that $\tilde{\epsilon}_N^{(n+1)} \ll 1$ and $\tilde{\epsilon}_N^{(n)} \ll 1$, we conclude that the order of the value of B is that of the second moment of random variable $\tilde{\epsilon}_N^{(n)}$, i.e., of the order $1/N$. Thus, the value of the bias in the estimator (1) is proportional to the inverse of the sample size N in each generation:

$$B \sim \frac{1}{N}. \quad (2)$$

The cause of the bias defined by the last expression is that the average of the ratio estimator does not generally equal the ratio of averages of the numerator and the denominator. The $1/N$ dependence of the bias in K_{eff} was rigorously obtained for the sampling procedure based on the discrete model of the neutron transport equation.⁷ To the best of our knowledge, a Markov chain analysis of Monte Carlo procedures for criticality calculation similar to the analysis existing for fixed source problems⁸ does not yet exist. In the following we attempt to apply such an analysis to a procedure based on a fixed number of fission points per generation. We analyze the limiting properties of the Markov chain showing that the amount of bias in K_{eff} does not exceed $C/N^{1/2}$, (C being a problem-dependent constant with a bias of the order N^{-1} , as we show in Ref. 9).

The standard methods for computing statistical errors and confidence limits in Monte Carlo calculations are invalid for eigenvalue calculations, because of the correlations between successive generations and deviations of the fission source from the fundamental mode for any finite generation.¹⁰ Certainly the lack of a rigorous theoretical basis for Monte Carlo eigenvalue calculations does not prevent successful practical applications of Monte Carlo methods for criticality calculations. Although it is not feasible to estimate the magnitude of the bias in K_{eff} , there are strong theoretical and numerical corroborations^{1,3,7} that the amount of the bias decreases as the inverse of the number of neutrons in a generation. Consequently, it is desirable to keep a large number of neutrons per generation.^b Practical calculations allowing more or less meaningful conclusions about the value of the bias

^bIn practical applications, the number of neutrons per generation varies in the range 500 ÷ 2000.

involved indicate that the value of the bias is not more than 0.25% for the majority of reactors.¹¹ Thus the value of the bias may approach the error in K_{eff} caused by uncertainties in the neutron cross sections; it becomes considerably less than any reasonably attainable statistical error of the calculation. Another class of problems where the bias in Monte Carlo eigenvalue calculations does not appear to be of great importance are Monte Carlo criticality safety calculations.¹² The Monte Carlo method is especially suitable for nuclear reactor safety calculations because of the complicated geometry of an actual nuclear power plant system. The adequate precision in K_{eff} appropriate for most safety calculations is of the order of $\sim 1\%$ (Ref. 12) or even of the order of $\sim 5\%$ for criticality clearance work.¹³ These values considerably exceed the conjectural amount of the bias in K_{eff} . Furthermore, the extremely slow convergence rate of the fission rate distribution to the fundamental reactor mode that is characteristic of many practical problems results in large errors in the eigenvalue and makes the problem of the bias less significant in those applications. However, the implementation of detailed cross-section libraries in modern sophisticated multipurpose Monte Carlo codes decreases considerably the uncertainty in K_{eff} caused by the errors in the cross sections. This fact and the increasing tendency to use Monte Carlo codes as numerical integral experiments and for testing other numerical methods make even the small values of the bias in K_{eff} unacceptable.

The effect of correlations between successive generations tends to underestimate the statistical error of the estimate of K_{eff} . This underestimation is not likely to be large for system-integrated parameters like eigenvalues but may become quite unacceptable for localized estimators of reaction rates and fluxes. The underestimation of the variance estimate caused by neglecting the correlations between successive generations depends strongly on the dominance ratio (the ratio of the modulus of the eigenvalue of the neutron transport equation λ_1 following the lowest eigenvalue λ_0 to λ_0) (Ref. 10). For systems with dominance ratios close to unity, the value of the variance estimate obtained with the assumption that the correlations are negligibly small (the standard practice in Monte Carlo criticality calculations) becomes quite unreliable and may differ strongly from the variance unless the correlation coefficient vanishes when the dominance ratio approaches unity. This situation appears to be quite unlikely.

The Monte Carlo methods used in eigenvalue calculations are based essentially on intuition with the general rule of thumb being to sample the maximum possible number of generations and the maximum possible number of neutrons per generation. This makes it difficult, if feasible at all, to pose the problem of devising efficient (with respect to variance per unit of computing time) Monte Carlo procedures for eigen-

value calculations. The purpose of the present work is to devise a rigorous formalism for the Monte Carlo procedure for K_{eff} estimation and thus to eliminate some of the above-mentioned difficulties characteristic of Monte Carlo eigenvalue calculations.

The general scheme of the Monte Carlo procedure for estimation of some quantity I in fixed-source calculations may be described as follows: Neutron histories are generated on the computer by random sampling from the appropriate stochastic model. A neutron history c is a sequence of points $[R_i]_{i=1}^k$ in a six-dimensional phase space R_6 of neutron energies E , directions of flight ω , and spatial coordinates r : $c = (R_1, \dots, R_k)$, constructed in a random fashion by sampling from the stochastic model and ending with the loss of a neutron. To each random walk c , a random variable $\xi(c) = \xi(R_1, \dots, R_k)$ is assigned. The random variable $\xi(c)$ is said to be an unbiased estimator of I if it fulfills

$$I = \langle \xi \rangle = \int_{\Omega_c} \xi(c) d\mu(c) \\ = \int_{\Omega_c} \xi(R_1, \dots, R_k) d\mu(R_1, \dots, R_k), \quad (3)$$

where Ω_c is the space of all possible random walks $c_i = (R_{1i}, \dots, R_{ki})$ and $d\mu(R_1, \dots, R_k)$ is the probability density function (pdf) of the random walk $c = (R_1, \dots, R_k)$. In practice, the estimate of I is obtained by taking the finite average:

$$\langle \xi \rangle_n = \frac{1}{n} \sum_{i=1}^n \xi[R_{1i}^{(i)}, \dots, R_{ki}^{(i)}] \quad (4)$$

The statistical error of this finite average and the confidence limits are calculated by the use of the central limit theorem for random variables $\xi(c_i)$:

$$\lim_{n \rightarrow \infty} \text{Prob} \left(\langle \xi \rangle_n - I < \frac{t\sigma}{\sqrt{n}} \right) \\ = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^t \exp \left(-\frac{z^2}{2} \right) dz, \quad (5)$$

where the variance σ^2 is defined by

$$\sigma^2 = \int_{\Omega_c} [\xi(c) - I]^2 d\mu(c). \quad (6)$$

The integral over the space of random walks Ω_c in Eq. (6) may be approximated by a finite average similar to expression (4).

In this paper we present a rigorous stochastic model for Monte Carlo eigenvalue calculations similar to that for the fixed-source scheme presented above. We also discuss in detail the origin of the bias in eigenvalue and derive an expression for the value of the bias useful for practical applications. We also derive an explicit formula for the value of the bias as

a function of a number of neutrons sampled in each generation, the bulk properties of a reactor, and some parameters indicating the deviation of the initial approximation from the fundamental reactor mode.

II. BASIC DEFINITIONS AND STATISTICAL MODEL

We consider only Monte Carlo procedures for estimation of K_{eff} with a constant number of fission points in each generation.^c Hereafter, a generation refers to an arbitrary set of N points $[R_i]_{i=1}^N$ in a six-dimensional phase space R_6 . A Monte Carlo procedure for the estimation of K_{eff} consists of transitions between successive generations. Transitions from one generation to another are governed by a set of probabilistic laws specified below such that the probability of transition from generation number $n: [R_i^{(n)}]_{i=1}^N$ to generation number $(n+1): [R_i^{(n+1)}]_{i=1}^N$ depends only on $[R_i^{(n)}]_{i=1}^N$. Thus, subsequent generations constitute a homogeneous Markov chain with infinitely many states.^{14,15} It is necessary to note that the properties of the homogeneous Markov chains with infinitely many states are different from those of Markov chains with absorbing states encountered in fixed-source calculations. The probabilistic laws governing the transitions between the states of the infinite Markov chain are chosen such that the number of points in a generation remains constant. To each state of the Markov chain $[R_i^{(n)}]_{i=1}^N$ a random variable $\xi[R_1^{(n)}, \dots, R_N^{(n)}]$ is assigned that is called K_{eff} estimator. Thus the Monte Carlo K_{eff} estimator is a linear functional operating in a space of state vectors $(R_1, \dots, R_N)$ of this Markov chain.

The preceding derivation is based on a refined version of the Monte Carlo procedure for K_{eff} estimation described in Ref. 3. Let the n 'th generation of neutrons be placed in points $[R_i^{(n)}]_{i=1}^N$ of phase space. The recurrent procedure of estimating K_{eff} by sampling a sequence of generations with a constant number of points in a generation is defined as follows: Fission neutrons are started from the points of the n 'th generation $[R_i^{(n)}]_{i=1}^N$ and are tracked until absorption, leakage, or fission occurs. The probability of selecting a point $R_i^{(n)}$ as a starting point is given by the expression

$$P[R_i^{(n)}] = \frac{\nu[R_i^{(n)}]}{\sum_{i=1}^N \nu[R_i^{(n)}]}, \quad (7)$$

^cAlthough Monte Carlo games with an increasing number of fission points per generation seem to provide asymptotically unbiased estimates of the effective multiplication factor,^{4,6} the Monte Carlo procedures with a constant number of fission points in a generation are still incorporated into any criticality code because of the simplicity of coding and processing of results.

where $\nu(R)$ is the mean number of secondary neutrons emitted in a fission process caused at point R . The fission sites caused by these neutrons constitute the points of the $(n+1)$ 'th generation $[R_i^{(n+1)}]_{i=1}^N$. Sampling of neutron histories from the points of the n 'th generation is repeated until the N fission points $[R_i^{(n+1)}]_{i=1}^N$ are obtained. Thus starting points for the next generation are obtained by sampling with replacement from probabilities defined by expression (7) from the finite population of points $[R_i^{(n)}]_{i=1}^N$. The points constituting the initial generation $[R_i^{(1)}]_{i=1}^N$ are chosen completely arbitrarily.^d This sampling scheme is guaranteed from extinction or explosion of the neutron population (except of course for the trivial case of zero fission). The transitions between generations are recognized easily as transitions between successive states of a homogeneous Markov chain^{15,16} with infinitely many states:

$$[R_1^{(1)}, \dots, R_N^{(1)}] \rightarrow [R_1^{(2)}, \dots, R_N^{(2)}] \\ \rightarrow \dots \rightarrow [R_1^{(n)}, \dots, R_N^{(n)}] \rightarrow \dots \quad (8)$$

To each state of the Markov chain¹⁰ $[R_1^{(n)}, \dots, R_N^{(n)}]$ we now assign the following random variable:

$$\xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] \\ = \frac{N-1}{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] - 1} \frac{1}{N} \sum_{i=1}^N \nu[R_i^{(n)}], \quad (9)$$

where $l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ is the number of neutron histories to be sampled from the points of the n 'th generation $[R_i^{(n)}]_{i=1}^N$ in order to obtain N fission points of the next generation $[R_i^{(n+1)}]_{i=1}^N$. The arithmetic average of the random variable $\xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ after sampling n_0 successive generations is given by

$$\bar{K}_N^{(n_0)} = \frac{1}{n_0} \sum_{k=1}^{n_0} \frac{N-1}{l^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}] - 1} \\ \times \frac{1}{N} \sum_{i=1}^N \nu[R_i^{(k)}]. \quad (10)$$

^dSuppose that the points of the initial generation are sampled from some initial probability density distribution. Certainly the closer the initial distribution is to the fundamental reactor mode, the fewer are the number of generations to be sampled in order to obtain the solution. In many practical cases a poor or successful choice of the initial distribution will be crucial for the realization of the Monte Carlo criticality calculations (the situation referred to in Ref. 12 as "the difficulty in calculating K_{eff} of the world"). We will prove below that the value of the bias in K_{eff} estimate also depends on this initial distribution. The value of the bias, however, can be made arbitrarily small by increasing the number of points in each generation N unless the initial distribution is orthogonal to the main eigenfunction of the transport equation.

In the following we will prove that the "one-generation average" of the random variable $\bar{K}_N^{(n_0)}$ {average over all possible values of $l^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}]$ for a given generation} converges with probability 1 (almost sure)¹⁵ to some value λ_N and that λ_N differs from the effective multiplication factor λ_0 by no more than $C/N^{1/2}$, with the constant C completely defined by some bulk properties of a reactor and fission importance function. Thus the random variable $\xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ is a Monte Carlo K_{eff} estimator with a known upper bound for the bias. In order to clarify the physical meaning of the estimator (9), consider expression (9) for large N . Since $l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ increases when N is being increased, expression (9) for large N becomes

$$\xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] \approx \frac{1}{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]} \sum_{i=1}^N \nu[R_i^{(n)}] . \quad (11)$$

The last expression is the ratio of secondary neutrons produced from the N fission points of the n 'th generation to the value $l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ —a sample of the number of neutron histories to be generated from the points of the n 'th generation in order to obtain N fission events in the same generation. Actually, it is a production-to-fission-rate ratio estimator of K_{eff} with production and fission rates being estimated from the same generation.

In order to proceed, consider the integral form of the neutron transport equation:

$$\lambda_l \phi_l(R) = \int_D \phi_l(R') K(R', R) dR' , \quad (12)$$

where $K(R', R)$ is the number density of fissions at point R caused by $\nu(R')$ fission neutrons emitted at R' , l is the order of the eigenfunction of integral Eq. (12), and D is the domain in phase space R_6 defined by the expression

$$D = V_r x(E_{min}, E_{max}) x V_\omega ,$$

where

x = direct product

V_r = convex bounded spatial domain with volume V

(E_{min}, E_{max}) = finite closed interval on the energy axis

V_ω = domain of all possible directions of neutron flights.

As follows from the definition, the domain D possesses finite measure

$$\mu(D) = 4\pi V(E_{max} - E_{min}) .$$

For $l = 0$, Eq. (12) becomes

$$\lambda_0 \phi_0(R) = \int_D \phi_0(R') K(R', R) dR' , \quad (13)$$

where $\phi_0(R)$ is the normalized equilibrium fission rate at R , i.e., the normalized pdf of fission point R in R_6 , and λ_0 is the lowest eigenvalue of the integral transport Eq. (12), i.e., the effective multiplication factor ($\lambda_0 \equiv K_{eff}$). The existence and uniqueness of a positive eigenfunction of Eq. (13), $\phi_0(R)$ with the positive eigenvalue λ_0 , which is greater than the modulus of any other eigenvalue λ_l , was proved in the framework of the theory of linear positive operators with invariant cone in a Banach space¹⁷ under varying assumptions^e of the medium type, cross sections, and scattering laws of energy dependence.¹⁸⁻²² It has been proven also that this positive eigenfunction is dominant,²² i.e., that the following limit exists:

$$\lim_{n \rightarrow \infty} \frac{1}{\lambda_0^n} \int K^{(n)}(R, P) F(R) dR = M(F) \phi_0(P) , \quad (14)$$

where $K^{(n)}(R, P)$ stands for the n 'th iterate of the kernel of the integral Eq. (12):

$$K^{(n)}(R, P) = \int_{D_1} \dots \int_{D_n} K(R, R_1) K(R_1, R_2) \dots K(R_n, P) dR_1 \dots dR_n , \quad (15)$$

where

$F(R)$ = arbitrary initial pdf

$M(F)$ = some linear functional operating in the Banach space of the solutions of Eq. (13), i.e., a constant dependent on the initial distribution $F(R)$

$\phi_0(R)$ = normalized equilibrium fission rate distribution

λ_0 = dominant eigenvalue of Eq. (12).

In order to proceed further, we now introduce the following functions:

$$\epsilon(R) = \begin{cases} \frac{1}{\mu(D)} , & R \in D \\ 0 , & R \notin D \end{cases} , \quad (16)$$

$$P^{(0)}(R) \equiv 1 , \quad (17)$$

$$P^{(1)}(R) = P(R) = \int_D K(R, Q) dQ , \quad (18)$$

^eNo attempt has been made to present a complete bibliography on the existence and uniqueness theory for criticality solution in neutron transport theory. More references can be found in the papers referred to.

and

$$P^{(n)}(R) = \int_D K^{(n)}(Q, R) \epsilon(Q) dQ, \quad n = 2, 3, \dots \quad (19)$$

[It should be noted that $P(R)$ physically yields the integrated number of fissions all over the phase space resulting from one particle entering fission at R , whereas $P^{(n)}(R)$ for $n > 1$ yields the number of fissions at R after n iterations due to a fission distribution $\epsilon(Q)$. This difference stems from the need to preserve the meaning of G^n of Eq. (20) for $n = 1$ and should not cause any ambiguity.]

$$G^{(n)}(R_1, \dots, R_N) = \frac{\sum_{i=1}^N P^{(n+1)}(R_i)}{\sum_{i=1}^N P^{(n)}(R_i)} \quad (20)$$

The function $\epsilon(R)$ may always be represented as follows:

$$\epsilon(R) = \epsilon_0 \phi_0(R) + \epsilon_1 \theta(R), \quad (21)$$

with $\phi_0(R)$ and $\theta(R)$ being normalized:

$$\int_D \phi_0(R) dR = \int_D \theta(R) dR = 1.$$

Substituting the function $\theta(R)$ into Eq. (14), we obtain

$$\lim_{n \rightarrow \infty} \frac{1}{\lambda_0^n} \int_D K^{(n)}(R, P) \theta(R) dR = c \phi_0(P) \quad (22)$$

Define the sequence of functions

$$\theta^{(n)}(P) = \int_D K^{(n)}(R, P) \theta(R) dR.$$

We may conclude from Eq. (22) that $\theta^{(n)}(R)$ may be represented as

$$\theta^{(n)}(R) = \lambda_0^n c \phi_0(R) + \psi^{(n)}(R),$$

where

$$\lim_{n \rightarrow \infty} \frac{1}{\lambda_0^n} \|\psi^{(n)}(R)\| = 0.$$

Hereafter we may assume that $c \equiv 0$, because if it is not so, we can always include the constant c into ϵ_0 in expansion (21). We define the norm in the space of the solutions of Eq. (12) as follows¹⁸ [the limit of Eq. (14) is in the sense of that norm]:

$$\|F(R)\| = \int_D |F(R)| dR \quad (23)$$

Now substituting Eq. (21) into the expression for $P^{(n)}(R)$ in Eq. (19), we obtain

$$P^{(n)}(R) = \epsilon_0 \lambda_0^n \phi_0(R) + \epsilon_1 \psi^{(n)}(R), \quad (24)$$

with

$$\psi^{(n)}(R) = \theta^{(n)}(R)$$

and

$$\lim_{n \rightarrow \infty} \|\theta^{(n)}\| \frac{1}{\lambda_0^n} = 0. \quad (25)$$

Since the integral operator of the integral Eq. (12) is a bounded operator with a norm λ_0 (Ref. 18),

$$\|K(P, Q)\| = \lambda_0.$$

Then,

$$\left\| \int_D K(R, Q) \theta(R) dR \right\| \leq \|K(R, Q)\| \|\theta(R)\| \leq \lambda_0 \|\theta(R)\|$$

and applying the last inequality successively we get

$$\|\theta^{(n)}(R)\| < \lambda_0^n \|\theta\|.$$

Thus the sequence of functions $\theta^{(n)}(R)$ is bounded. Equation (25) will also be satisfied if we assume that

$$\|\theta^{(n)}\| < \gamma |\lambda_1|^n,$$

where γ and λ_1 are some constants and $|\lambda_1| < \lambda_0$. In such a case one may write

$$\epsilon_1 \|\psi^{(n)}(R)\| \leq (1 - \epsilon_0) \gamma |\lambda_1|^n. \quad (26)$$

Now we present a case when λ_1 entering inequality (26) coincides with the eigenvalue λ_1 of Eq. (12) following the dominant eigenvalue λ_0 . Suppose that the following expansion is valid^f uniformly:

$$\theta(R) = \sum_{l=1}^{\infty} \alpha_l \phi_l(R),$$

with

$$\sum_{l=1}^{\infty} |\alpha_l| = \gamma < \infty.$$

Then substituting the last expansion for $\theta(R)$ into the expansion (21) and using Eq. (19) we get again

$$P^{(n)}(R) = \epsilon_0 \lambda_0^n \phi_0(R) + \psi^{(n)}(R),$$

with

$$\|\psi^{(n)}(R)\| = \epsilon_1 \left\| \sum_{l=1}^{\infty} \alpha_l \lambda_l \phi_l(R) \right\| \leq \epsilon_1 \sum_{l=1}^{\infty} \|\alpha_l \lambda_l \phi_l(R)\|.$$

Suppose that the eigenfunctions of Eq. (12) are normalized with unit norm

$$\|\phi_l(R)\| = \int_D |\phi_l(R)| dR = 1.$$

^fThe integral operator of Eq. (12) is not a self-adjoint operator with an orthonormal complete set of eigenfunctions $[\phi_l(R)]_{l=0}^{\infty}$, so that the infinite series expression for $\theta(R)$ is not always valid. Note also that a $\phi_0(R)$ component is not included in the expansion. This is so because any such component is removed from the expansion and attached to $\xi_0 \phi_0(R)$ of Eq. (21).

Then, since $\lambda_0 > |\lambda_l|$ for all l ,

$$\epsilon_1 \|\psi^{(n)}(R)\| \leq \epsilon_1 \sum_{l=1}^{\infty} |\alpha_l| |\lambda_l|^n \leq \gamma |\lambda_1|^n (1 - \epsilon_0) .$$

The last inequality is different from inequality (26), since in inequality (26) λ_1 is some constant, satisfying $|\lambda_1| < \lambda_0$, but not necessarily equal to the eigenvalue of the transport equation. Hereafter we will use the same notation for both meanings of λ_1 , keeping in mind that λ_1 of inequality (26) equals in some special cases the eigenvalue of the neutron transport equation λ_1 following the dominant eigenvalue λ_0 . The constant ϵ_0 entering inequality (26) may be interpreted as some measure of the deviation of the initial approximation $\epsilon(R)$ from the fundamental reactor mode $\phi_0(R)$.

Substitution of expression $P^{(n)}(R)$ [Eq. (24)] into the definition of $G^{(n)}(R_1, \dots, R_N)$ [Eq. (20)] yields

$$G^{(n)}(R_1, \dots, R_N) = \frac{\sum_{i=1}^N [\epsilon_0 \lambda_0^{n+1} \phi_0(R_i) + \psi^{(n+1)}(R_i)]}{\sum_{i=1}^N [\epsilon_0 \lambda_0^n \phi_0(R_i) + \psi^{(n)}(R_i)]} .$$

Now taking the limit as $n \rightarrow \infty$ and using inequality (26) we get

$$\lim_{n \rightarrow \infty} G^{(n)}(R_1, \dots, R_N) = \lambda_0 . \quad (27)$$

The kernel of integral Eq. (12) may be represented in the form

$$K(R', R) = \nu(R') G_f(R', R) , \quad (28)$$

where $G_f(R', R)$ is the fission Green function of the neutron transport equation. The value $G_f(R', R)$ equals the number density of fission events at R due to one fission neutron born at point R' . Then from the definition of $P(R)$ of Eq. (18) we get

$$P(R') = \int_D K(R', R) dR = \nu(R') \int_D G_f(R', R) dR .$$

The average number of fission events produced by one fission neutron started with probability (7) from fission points $[R_1^{(n)}, \dots, R_N^{(n)}]$ of the n 'th generation is given by the expression

$$\begin{aligned} & P_f^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] \\ &= \sum_{j=1}^N \left\{ \frac{\nu[R_j^{(n)}]}{\sum_{i=1}^N \nu[R_i^{(n)}]} \cdot \int_D G_f[R_j^{(n)}, P] dP \right\} \\ &= \frac{\sum_{j=1}^N P[R_j^{(n)}]}{\sum_{i=1}^N \nu[R_i^{(n)}]} . \end{aligned} \quad (29)$$

This is also the probability of obtaining a fission event.

Now we will derive the expression for the value of $P_f^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}][R_1^{(n)}, \dots, R_N^{(n)}]$, which is the probability that for a given state of the Markov chain $[R_1^{(n)}, \dots, R_N^{(n)}]$ $l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ source particles will be needed to sample according to the above specified probabilistic laws in order to obtain N fission points. First, we must recall that if $l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ source particles have to be sampled until N fissions are obtained, then the l 'th particle must yield a fission event. Thus the sought value is given by the probability that $l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] - 1$ source particles will yield $N - 1$ fissions and the l 'th particle will yield fission. Since the probability of the first event is given by the formulas for the probability of $N - 1$ successes in a simple binomial experiment with the probability of success given by expression (29), we have

$$\begin{aligned} & P_f^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}][R_1^{(n)}, \dots, R_N^{(n)}] \\ &= \left\{ l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] - 1 \right\} \\ & \quad \times \{1 - P_f^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]\}^{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] - N} \\ & \quad \times \{P_f^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]\}^{N-1+1} . \end{aligned} \quad (30)$$

We will now derive an alternative expression for the probability $P_f^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$, given by Eq. (29). The probability in Eq. (29) is basically derived from the concept of an average over N batches of trials with a varying number of successes (fission events) n_i and a fixed number of trials N in each batch:

$$P = \frac{1}{N} \sum_{i=1}^N \frac{n_i}{N} .$$

However, the probability of a success P may be learned in a different manner as an average over N batches of trials with a varying number of trials l_i necessary in order to obtain a fixed number of successes, N , namely,

$$P = \frac{1}{N} \sum_{i=1}^N \frac{N}{l_i} .$$

The meaning of the relative frequencies n_i/N and N/l_i is quite different because in n_i/N we know only that n_i successes occurred in N trials while in N/l_i we know that $N - 1$ successes occurred in $l_i - 1$ trials and that the l_i 'th trial was a success. Then to retain the same meaning in both equivalent expressions for P we should take $(N - 1)/(l_i - 1)$ in the last expression rather than N/l_i . Grouping terms by frequencies of l_i leads to

$$P = \frac{1}{N} \sum_{l_i=N}^{\infty} \frac{N-1}{l_i-1} N(l_i) = \sum_{l_i=N}^{\infty} \frac{N-1}{l_i-1} P(l_i) .$$

Thus the following alternative expression for $P_f^{(n)} \times [R_1^{(n)}, \dots, R_N^{(n)}]$ is valid[§]:

$$\begin{aligned} & \sum_{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] = N}^{\infty} \frac{N-1}{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] - 1} \\ & \times P_{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]}[R_1^{(n)}, \dots, R_N^{(n)}] \\ & = P_f^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] . \end{aligned} \quad (31)$$

Consider the average of the random variable $\xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ defined by Eq. (9) over all possible values of $l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$:

$$\begin{aligned} & \langle \xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] \rangle_{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]} \\ & = \sum_{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] = N}^{\infty} \xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] \\ & \times P_{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]}[R_1^{(n)}, \dots, R_N^{(n)}] . \end{aligned} \quad (32)$$

Substituting Eq. (9) into Eq. (32) and using Eqs. (29) and (31), we get

$$\begin{aligned} & \langle \xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] \rangle_{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]} \\ & = \sum_{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] = N}^{\infty} \left\{ \frac{N-1}{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] - 1} \right. \\ & \times \left. \frac{1}{N} \sum_{i=1}^N \nu[R_i^{(n)}] \right\} P_{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]}^{(n)} \\ & \times [R_1^{(n)}, \dots, R_N^{(n)}] = \frac{1}{N} \sum_{i=1}^N P[R_i^{(n)}] . \end{aligned} \quad (33)$$

Note that the above average is in fact the expected value of $\xi_N^{(n)}$ in the n 'th generation with a fixed and limited number of fission points N . To be more specific, the game played is the following. The fission points of the n 'th generation $[R_1^{(n)}, \dots, R_N^{(n)}]$ are assumed to be already given by the $(n-1)$ 'th generation. Thus, in Eq. (9), $\sum_{i=1}^N \nu[R_i^{(n)}]$ and N are already fixed and neutrons are now sampled starting at $[R_1^{(n)}, \dots, R_N^{(n)}]$ according to the probabilities of Eq. (7) and are transported in the medium until leakage or absorption or fission occurs. This process is continued until N fission points [of the $(n+1)$ 'th generation] are obtained $[R_1^{(n+1)}, \dots, R_N^{(n+1)}]$. This will require $l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ neutrons to be sampled. This $l^{(n)}$ will then be introduced into Eq. (9) to obtain one sample value of $\xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$. Repeating that game with the same points $[R_1^{(n)}, \dots, R_N^{(n)}]$ and calculating the arithmetic average value of $\xi_N^{(n)}$ will yield a quantity converging to $\langle \xi_N^{(n)} \rangle_l$ of Eq. (33).

Let us now introduce the shorthand notation for the average:

[§]Equation (31) can also be proven formally by induction. See Appendix A.

$$\begin{aligned} & \langle \xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] \rangle_{l^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]} \\ & = \tilde{\kappa}_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] . \end{aligned} \quad (34)$$

Then Eq. (33) may be written in an equivalent form:

$$\tilde{\kappa}_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] = \frac{1}{N} \sum_{i=1}^N P[R_i^{(n)}] . \quad (35)$$

The one-generation average defined by Eq. (35) is the random variable defined for each state of the Markov chain, expression (8). We now derive the expression for the transition probability of the Markov chain (8), i.e., the conditional probability that with the n 'th generation fission points $[R_1^{(n)}, \dots, R_N^{(n)}]$ given, the fission points of the $(n+1)$ 'th generation in $dR_1^{(n+1)}, \dots, dR_N^{(n+1)}$ are at $[R_1^{(n+1)}, \dots, R_N^{(n+1)}]$. The conditional probability to get a fission event in $dR_j^{(n+1)}$ at $R_j^{(n+1)}$ starting from the points of the n 'th generation is given by

$$P_f[R_j^{(n+1)}] dR_j^{(n+1)} = \frac{\sum_{i=1}^N K[R_i^{(n)}, R_j^{(n+1)}] dR_j^{(n+1)}}{\sum_{k=1}^N P[R_k^{(n)}]} . \quad (36)$$

Expression (36) is the ratio of the total number of fissions in $dR_j^{(n+1)}$ at $R_j^{(n+1)}$ due to $\sum_{i=1}^N \nu[R_i^{(n)}]$ particles emitted at $[R_1^{(n)}, \dots, R_N^{(n)}]$ to the total number of fissions. Since the transition from the n 'th generation to the $(n+1)$ 'th generation consists in obtaining N fission points starting from the points of the n 'th generation, the probability of this event is given by the product of the probabilities defined by expression (36). Thus the transition probability for the Markov chain (8) is

$$\begin{aligned} & k[R_1^{(n)}, \dots, R_N^{(n)} | R_1^{(n+1)}, \dots, R_N^{(n+1)}] \\ & = \prod_{m=1}^N \frac{\sum_{k=1}^N K[R_k^{(n)}, R_m^{(n+1)}]}{\sum_{l=1}^N P[R_l^{(n)}]} . \end{aligned} \quad (37)$$

From definition (37) it follows that the transition probability is normalized, e.g.,

$$\begin{aligned} & \int_{D_1} \dots \int_{D_N} k[R_1^{(n)}, \dots, R_N^{(n)}] \\ & \times [R_1^{(n+1)}, \dots, R_N^{(n+1)}] dR_1^{(n+1)} \dots dR_N^{(n+1)} = 1 . \end{aligned} \quad (38)$$

So far we have considered the one-generation average of the estimator along with definitions and properties of the Markov chain. The global average is, however, obtained by averaging further over the generations, by

looking at $\langle \xi_N^{(n)} \rangle_i$ in the limit as $n \rightarrow \infty$. To study this limit we need first to consider some limit properties of the Markov chains.

III. LIMIT PROPERTIES OF THE MARKOV CHAIN MODEL FOR K_{eff} ESTIMATION

We will now recall some basic results from the theory of Markov chains.^{15,16,23} Let $X \in E$ denote a state of a Markov chain with the transition probability $P(X, Y)$ and f some function of x . Then the strong law of large numbers for Markov chains states that for any initial state x_1 of a Markov chain the following limit exists:

$$Prob \left[\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n f(X_i) = \int_E f(Z) \pi(Z) dZ \right] = 1, \quad (39)$$

where $\pi(Z)$ is the stationary probability density distribution of the Markov chain, which is the solution of the following integral equation:

$$\pi(Z) = \int_E P(X, Z) \pi(X) dX. \quad (40)$$

It is also proved¹⁵ that the following limiting relation exists:

$$\lim_{n \rightarrow \infty} P^{(n)}(X, Z) = \pi(Z) \quad (41)$$

and

$$\|P^{(n)}(X, Z) - \pi(Z)\| < \gamma \rho^n, \quad (42)$$

with γ and $0 < \rho < 1$ independent of n and X . The expression $P^{(n)}(X, Z)$ in Eq. (41) is the n -step transition probability of the Markov chain, which is defined by the following recurrent formulas [this definition is equivalent to that of k^n in Eq. (15)]:

$$P^{(n+1)}(X, Z) = \int_E P^{(n)}(X, Y) P(Y, Z) dY. \quad (43)$$

For the Markov chain defined in Sec. II, the expression for the function $f(X)$ of the state of a Markov chain is given by Eq. (35), with $X_i \equiv [R_1^{(i)}, \dots, R_N^{(i)}]$. Then, applying the strong law of large numbers for the fission Markov chain of Eq. (8), we get that for any initial generation $[R_1^{(i)}]_{i=1}^N$ the following expression is valid:

$$Prob \left\{ \lim_{n \rightarrow \infty} \frac{1}{n_0} \sum_{n=1}^{n_0} \tilde{k}_N^{(n)} [R_1^{(n)}, \dots, R_N^{(n)}] = \int_{D_1} \dots \int_{D_N} \tilde{k}_N^{(n)} [R_1^{(n)}, \dots, R_N^{(n)}] \times F_s[R_1^{(n)}, \dots, R_N^{(n)}] dR_1^{(n)} \dots dR_N^{(n)} \right\} = 1, \quad (44)$$

where $F_s(R_1, \dots, R_N)$ is the stationary distribution of the Markov chain of Eq. (8), which in our case satisfies the equation

$$\begin{aligned} F_s(R_1, \dots, R_N) \\ = \int_{D_1} \dots \int_{D_N} k(P_1, \dots, P_N | R_1, \dots, R_N) \\ \times F_s(P_1, \dots, P_N) dP_1 \dots dP_N. \end{aligned} \quad (45)$$

Expression (41) for the fission Markov chain then takes the form

$$\begin{aligned} \lim_{n \rightarrow \infty} k^{(n)}(P_1, \dots, P_N | R_1, \dots, R_N) \\ = F_s(R_1, \dots, R_N), \end{aligned} \quad (46)$$

where $k^{(n)}(P_1, \dots, P_N | R_1, \dots, R_N)$ is defined by the following recurrence relation called the Chapman-Kolmogorov equation in the theory of Markov chains²³:

$$\begin{aligned} k^{(n+1)}(P_1, \dots, P_N | R_1, \dots, R_N) \\ = \int_{D_1} \dots \int_{D_N} k^{(n)}(P_1, \dots, P_N | Q_1, \dots, Q_N) \\ \times k(Q_1, \dots, Q_N | R_1, \dots, R_N) dQ_1, \dots, dQ_N, \end{aligned} \quad (47)$$

with

$$k^{(0)}(P_1, \dots, P_N, Q_1, \dots, Q_N) = \prod_{i=1}^N \delta(P_i - Q_i).$$

It is necessary to note that the limit in Eq. (46) does not depend on $(P_1, \dots, P_N)$. In the actual procedure for K_{eff} estimation, we generate a sequence of generations according to Eq. (37). At each generation we calculate the random variable $\xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$, and the average of this random variable over n generations is used as an estimate $\tilde{\lambda}_N^{(n)}$ of the effective multiplication factor λ_0 :

$$\tilde{\lambda}_N^{(n)} = \frac{1}{n} \sum_{k=1}^n \xi_N^{(k)} [R_1^{(k)}, \dots, R_N^{(k)}]_{l^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}]}. \quad (48)$$

In order to verify the validity of this procedure, one has to look at the expectation value of $\tilde{\lambda}_N^{(n)}$ and check whether it equals λ_0 or not. The expectation value of $\tilde{\lambda}_N^{(n)}$ is obtained by averaging $\xi_N^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}]$ in each generation, substituting the average value of $\xi_N^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}]$ in each generation k into Eq. (48) and taking the limit as $n \rightarrow \infty$. The average of $\xi_N^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}]$ in the k 'th generation can be obtained by averaging over all possible values of $l^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}]$ according to Eq. (32). The value

$\xi_N^{(n)}(R_1, \dots, R_N)$ then serves as a one sample estimate of $\langle \xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] \rangle_{I^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]}$. Thus the expectation of the K_{eff} estimator of Eq. (48) is given by

$$\langle \tilde{\lambda}_N^{(n)} \rangle = \lim_{n \rightarrow \infty} \frac{1}{n} \times \sum_{k=1}^n \langle \xi_N^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}] \rangle_{I^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]} \quad (49)$$

or

$$\langle \tilde{\lambda}_N^{(n)} \rangle = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=1}^n \tilde{k}_N^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}] \quad (50)$$

According to Eq. (44) the average over successive generations in Eq. (50) exists and equals with probability 1 the average over the stationary distribution. Thus,

$$\langle \tilde{\lambda}_N^{(n)} \rangle = \int_{D_1} \dots \int_{D_N} k_N^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}] \times F_s[R_1^{(k)}, \dots, R_N^{(k)}] dR_1^{(k)} \dots dR_N^{(k)} \quad (51)$$

Substituting the expression for $k_N^{(k)}(R_1, \dots, R_N)$ from Eq. (35) into Eq. (51), we obtain

$$\langle \tilde{\lambda}_N^{(n)} \rangle = \int_{D_1} \dots \int_{D_N} \frac{1}{N} \times \sum_{i=1}^N P(R_i) F_s(R_1, \dots, R_N) dR_1 \dots dR_N \quad (52)$$

In Sec. IV we show that the estimator of Eq. (48) is an asymptotically unbiased estimator of λ_0 , i.e.,

$$\lim_{N \rightarrow \infty} \langle \tilde{\lambda}_N^{(n)} \rangle = \lambda_0 \quad (53)$$

IV. CONVERGENCE OF THE K_{eff} ESTIMATOR

In this section we estimate the modulus of the difference between the average of the K_{eff} estimator and λ_0 . Substituting expression (46) for $F_s(R_1, \dots, R_N)$ into Eq. (52), we obtain

$$\langle \lambda_N^{(n)} \rangle = \lim_{n \rightarrow \infty} \int_{D_1} \dots \int_{D_N} k^{(n)}(P_1, \dots, P_N | R_1, \dots, R_N) \frac{1}{N} \sum_{i=1}^N P(R_i) dR_1 \dots dR_N \quad (54)$$

From definitions (17) through (20), it follows that

$$\frac{1}{N} \sum_{i=1}^N P(R_i) = G^{(0)}(R_1, \dots, R_N) \quad (55)$$

Then, using expression (27) for λ_0 , we can write

$$\langle \lambda_N^{(n)} \rangle - \lambda_0 = \lim_{n \rightarrow \infty} \int_{D_1} \dots \int_{D_N} k^{(n)}(P_1, \dots, P_N | R_1, \dots, R_N) \times G^{(0)}(R_1, \dots, R_N) dR_1 \dots dR_N - G^{(n)}(P_1, \dots, P_N) \quad (56)$$

Now we will verify the following identity:

$$\begin{aligned} & \int_{D_1} \dots \int_{D_N} k^{(n)}(P_1, \dots, P_N | R_1, \dots, R_N) G^{(0)}(R_1, \dots, R_N) dR_1 \dots dR_N - G^{(n)}(P_1, \dots, P_N) \\ &= \sum_{l=0}^{n-1} \int_{D_1} \dots \int_{D_{2N}} [G^{(l)}(R_1, \dots, R_N) - G^{(l+1)}(Q_1, \dots, Q_N)] k(Q_1, \dots, Q_N | R_1, \dots, R_N) dR_1 \dots dR_N \\ & \quad \times k^{(n-l-1)}(P_1, \dots, P_N | Q_1, \dots, Q_N) dQ_1 \dots dQ_N \end{aligned} \quad (57)$$

Denoting the terms in the sum of identity (57) by a_l , we get for $l=0$:

$$\begin{aligned} a_0 &= \int_{D_1} \dots \int_{D_{2N}} G^{(0)}(R_1, \dots, R_N) k(Q_1, \dots, Q_N | R_1, \dots, R_N) dR_1 \dots dR_N \\ & \quad \times k^{(n-1)}(P_1, \dots, P_N | Q_1, \dots, Q_N) dQ_1 \dots dQ_N - \int_{D_1} \dots \int_{D_{2N}} G^{(1)}(Q_1, \dots, Q_N) \\ & \quad \times k(Q_1, \dots, Q_N | R_1, \dots, R_N) dR_1 \dots dR_N k^{(n-1)}(P_1, \dots, P_N | Q_1, \dots, Q_N) dQ_1 \dots dQ_N \end{aligned}$$

Applying the Chapman-Kolmogorov Eq. (47) and the normalization condition Eq. (38), we obtain

$$a_0 = \int_{D_1} \dots \int_{D_N} G^{(0)}(R_1, \dots, R_N) k^{(n)}(P_1, \dots, P_N | R_1, \dots, R_N) dR_1 \dots dR_N \\ - \int_{D_1} \dots \int_{D_N} G^{(1)}(Q_1, \dots, Q_N) k^{(n-1)}(P_1, \dots, P_N | Q_1, \dots, Q_N) dQ_1 \dots dQ_N = A_0 - A_1 .$$

Similarly the term with $l = 1$ is

$$a_1 = \int_{D_1} \dots \int_{D_{2N}} G^{(1)}(R_1, \dots, R_N) k(Q_1, \dots, Q_N | R_1, \dots, R_N) dR_1 \dots dR_N \\ \times k^{(n-2)}(P_1, \dots, P_N | Q_1, \dots, Q_N) dQ_1 \dots dQ_N - \int_{D_1} \dots \int_{D_{2N}} G^{(2)}(Q_1, \dots, Q_N) \\ \times k(Q_1, \dots, Q_N | R_1, \dots, R_N) dR_1 \dots dR_N k^{(n-2)}(P_1, \dots, P_N | Q_1, \dots, Q_N) dQ_1 \dots dQ_N .$$

Again applying the Chapman-Kolmogorov Eq. (47) and normalization condition Eq. (38), we obtain

$$a_1 = \int_{D_1} \dots \int_{D_N} G^{(1)}(R_1, \dots, R_N) k^{(n-1)}(P_1, \dots, P_N | R_1, \dots, R_N) dR_1 \dots dR_N \\ - \int_{D_1} \dots \int_{D_N} G^{(2)}(Q_1, \dots, Q_N) k^{(n-2)}(P_1, \dots, P_N | Q_1, \dots, Q_N) dQ_1 \dots dQ_N = A_1 - A_2 .$$

Similarly, one can show that for each a_l we get $a_l = A_l - A_{l+1}$, and thus the sum of the right side of Eq. (57) takes the form

$$A_0 - A_1 + A_1 - \dots + A_{n-1} - A_n = A_0 - A_n .$$

All the terms are cancelled, except A_0 and A_n , which are identical to the left side of the identity. Thus identity (57) is valid.

According to the definition of norm (25) and the definitions of the one-step transition probability $k(P_1, \dots, P_N | Q_1, \dots, Q_N)$ [Eq. (37)] and the n -step transition probability $k^{(n)}(P_1, \dots, P_N | Q_1, \dots, Q_N)$ [Eq. (47)], the following equalities are valid:

$$\|k(P_1, \dots, P_N | Q_1, \dots, Q_N)\| = 1$$

and

$$\|k^{(n)}(P_1, \dots, P_N | Q_1, \dots, Q_N)\| = 1 . \quad (58)$$

Then, substituting the left side of identity (57) into Eq. (56), we obtain

$$\langle \lambda_N^{(n)} \rangle - \lambda_0 = \lim_{n \rightarrow \infty} \sum_{l=0}^{n-1} \int_{D_1} \dots \int_{D_N} [G^{(l)}(R_1, \dots, R_N) k^{(n-l)}(P_1, \dots, P_N | R_1, \dots, R_N) dR_1 \dots dR_N \\ - G^{(l+1)}(Q_1, \dots, Q_N) k^{(n-l-1)}(P_1, \dots, P_N | Q_1, \dots, Q_N) dQ_1 \dots dQ_N] . \quad (59)$$

Substituting expression (24) for $p^{(n)}(R)$ into definition (20) of $G^{(n)}(R_1, \dots, R_N)$, we get

$$G^{(l)}(R_1, \dots, R_N) = \frac{\sum_{i=1}^N \left[\epsilon_0 \lambda_0^{l+1} \phi_0(R_i) + \sum_{i=1}^N \epsilon_i \psi^{(l+1)}(R_i) \right]}{\sum_{i=1}^N \left[\epsilon_0 \lambda_0^l \phi_0(R_i) + \sum_{i=1}^N \epsilon_i \psi^{(l)}(R_i) \right]} = \frac{D^{(l+1)}(R_1, \dots, R_N)}{D^{(l)}(R_1, \dots, R_N)}$$

and

$$G^{(l+1)}(Q_1, \dots, Q_N) = \frac{\sum_{i=1}^N \left[\epsilon_0 \lambda_0^{l+2} \Phi_0(Q_i) + \sum_{i=1}^N \epsilon_i \psi^{(l+2)}(Q_i) \right]}{\sum_{i=1}^N \left[\epsilon_0 \lambda_0^{l+1} \Phi_0(Q_i) + \sum_{i=1}^N \epsilon_i \psi^{(l+1)}(Q_i) \right]} = \frac{D^{(l+2)}(Q_1, \dots, Q_N)}{D^{(l+1)}(Q_1, \dots, Q_N)} .$$

Denote $(R_1, \dots, R_N) = X$ and $(Q_1, \dots, Q_N) = Y$. Then from definition (19) and Eq. (29) follows

$$G^{(l+1)}(Y) = \frac{\hat{K}D^{(l+1)}(X)}{\hat{K}D^{(l)}(X)}, \quad (60)$$

where $\hat{K}$ is the transport operator of Eq. (13). Since $\hat{K}$ is a positive linear operator, the following inequalities are valid²⁴:

$$\inf_Y \frac{f}{p} \leq \inf_X \frac{\hat{K}f}{\hat{K}p} \leq \sup_X \frac{\hat{K}f}{\hat{K}p} \leq \sup_Y \frac{f}{p}.$$

Using these inequalities^h we obtain from Eqs. (58) and (59):

$$|\langle \lambda_N^{(n)} \rangle - \lambda_0| \leq \lim_{n \rightarrow \infty} \sum_{l=0}^{n-1} |\sup G^{(l)}(R_1, \dots, R_N) - \inf G^{(l)}(R_1, \dots, R_N)|. \quad (61)$$

For every l the points $(R_1, \dots, R_N)$ are sampled from the pdf $k^{(l)}(P_1, \dots, P_N | R_1, \dots, R_N)$. Since the sums appearing in the definition of $G^{(l)}(R_1, \dots, R_N)$ can be viewed as sample averages, they approach in probability the expected values as $N \rightarrow \infty$. We obtain

$$\begin{aligned} \lim_{N \rightarrow \infty} G^{(l)}(R_1, \dots, R_N) \\ = C_l = \text{const} = \sup G^l(\cdot) = \inf G^l(\cdot). \end{aligned}$$

Then we obtain from inequality (61):

$$\lim_{N \rightarrow \infty} |\langle \lambda_N^{(n)} \rangle - \lambda_0| = 0.$$

Therefore, the devised Markov procedure for estimation of K_{eff} provides an asymptotically unbiased estimate of the effective multiplication factor of λ_0 . Now we will estimate the difference between the expected value of the Monte Carlo K_{eff} estimator (9), $\langle \lambda_N^{(n)} \rangle \equiv \lambda_N$, and the eigenvalue λ_0 for finite N . In order to do this, we must investigate the structure of the stationary distribution of the fission Markov chain $F_s(R_1, \dots, R_N)$. This distribution with independent R_i is invariant under finite permutations of the variables R_i . The random variables $R_1, \dots, R_N$ are called exchangeable if the $n!$ permutations $R_{i1}, \dots, R_{iN}$ have the same N -dimensional probability distribution. The theory of exchangeable probability distributions was developed in Refs. 25 and 9. In further considerations we will use only the symmetry of $F_s(R_1, \dots, R_N)$ in respect to all permutations of the arguments.

Introduce the following one-dimensional pdf's:

$$\begin{aligned} f_j(R, N) = \int_{D_1} \dots \int_{D_N} F_s(R_1, \dots, R_N) \\ \times \delta(R_j - R) dR_1 \dots dR_N. \end{aligned}$$

From the symmetry of the stationary distribution of fission Markov chain $F_s(R_1, \dots, R_N)$ it follows that $f_j(R, N) = f_N(R)$ for $j = 1, \dots, N$. Then, from the formula for the total probability, we obtain

$$\begin{aligned} f_N(R) = \int_{D_1} \dots \int_{D_N} \frac{\sum_{j=1}^N K(P_j, R)}{\sum_{i=1}^N p(P_i)} \\ \times f_N(P_1) \dots f_N(P_N) dP_1 \dots dP_N. \quad (62) \end{aligned}$$

It is necessary to note that Eq. (62) for the marginal pdf $F_N(R)$ is a nonlinear integral equation while the integral equation for the stationary probability distribution of the fission Markov chain is a linear one.

Now consider the adjoint equation for the equilibrium fission importance function $\Phi_0^*(R)$:

$$\lambda_0 \Phi_0^*(R) = \int_D K(R, P) \Phi_0^*(P) dP. \quad (63)$$

Multiplying Eq. (62) by $\Phi_0^*(R)$, integrating over R , and utilizing Eq. (63), we arrive at the following expression:

$$\begin{aligned} \int_D \Phi_0^*(R) f_N(R) dR = \lambda_0 \int_{D_1} \dots \int_{D_N} \frac{\sum_{j=1}^N \Phi_0^*(P_j)}{\sum_{i=1}^N p(P_i)} \\ \times f_N(P_1) \dots f_N(P_N) dP_1 \dots dP_N. \quad (64) \end{aligned}$$

From the definition of $f_N(R)$ and expression (52), it can be easily verified that

$$\lambda_N = \int_D f_N(R) p(R) dR.$$

Subtracting the expression

$$\lambda_0 \left[\int_D \Phi_0^*(P) f_N(P) dP \right] / \left[\int_D p(P) f_N(P) dP \right]$$

from each side of expression (64), we obtain after some algebraic transformations:

$$\lambda_N - \lambda_0 = I_N \lambda_0 \frac{\int_D p(R) f_N(R) dR}{\int_D \Phi_0^*(R) f_N(R) dR},$$

where I_N is given by

$$\begin{aligned} I_N = \int_{D_1} \dots \int_{D_N} \left[\frac{\sum_{i=1}^N \Phi_0^*(P_i)}{\sum_{j=1}^N p(P_j)} - \frac{\int_D \Phi_0^*(P) f_N(P) dP}{\int_D p(P) f_N(P) dP} \right] \\ \times f_N(P_1) \dots f_N(P_N) dP_1 \dots dP_N. \end{aligned}$$

^hThe same inequalities are valid for the adjoint operator and are used for $l = 0$.

Applying to the last expression the theorem¹ of Appendix B with $u(t) = \Phi_0^*(P)$ and $v(t) = P(P)$, we obtain

$$|\lambda_N - \lambda_0| \leq \frac{C}{N^{1/2}}, \quad (65)$$

where C is some linear functional of the adjoint equilibrium fission density $\Phi_0^*(R)$, $p(R)$, and $f_N(R)$, i.e., some problem-dependent constant.

Some useful conclusions may be drawn from the analysis of inequality (65). As we can see from inequality (65), the K_{eff} estimator (9) is an asymptotically unbiased estimate of K_{eff} since its expected value approaches λ_0 as $N \rightarrow \infty$. Thus expression (53) is valid. An upper limit bound for the amount of the bias for finite N is given by the right side of inequality (65):

$$B = \frac{C}{\sqrt{N}}.$$

The value of B is proportional to the inverse of the square root of the number of fission points in a generation N . Since $I_N = 0$ when $p(R) = \text{const}$ (see Appendix B), the bias in this case equals zero, i.e., $\lambda_N = \lambda_0$. In this case the equilibrium fission rate distribution is constant over the reactor. Then the Monte Carlo estimator (9) simply becomes an unbiased batch estimator since in each generation the expected value of the estimator equals K_{eff} . It must be noted that the causes of the bias in K_{eff} are the statistical errors of the numerator and denominator of expression (59). For large N we can assume that

$$\begin{aligned} \sup G^{(l)}(R_1, \dots, R_N) &\approx \frac{C_l + \frac{d_l}{\sqrt{N}}}{C_l - \frac{d_l}{\sqrt{N}}} \\ \inf G^{(l)}(R_1, \dots, R_N) &\approx \frac{C_l - \frac{d_l}{\sqrt{N}}}{C_l + \frac{d_l}{\sqrt{N}}}. \end{aligned}$$

Substituting these expressions into (61), we obtain inequality (65). It is necessary to note that inequality (65) is valid, however, for all values of N , not necessarily large ones. The constant C entering the inequality (65) is prohibitively difficult to calculate. In Ref. 9 we derived an expression for the value of the bias that is valid for large N and is appropriate for practical calculations.

V. ASYMPTOTIC STATISTICAL PROPERTIES OF THE K_{eff} ESTIMATOR

In this section we present some statistical properties of the one-generation average of the estimator (48), $\bar{k}_N^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}]$. From the definition of the n -step transition probability of the Markov chain expression (47), it follows that

$$\begin{aligned} \sup_{Q_i, P_i, R_i \in D} |k^{(n)}(P_1, \dots, P_N | R_1, \dots, R_N) \\ - k^{(n)}(Q_1, \dots, Q_N | R_1, \dots, R_N)| = \alpha < 1. \end{aligned} \quad (66)$$

Under condition (66), the stationary distribution of the Markov chain (8) exists and the following estimate of the convergence rate in (46) is valid²³:

$$\begin{aligned} \|F_s(R_1, \dots, R_N) - k^{(n)}(Q_1, \dots, Q_N | R_1, \dots, R_N)\| \\ \leq \alpha^n. \end{aligned} \quad (67)$$

Inequality (67) is valid for any initial state of a Markov chain $(Q_i)_{i=1}^N$. Now suppose that the following limit exists:

$$\begin{aligned} \lim_{n \rightarrow \infty} \left(\frac{1}{n} \sum_{k=1}^n \{ \bar{k}_N^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}] - \langle \bar{\lambda}_N^{(n)} \rangle \}^2 \right) \\ = \sigma^2 \geq 0. \end{aligned} \quad (68)$$

According to Eq. (39) with probability one, this limit equals the average over the stationary distribution:

$$\begin{aligned} \sigma^2 = \int_{D_1} \dots \int_{D_N} \left[\frac{1}{N} \sum_{i=1}^N P(R_i) - \langle \bar{\lambda}_N^{(n)} \rangle \right]^2 \\ \times F_s(R_1, \dots, R_N) dR_1 \dots dR_N. \end{aligned}$$

Under conditions (66), (67), and (68), the central limit theorem for Markov chains¹⁶ is valid and the following limit exists:

$$\begin{aligned} \lim_{n \rightarrow \infty} \text{Prob} \left(\frac{1}{n} \sum_{k=1}^n \{ \bar{k}_N^{(k)}[R_1^{(k)}, \dots, R_N^{(k)}] \right. \\ \left. - \langle \bar{\lambda}_N^{(n)} \rangle \} < \frac{t\sigma}{\sqrt{n}} \right) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^t \exp\left(-\frac{z^2}{2}\right) dz. \end{aligned} \quad (69)$$

The last expression, Eq. (69), states that the one-generation average of the K_{eff} estimator (48) is asymptotically normally distributed around its mean value $\langle \bar{\lambda}_N^{(n)} \rangle$. Thus the confidence limits and statistical error of estimator (48) may be calculated, provided that variance σ is calculated. The total mean square error of the estimator (48), d^2 , is given by the expression

$$d^2 = \sigma^2 + B^2.$$

VI. CONCLUSIONS

We have presented the rigorous stochastic procedure for Monte Carlo estimation of the effective multiplication factor of a nuclear reactor. An upper limit

¹Several similar theorems were proved in Ref. 26.

bound of the bias in the K_{eff} estimator was obtained which follows a $N^{-1/2}$ behavior. It is worthwhile to note that the value of the upper bound of the bias does not depend on the details of the Monte Carlo game, i.e., on the explicit expression for the Markov chain transition probability, Eq. (37). Inequality (65) could probably be sharpened, however, in the case when the detailed structure of the transition probability $k[R_1^{(n)}, \dots, R_N^{(n)} | R_1^{(n+1)}, \dots, R_N^{(n+1)}]$ is considered. It is also necessary to note that all the results presented are still valid for any Monte Carlo K_{eff} estimator $\xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ defined on the states of some Markov chain with the transition probabilities different from Eq. (37), if the one-generation average of $\xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}]$ is given by Eq. (35).[†] The results presented above will still be valid if the Monte Carlo estimator depends on two successive states of the Markov chain, provided that the one-generation average satisfies an equation of the form

$$\begin{aligned} & \langle \xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}, R_1^{(n+1)}, \dots, R_N^{(n+1)}] \rangle \\ &= \frac{1}{N} \sum_{i=1}^N P[R_i^{(n)}] + \theta^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] \end{aligned}$$

with

$$\lim_{n \rightarrow \infty} \theta^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] = 0.$$

This can be verified by substitution of the one-generation average from Eq. (69) into expression (56) for the difference between the expectation of the estimator and the eigenvalue. Then, repeating the above performed transformations and taking the limit as $n \rightarrow \infty$, we arrive at inequality (65).

APPENDIX A

Theorem:

$$p = \sum_{n=N}^{\infty} \frac{N-1}{n-1} \frac{(n-1)!}{(N-1)!(n-N)!} p^N (1-p)^{n-N}.$$

Proof: The theorem is proved by induction. Define

$$\begin{aligned} f_N &= \sum_{n=N}^{\infty} \frac{N-1}{n-1} \frac{(n-1)!}{(N-1)!(n-N)!} p^N (1-p)^{n-N} \\ &= \sum_{n=N}^{\infty} \frac{(n-2)! p^N (1-p)^{n-N}}{(N-2)!(n-N)!}. \end{aligned}$$

Setting $N=2$, we find that

$$f_2 = \sum_{n=2}^{\infty} p^2 (1-p)^{n-2} = \frac{p^2}{1-(1-p)} = p.$$

Now suppose that $f_N = p$ and consider f_{N+1} :

$$\begin{aligned} f_{N+1} &= \sum_{n=N+1}^{\infty} \frac{(n-2)!}{(N-1)!(n-N-1)!} \\ &\quad \times p^{N+1} (1-p)^{n-N-1}. \end{aligned}$$

Denoting $m = n - 1$, we get

$$\begin{aligned} f_{N+1} &= \sum_{m=N}^{\infty} \frac{(m-1)!}{(N-1)!(m-N)!} p^{N+1} (1-p)^{m-N} \\ &= \frac{(1-p)}{(N-1)!} \left(\frac{p}{1-p} \right)^{N+1} \sum_{m=N}^{\infty} \frac{(m-1)!}{(m-N)!} (1-p)^m. \end{aligned}$$

Denote

$$g_N = \sum_{n=N}^{\infty} \frac{(n-2)!}{(n-N)!} (1-p)^{n-1}.$$

Since $f_N = p$, then

$$g_N = (N-2)! \left(\frac{1-p}{p} \right)^{N-1}.$$

Therefore,

$$\begin{aligned} -\frac{\partial g_N}{\partial p} &= \sum_{m=N}^{\infty} \frac{(m-1)!}{(m-N)!} (1-p)^{m-2} \\ &= (N-1)! \left(\frac{1-p}{p} \right)^{N-1} \left(\frac{1}{p} + \frac{1}{1-p} \right). \end{aligned}$$

Thus

$$\begin{aligned} & \sum_{m=N}^{\infty} \frac{(m-1)!}{(m-N)!} (1-p)^m \\ &= \frac{(N-1)!(1-p)^2}{p(1-p)} \left(\frac{1-p}{p} \right)^{N-1} \\ &= (N-1)! \left(\frac{1-p}{p} \right)^N. \end{aligned}$$

Therefore, $f_{N+1} = p$. Thus, by induction we conclude that $f_N = p$ for all N .

APPENDIX B

[†]It is necessary to note that not all the Markov procedures for K_{eff} estimation yield an asymptotically unbiased estimate of K_{eff} . An example of a Markovian Monte Carlo game providing a biased estimate of K_{eff} is presented in Appendix C.

Theorem: Let $u(P) > 0$, $v(P) > 0$, and $f(P) > 0$ be some bounded functions defined in domain S and $\int_S f(P) dP = 1$. Then for every N the following inequality is valid:

$$I_N = \left| \int_{S_1} \cdots \int_{S_N} \left[\frac{\sum_{i=1}^N u(P_i)}{\sum_{j=1}^N v(P_j)} - \frac{\int_S u(P)f(P) dP}{\int_S v(P)f(P) dP} \right] \prod_{l=1}^N f(P_l) dP_l \right| \leq \frac{C}{N^{1/2}} . \quad (\text{B.1})$$

Proof: Since

$$\int_S u(P)f(P) dP = \int_{S_1} \cdots \int_{S_N} \frac{\sum_{i=1}^N u(P_i)}{N} \prod_{l=1}^N f(P_l) dP_l ,$$

then

$$\begin{aligned} I_N &= \frac{1}{\int_S v(P)f(P) dP} \left| \int_{S_1} \cdots \int_{S_N} \left[\frac{\sum_{i=1}^N u(P_i)}{\sum_{j=1}^N v(P_j)} \int_S v(P)f(P) dP - \frac{\sum_{i=1}^N u(P_i)}{N} \prod_{l=1}^N f(P_l) dP_l \right] \right| \\ &= \frac{1}{\int_S v(P)f(P) dP} \left| \int_{S_1} \cdots \int_{S_N} \frac{\sum_{i=1}^N u(P_i)}{\sum_{j=1}^N v(P_j)} \frac{1}{N} \sum_{i=1}^N \left[\int_S v(P)f(P) dP - v(P_i) \right] \prod_{l=1}^N f(P_l) dP \right| . \end{aligned}$$

Applying the Schwartz inequality

$$\left| \int_D g_1(z)g_2(z)g_3(z) dz \right| \leq \left[\int_D g_1(z)g_2^2(z) dz \right]^{1/2} \left[\int_D g_1(z)g_3^2(z) dz \right]^{1/2}$$

with

$$\begin{aligned} g_1(z) &= \frac{1}{N} \prod_{l=1}^N f(P_l) ; \quad g_2(z) = \frac{\sum_{i=1}^N u(P_i)}{\sum_{j=1}^N v(P_j)} ; \\ g_3(z) &= \sum_{i=1}^N \left[\int_S v(P)f(P) dP - v(P_i) \right] \end{aligned}$$

and the identity

$$\int_{S_1} \cdots \int_{S_N} \left\{ \sum_{i=1}^N \left[\int_S v(P)f(P) dP - v(P_i) \right] \right\}^2 \prod_{l=1}^N f(P_l) dP_l = N \cdot \int_S \left[v(P) - \int_S v(P)f(P) dP \right]^2 f(P) dP ,$$

we obtain

$$\begin{aligned} I_N &\leq \frac{1}{\int_S v(P)f(P) dP} \left\{ \int_{S_1} \cdots \int_{S_N} \left[\frac{\sum_{i=1}^N u(P_i)}{\sum_{j=1}^N v(P_j)} \right]^2 \prod_{l=1}^N f(P_l) dP_l \right\}^{1/2} \\ &\quad \times \left\{ \frac{1}{N} \int_S \left[v(P) - \int_S v(P)f(P) dP \right]^2 f(P) dP \right\}^{1/2} . \end{aligned}$$

Since functions $u(P)$ and $v(P)$ are bounded,

$$I_N \leq \frac{C}{\int_S v(P)f(P) dP} \cdot \frac{1}{\sqrt{N}} \left\{ \int_S \left[v(P) - \int_S v(P)f(P) dP \right]^2 f(P) dP \right\}^{1/2} .$$

This completes the proof. In the case in which $v(P) = \text{const}$, $I_N \equiv 0$. The sequence of points $(P_i)_{i=1}^N$ of inequality (A.1) is an arbitrary sequence of points in domain S . In the case when this sequence is a finite sample of size N from the pdf $f(P)$, the inequality (A.1) cannot be improved. Then inequality (A.1) has the clear probabilistic meaning since the sums entering (A.1) become Monte Carlo estimates of the corresponding integrals with the statistical error proportional to $1/\sqrt{N}$. In the case, however, when this sequence is the sequence of uniform numbers (see Ref. 27), inequality (A.1) may be sharpened and becomes

$$I_N \leq \frac{C}{N}.$$

APPENDIX C

EXAMPLE OF THE MARKOVIAN MONTE CARLO GAME THAT PROVIDES A BIASED ESTIMATE OF K_{eff} EVEN WHEN THE NUMBER OF FISSION POINTS IN A GENERATION IS INFINITE

Suppose that in order to obtain N fission points of the $(n+1)$ 'th generation from the fission points of the n 'th generation, fission neutrons are started from the fission points of the n 'th generation $R_i^{(n)}$ until the fission event occurs. The probability of accepting point $R_i^{(n)}$ as a starting point is given by the expression

$$P[R_i^{(n)}] = \frac{\nu[R_i^{(n)}]}{\sum_{i=1}^N \nu[R_i^{(n)}]}.$$

The difference between this procedure and the procedure described in Sec. II is that once point $R_i^{(n)}$ was accepted as a starting point, fission neutrons are sampled from this specific point until the first fission occurs. Thus, the starting points of each history are sampled N times. The points of fission events produced by these neutrons are accepted as the points of the $(n+1)$ 'th generation. The K_{eff} estimator for this game is given by the expression

$$\xi_N^{(n)}[R_1^{(n)}, \dots, R_N^{(n)}] = \frac{1}{N} \sum_{i=1}^N \nu[R_i^{(n)}] \frac{1}{N_i^{(n)}[R_i^{(n)}]}, \quad (C.1)$$

where $N_i^{(n)}[R_i^{(n)}]$ is the number of fission neutrons to be sampled from the points $R_i^{(n)}$ until the first fission occurs. Averaging of this estimator over all possible values of $N_i^{(n)}[R_i^{(n)}]$ yields

$$\left\langle \frac{1}{N_i^{(n)}[R_i^{(n)}]} \right\rangle = \int_D G_f[R_i^{(n)}, R] dR. \quad (C.2)$$

The transition probability of the Markov chain corresponding to this game is given by the following expression:

$$K(R_1, \dots, R_N | P_1, \dots, P_N) = \prod_{i=1}^N \sum_{j=1}^N \frac{G_f(R_j, P_i)}{G_f(R_j)} \cdot \frac{\nu(R_j)}{\sum_{m=1}^N \nu(R_m)}, \quad (C.3)$$

where

$$G_f(R) = \int_D G_f(R, P) dP. \quad (C.4)$$

Then

$$\begin{aligned} \lambda_N^{(n)} &= \frac{1}{N} \sum_{i=1}^N K^{(n)}(P_1, \dots, P_N | R_1, \dots, R_N) \\ &\quad \times p(R_i) dR_1 \dots dR_N \\ &= \frac{1}{N} \sum_{i=1}^N \int_{D_1} \dots \int_{D_{2N}} K^{(n-1)}(P_1, \dots, P_N | X_1, \dots, X_N) \\ &\quad \times \prod_{j=1}^N \sum_{l=1}^N \frac{\nu(X_l)}{\sum_{m=1}^N \nu(X_m)} \cdot \frac{G_f(X_l, R_j)}{G_f(X_l)} \\ &\quad \times p(R_i) \cdot dX_1 \dots dX_N dR_1 \dots dR_n. \end{aligned}$$

Integrating the terms with $j \neq i$, we get

$$\begin{aligned} \lambda_N^{(n)} &= \int_{D_1} \dots \int_{D_{N+1}} K^{(n-1)}(P_1, \dots, P_N | X_1, \dots, X_N) \\ &\quad \times \sum_{l=1}^N \frac{\nu(X_l)}{\sum_{m=1}^N \nu(X_m)} \cdot \frac{G_f(X_l, R)}{G_f(X_l)} \\ &\quad \times p(R) dR dX_1 \dots dX_n. \end{aligned}$$

In order to simplify the calculations, we assume further that the number of secondary neutrons generation per fission event is constant:

$$\nu(R) \equiv \nu_0 = \text{const}.$$

This is not too severe an approximation since in reality $\nu(R)$ varies in a rather narrow interval. Then

$$\frac{\nu(X_l)}{\sum_{m=1}^N \nu(X_m)} = \frac{1}{N}$$

and

$$\begin{aligned}\lambda_N^{(n)} &= \frac{1}{N} \sum_{i=1}^N \int_{D_1} \dots \int_{D_{2N+1}} K^{(n-2)}(P_1, \dots, P_N | Y_1, \dots, Y_N) \\ &\times \left[\prod_{j=1}^N \frac{1}{N} \sum_{l=1}^N \frac{G_f(Y_l, X_j)}{G_f(Y_l)} \right] \\ &\times \frac{G_f(X_i, R)}{G_f(X_i)} p(R) dR dY_1 \dots dY_N dX_1 \dots dX_N \\ &= \frac{1}{N} \sum_{l=1}^N \int_{D_1} \dots \int_{D_{N+2}} K^{(n-2)}(P_1, \dots, P_N | Y_1, \dots, Y_N) \\ &\times \frac{G_f(Y_l, X)}{G_f(Y_l)} \frac{G_f(X, R)}{G_f(X)} p(R) dX dR dY_1 \dots dY_N.\end{aligned}$$

Repeating this procedure successively, we obtain

$$\begin{aligned}\lambda_N^{(n)} &= \frac{1}{N} \sum_{l=1}^N \int_{D_1} \dots \int_{D_N} \frac{G_f(P_l, R_1)}{G_f(P_l)} \\ &\times \frac{G_f(R_1, R_2)}{G_f(R_1)} \dots \frac{G_f(R_{n-1}, R_n)}{G_f(R_{n-1})} \\ &\times p(R_n) dR_1 \dots dR_n.\end{aligned}$$

The last expression is the Monte Carlo estimate of the functional

$$I = \int_D f(R) p(R) dR$$

from the solution of the integral equation

$$f(R) = \int_D \frac{G_f(P, R)}{G_f(P)} f(P) dP, \quad (C.5)$$

which does not coincide with the criticality equation. Thus the procedure presented is not "sufficiently stochastic" to provide the convergence to the equilibrium distribution. The Monte Carlo estimate $\lambda_N^{(n)}$ differs from λ_0 when $n \rightarrow \infty$, and $N \rightarrow \infty$, as can be deduced when comparing Eq. (C.5) with the criticality equation

$$\lambda_0 f_0(R) = \nu_0 \int_D G_f(P, R) f_0(P) dP. \quad (C.6)$$

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REFERENCES

1. E. L. KAPLAN, "Monte Carlo Methods for Equilibrium Solutions in Neutron Multiplication," UCRL-5275-T, Lawrence Livermore National Laboratory (1958).
2. J. B. PARKER and E. R. WOODCOCK, *Prog. Nucl. Energy Ser.*, **4**, 435 (1961).
3. J. LIEBEROTH, *Nukleonik*, **11**, 213 (1968).
4. R. C. GAST, "Monte Carlo Eigenfunction Iteration Strategies That Are and Are Not Fair Games," WAPD-TM-878, Westinghouse Electric Corporation (1969).
5. R. C. GAST and N. R. CANDELORE, *Trans. Am. Nucl. Soc.*, **14**, 219 (1971).
6. R. C. GAST and N. R. CANDELORE, "Monte Carlo Eigenfunction Strategies and Uncertainties," *Proc. NEACRP Mtg. Monte Carlo Study Group*, Argonne, Illinois, July 1-3, 1974, ANL-75-2, p. 161, Argonne National Laboratory (1975).
7. E. M. GELBARD and R. E. PRAEL, "Monte Carlo Work at Argonne National Laboratory," *Proc. NEACRP Mtg. Monte Carlo Study Group*, Argonne, Illinois, July 1-3, 1974, ANL-75-2, p. 201, Argonne National Laboratory (1975).
8. J. SPANIER and E. M. GELBARD, *Monte Carlo Principles and Neutron Transport Problems*, p. 27, Addison-Wesley, Publishing Company, Inc., Reading, Massachusetts (1969).
9. A. DUBI and T. ELPERIN, submitted for publication in *Nucl. Sci. Eng.*
10. D. B. MacMILLAN, *Nucl. Sci. Eng.*, **50**, 73 (1973).
11. H. BOWSER, E. M. GELBARD, P. GEMMEL, and G. PACK, *Trans. Am. Nucl. Soc.*, **45**, 324 (1983).
12. D. DICKENSON and G. E. WHITESIDES, *Nucl. Technol.*, **30**, 73 (1976).
13. J. G. MOORE, *Adv. Nucl. Sci. Technol.*, **9**, 73 (1976).
14. J. KYNČL and I. MAREK, *Lect. Notes Math.*, **703**, 224 (1979).
15. S. OREY, *Lecture Notes on Limit Theorems for Markov Chain Transition Probabilities*, Van Nostrand Reinhold Company, London (1971).
16. J. L. DOOB, *Stochastic Processes*, John Wiley & Sons, Inc., New York (1953).
17. H. H. SCHAEFFER, *Banach Lattices and Positive Operators*, Springer Verlag, New York (1974).
18. L. V. KANTOROVICH and G. P. AKILOV, *Functional Analysis in Normed Spaces*, Macmillan, Inc., New York (1964).

19. M. BORYSIEVICZ, *Trans. Theory Stat. Phys.*, **7**, 139 (1978).
20. S. UKAI and T. HIRAOKA, *J. Nucl. Sci. Technol.*, **9**, 36 (1972).
21. F. PREMUDA and G. SPIGA, *Nucl. Sci. Eng.*, **63**, 1 (1977).
22. G. BIRKHOFF, *Rend. Mater.*, **22**, 102 (1963).
23. K. L. CHANG, *Markov Chains with Stationary Transition Probabilities*, Springer Verlag, New York (1967).
24. E. HOPF, *J. Math. Mech.*, **12**, 683 (1963).
25. L. J. SAVAGE and E. HEWITT, *Trans. Amer. Math. Soc.*, **80**, 470 (1955).
26. M. J. POWELL and J. SWANN, *J. Inst. Math. Its Appl.*, **2**, 228 (1966).
27. J. H. HALTON, *SIAM Rev.*, **12**, 1 (1970).
28. W. FELLER, *An Introduction to Probability Theory and Its Applications*, Vol. 2, John Wiley & Sons, Inc., New York (1966).