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*Title:* Intergenerational Correlation in Monte Carlo K-Eigenvalue Calculations

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**ABSTRACT**

This paper investigates intergenerational correlation in the Monte Carlo k-eigenvalue calculation of a neutron effective multiplicative factor. To this end, the exponential transform for path-stretching has been applied to large fissionable media with localized highly multiplying regions because in such media exponentially-decaying shape is rough representation of the importance of source particles. The numerical results show that the difference between real and apparent variances virtually vanishes for an appropriate value of the exponential transform parameter. This indicates that the intergenerational correlation of k-eigenvalue samples could be eliminated by the adjoint biasing of particle transport. The relation between the biasing of particle transport and the intergenerational correlation is therefore investigated in the framework of collision estimators and the following conclusion has been obtained: Within the leading order approximation with respect to the number of histories per generation, the intergenerational correlation vanishes when immediate importance is constant, and the immediate importance under simulation can be made constant by the biasing of particle transport with a function adjoint to source neutron's distribution, i.e., the importance over all future generations.

## I. INTRODUCTION

In Monte Carlo computing, statistical error is estimated through sample variance by many practitioners. As shown in standard introductory statistics textbooks,[1] sample variance is unbiased when there exists no correlation among samples. However, in the Monte Carlo $k-$eigenvalue calculation of a neutron effective multiplicative factor, source generations iterated in a recursive manner yield correlated samples. A straightforward method to cope with such correlation is to compute the sample variance of the batches of the $k-$eigenvalues from consecutive generations since the virtual generation-lag between the adjacent batches increases.[2] There are several relations among real and apparent variances and lag-covariances, where "real" refers to the variance of sample mean and the lag-covariance of samples, and "apparent" to the expected value of the sample variance and lag-covariances. Based on these relations, an iterative method was proposed to estimate real variance.[3] Demaret et al. and Jacquet et al. proposed a fitting method of estimating lag-covariances based on time series methodologies and showed that it stably performs.[4,5] In all these methods, the algorithm of source iteration and normalization remains intact. On the other hand, superhistory powering employs the modified procedures of source normalization and iteration to reduce the correlation of k-eigenvalue samples.[6]

In this paper, the possibility of reducing the intergenerational correlation of $k-$eigenvalue samples is investigated using the biasing of particle transport. To motivate the investigation, the exponential transform for path stretching[7,8] has been applied to large fissionable media with localized highly multiplying regions. From practical viewpoints, such media capture the essence of rod drop accidents of boiling water reactors at cold or hot standby. Qualitatively, a certain fraction of the particles in a sharp distribution peak tend to escape from that peak and spread over the surrounding region. Since the trace of one particle usually covers small area during one generation, the statistical fluctuation of source distribution caused by those spreading particles at one generation tends to be transfered to the next generation and the intergenerational correlation consequently becomes positively large. The exponential transform can be utilized to suppress such a phenomenon by virtually confining particles in highly multiplying regions. On the other hand, exponentially-decaying shape is rough representation of the importance of source neutrons for a large fissionable medium with a localized highly multiplying region. Therefore, one may pose the following question: Is there mathematical relation between the adjoint biasing of particle transport and the intergenerational correlation of sources?

This paper is organized as follows. Statistical treatments of k-eigenvalue samples and the spatial transform of k-eigenvalue transport equation are explained in Secs. II and III, respectively. The numerical results with exponential transform are presented in Sec. IV. In Sec. V, the relation between the biasing of particle transport and the intergenerational correlation of k-eigenvalue samples is analyzed. Conclusions are stated in Sec. VI.

## II. STATISTICAL TREATMENTS

A quantity of interest is the variance of the $k$-eigenvalue estimate:

$$k = \frac{1}{N}\sum_{j=1}^{N} k_j. \tag{1}$$

where $N$ is the number of stationary generations in a Monte Carlo $k$-eigenvalue computation and $k_j$ is a $k$-eigenvalue sample for the $j$-th stationary generation. A standard estimator of the variance of $k$ is sample variance:

$$\sigma_S^2 = \frac{1}{N(N-1)}\sum_{i=1}^{N}(k_i - k)^2. \tag{2}$$

The expected value of $\sigma_S^2$, which is called apparent variance and denoted by $\sigma_A^2$, is computed by

$$\sigma_A^2 \equiv E[\sigma_S^2] \approx \frac{1}{M}\sum_{i=1}^{M}\frac{1}{N(N-1)}\sum_{j=1}^{N}\left( k_j^i - \frac{1}{N}\sum_{m=1}^{N} k_m^i \right)^2 \tag{3}$$

where $E[\,\cdot\,]$ denotes an expected value, $M$ is the number of independently replicated Monte Carlo runs, $N$ is the number of stationary generations per run and $k_j^i$ is the eigenvalue sample for the $j$-th stationary generation of the $i$-th run. In general, apparent variance is not equal to real variance that is denoted by $\sigma_R^2$ and defined by

$$\sigma_R^2 \equiv E[k^2] - E[k]^2. \tag{4}$$

The difference between apparent and real variances is[3]:

$$\sigma_A^2 - \sigma_R^2 = -\frac{2}{N(N-1)}\sum_{i=1}^{N}(N-i)C_R[i], \tag{5}$$

where $C_R[i]$ is real lag-i covariance:

$$C_R[i] = E[(k_m - E[k_m])(k_{m+i} - E[k_{m+i}])],\ m = 1, \ldots, N-i. \tag{6}$$

Note that the stationarity introduced above has dictated that $E[k] = E[k_m] = E[k_{m+i}]$ and $C_R[i]$ is independent of $m$. Real variance is computed by

$$\sigma_R^2 \approx \frac{1}{M-1}\sum_{i=1}^{M}\Big( \frac{1}{N}\sum_{j=1}^{N} k_j^i - \frac{1}{M}\sum_{i=1}^{M}\frac{1}{N}\sum_{j=1}^{N} k_j^i \Big)^2. \tag{7}$$

## III. SPATIAL TRANSFORM OF TRANSPORT EQUATION

This section describes the spatial transform of k-eigenvalue transport equation:

$$\vec{\Omega}\cdot\vec{\nabla}\psi(\vec{r},\vec{\Omega},E) + \Sigma_t(\vec{r},E)\psi(\vec{r},\vec{\Omega},E) = \int_0^{E_{max}}\int_{4\pi}\Sigma_s(\vec{r},\vec{\Omega}',E'\rightarrow\vec{\Omega},E)\psi(\vec{r},\vec{\Omega}',E')d^2\Omega' dE'$$
$$+\frac{1}{k}\frac{\chi(E)}{4\pi}\int_0^{E_{max}}\int_{4\pi}\nu\Sigma_f(\vec{r},E')\psi(\vec{r},\vec{\Omega}',E')d^2\Omega' dE',\ \vec{r}\in D, \tag{8}$$

$$\psi(\vec{r},\vec{\Omega},E) = 0,\ \vec{r}\in\partial D,\ \vec{n}\cdot\Omega < 0, \tag{9}$$

where $\psi$ is flux density, $\vec{r}$ position vector, $\vec{\Omega}$ the unit vector of direction of movement, $E$ energy, $\Sigma_t$ total macroscopic cross section, $\Sigma_s$ differential scattering macroscopic cross section, $\Sigma_f$ macroscopic fission cross section, $\nu$ the mean number of neutrons emerging from a fission event, $\chi$ is the energy spectrum of these neutrons, $(0, E_{max})$ the energy domain and $D$ the spatial domain. We transform the solution of Eqs. (8)-(9) by $S^*(\vec{r})$:

$$\Psi(\vec{r},\vec{\Omega},E) = S^*(\vec{r})\psi(\vec{r},\vec{\Omega},E). \tag{10}$$

Eqs. (8) and (9) then become

$$\vec{\Omega}\cdot\vec{\nabla}\Psi(\vec{r},\vec{\Omega},E) + \left[\Sigma_t(\vec{r},E) - \frac{\vec{\Omega}\cdot\vec{\nabla}S^*(\vec{r})}{S^*(\vec{r})}\right]\Psi(\vec{r},\vec{\Omega},E)$$
$$= \int_0^{E_{max}}\int_{4\pi}\Sigma_s(\vec{r},\vec{\Omega}'\rightarrow\vec{\Omega},E'\rightarrow E)\Psi(\vec{r},\vec{\Omega}',E')d^2\Omega' dE'$$
$$+\frac{1}{k}\frac{\chi(E)}{4\pi}\int_0^{E_{max}}\int_{4\pi}\nu\Sigma_f(\vec{r},E')\Psi(\vec{r},\vec{\Omega}',E')d^2\Omega' dE',\ \vec{r}\in D, \tag{11}$$

$$\Psi(\vec{r},\vec{\Omega},E) = 0,\ \vec{r}\in\partial D,\ \vec{n}\cdot\Omega < 0\,. \tag{12}$$

In the particle transport ruled by Eq. (11), total macroscopic cross section, the mean number of scattering events per collision, and the mean number of fission events per collision are, respectively, modified to

$\Sigma_t - \vec{\Omega} \cdot \vec{\nabla} S^*/S^*$,

$\int_0^{E_{max}} \int_{4\pi} \Sigma_s(\vec{r}, \vec{\Omega} \to \vec{\Omega}', E \to E') d^2\Omega' dE' / [\Sigma_t - \vec{\Omega} \cdot \vec{\nabla} S^*/S^*]$, and

$\Sigma_f(\vec{r}, E)/[\Sigma_t - \vec{\Omega} \cdot \vec{\nabla} S^*/S^*]$.

Other transport-governing quantities remain unchanged.

## IV. EXPONENTIAL TRANSFORM AND TWO STANDARD DEVIATIONS

In this section, the exponential transform for path stretching[7,8] is applied to energy-independent and isotropically-scattering media. Real and apparent standard deviations ($\sigma_R$ and $\sigma_A$) are then evaluated by (3) and (7) in Sec. II. The first problem is shown in Figure 1, for which $S^*$ in Sec.III is chosen as

$$S^*(\vec{r}) = \begin{cases} e^{-\lambda_x \Sigma_t (x-a) - \lambda_y \sigma_t (y-b)}, & a < x < d,\ b < y < e, \\ e^{-\lambda_y \Sigma_t (y-b)}, & -a < x < a,\ b < y < e, \\ e^{\lambda_x \Sigma_t (x+a) - \lambda_y \sigma_t (y-b)}, & -d < x < -a,\ b < y < e, \\ e^{\lambda_x \Sigma_t (x+a)}, & -d < x < -a,\ -b < y < b, \\ e^{\lambda_x \Sigma_t (x+a) + \lambda_y \sigma_t (y+b)}, & -d < x < -a,\ -e < y < -b, \\ e^{\lambda_y \Sigma_t (y+b)}, & -a < x < a,\ -e < y < -b, \\ e^{-\lambda_x \Sigma_t (x-a) + \lambda_y \sigma_t (y+b)}, & a < x < d,\ -e < y < -b, \\ e^{-\lambda_x \Sigma_t (x-a)}, & a < x < d,\ -b < y < b, \\ 1, & -a < x < a,\ -b < y < b. \end{cases} \tag{13}$$

Note that the region defined by $-a < x < a$ and $-b < y < b$ is a localized highly multiplying region and exponential transform is not applied to that region. Apparent and real standard deviations for various values of $\lambda_x$ and $\lambda_y$ are shown in Figure 2 wherein implicit capture with Russian roulette was employed, $k_j^i$ were estimated by a collision estimator through independently replicating 500 runs with 300 generations whose first 100 generations were disposed to secure stationarity, and the number of particle histories per generation is 2000. It was observed that $|\sigma_A - \sigma_R|$ significantly reduced together with the decrease of $\sigma_R$ when the transform parameter was chosen optimally. It was also observed that both $|\sigma_A - \sigma_R|$ and $\sigma_R$ started to increase beyond that optimal value.

The second problem is shown in Figure 3, for which $S^*$ is chosen as

$$S^*(\vec{r}) = \begin{cases} e^{\lambda\Sigma_t(x+a+h)}, & \text{if } -b < x < -(a+h), \\ 1 & \text{if } -(a+h) < x < -a, \\ e^{-\lambda\Sigma_t(x+a)}, & \text{if } -a < x < 0, \\ e^{\lambda\Sigma_t(x-a)}, & \text{if } 0 < x < a, \\ 1 & \text{if } a < x < a+h, \\ e^{-\lambda\Sigma_t(x-a-h)}, & \text{if } a+h < x < b. \end{cases} \tag{14}$$

Note that the region defined by $-(a+h) < x < -a$ or $a < x < a+h$ is a localized highly multiplying region and exponential transform is not applied to that region. Apparent and real standard deviations for various values of $\lambda$ are shown in Figure 4 wherein the number of particle histories per generation is 1000 and other computational conditions are the same as those for Figure 2. Results similar to those in Figure 2 are observed in Figure 4. Both the results indicate that the exponential transform for path stretching may reduce the intergenerational correlation of k-eigenvalue samples for a certain class of problems.

The problems treated above capture the essential property of the rod drop accidents of boiling water reactors at cold or hot standby in the sense that there are sharp distribution peaks of the neutrons born from fission. Exponential shape is rough representation of the decaying of these peaks. Since fissionable isotopes are both sources and detectors, exponential shape is also rough representation of the importance of the source particles around these peaks. Therefore, one may pose the following question: Is there mathematical relation between the adjoint biasing of particle transport and the intergenarational correlation of k-eigenvalue samples? This question is the subject of the next secticon.

## V. INTERGENERATIONAL CORRELATION AND PARTICLE TRANSPORT

This section investigates the relation between the biasing of particle transport and the intergenerational correlation of k-eigenvalue samples. To this end, part of Brissenden and Garlick's work[6] on the estimation bias of $k-$eigenvalue calculation for a discretized model is extended to continuous models based on Sutton and Brown's unpublished work[9].

To start analysis, Eq. (8) is rewritten in terms of the spatial source distribution $S_0(\vec{r})$:

$$S_0(\vec{r}) = \frac{1}{k_0}\mathbf{F}\mathbf{T}^{-1}\left(\frac{\chi(E)}{4\pi}S_0(\vec{r})\right) = \frac{1}{k_0}\int_D H(\vec{r}\,' \to \vec{r})S_0(\vec{r}\,')d^3r', \tag{15}$$

where $\mathbf{F}$ and $\mathbf{T}$ are fission and transport operators:

$$\begin{aligned}
\mathbf{F}\phi &= \int_0^{E_{max}}\int_{4\pi} \nu\Sigma_f(\vec{r}, E')\phi(\vec{r}, \vec{\Omega}', E')d^2\Omega' dE' \,, \\
\mathbf{T}\phi &= \vec{\Omega}\cdot\vec{\nabla}\phi(\vec{r}, \vec{\Omega}, E) + \Sigma_t(\vec{r}, E)\phi(\vec{r}, \vec{\Omega}, E) \\
&\quad - \int_0^{E_{max}}\int_{4\pi} \Sigma_s(\vec{r}, \vec{\Omega}', E' \to \vec{\Omega}, E)\phi(\vec{r}, \vec{\Omega}', E')d^2\Omega' dE' \,,
\end{aligned}$$

and $H(\vec{r}\,' \to \vec{r})$ is an integral kernel that can be interpreted as the expected number of source particles per unit volume at $\vec{r}$ directly resulting from a starter particle at $\vec{r}\,'$. Note that this interpretation of $H(\vec{r}\,' \to \vec{r})$ excludes the starter particles produced by the daughter particles. The subscript "zero" in $S_0$ and $k_0$ is employed to indicate unbiased quantities because their Monte Carlo estimation is biased.[6,9,10] In passing, $S_0 = \mathbf{F}\psi_0$ where $\psi_0$ is the solution of Eqs. (8) and (9) with $k = k_0$.

A realization of the unnormalized distribution of source particles after simulating the m-th stationary generation may be written as

$$\hat{S}^{(m)}(\vec{r}) \equiv S^{(m)}(\vec{r}) + \hat{s}^{(m)}(\vec{r}), \tag{16}$$

where $S^{(m)}(\vec{r})$ is the expected value (ensemble average) of $\hat{S}^{(m)}(\vec{r})$ and $\hat{s}^{(m)}$ is the statistically fluctuating component. Throughout this section, the hat $(\hat{\cdot})$ denotes a realization of stochastic quantities. An explicit form of $\hat{S}^{(m)}(\vec{r})$ is written as

$$\hat{S}^{(m)}(\vec{r}) = \sum_{i=1}^{I(m)} w_i \delta(\vec{r} - \vec{r}_i),$$

where $I(m)$ is the number of the fission or collision sites during the m-th stationary generation and $w_i$ is statistical weight. However, any explicit form will not be used in the following analysis. Instead, several general properties associated with the formulation in (16) will be used. The total number of histories per generation, which is denoted by $L$ and defined to take into account the weights of the history starter paticles, is assumed to be constant over all generations. $S^{(m)}$ is then proportional to $L$. When $L$ is sufficiently large, $S^{(m)}$ and $\hat{s}^{(m)}$ are related by

$$\frac{\int_D \hat{s}^{(m)} d^3 r}{\int_D S^{(m)} d^3 r} = O(1/\sqrt{L}),$$

where $O$ is the order notation defined by $\lim_{x \to 0} O(x)/x = \; const \; w.r.t. \; x$. Therefore, the following scalings are employed to make both $S^{(m)}$ and $\hat{s}^{(m)}$ $O(1)$-quantities:

$$S^{(m)} \leftarrow L S^{(m)}, \; \hat{s}^{(m)} \leftarrow \sqrt{L} \hat{s}^{(m)}.$$

Since the stationarity dictates that $S^{(m)}$ is independent of $m$:

$$S^{(m)}(\vec{r}) \leftarrow S(\vec{r}).$$

the formulation in (16) is rewritten as

$$\hat{S}^{(m)}(\vec{r}) \equiv LS(\vec{r}) + \sqrt{L}\hat{s}^{(m)}(\vec{r}). \tag{17}$$

The fluctuating component satisfies

$$E[\hat{s}^{(m)}] = 0, \tag{18}$$

where in this section $E$ with an argument ($E[\cdot]$) denotes an expected value and $E$ with no argument denotes energy. $K-$eigenvalue samples are denoted by $\hat{k}^{(m)}$ and expressed as

$$\hat{k}^{(m)} = \frac{\int_D \hat{S}^{(m)}(\vec{r})d^3r}{L}.$$

This is equivalent to assuming collision estimators; and $\hat{k}^{(m)}$ corresponds to $k_m$ in Sec.II. The integration of $S(\vec{r})$ over the whole spatial domain $D$ is the expected value of $\hat{k}^{(m)}$:

$$k \equiv \int_D S(\vec{r})d^3r = E[\hat{k}^{(m)}] = E\left[\frac{\int_D \hat{S}^{(m)}(\vec{r})d^3r}{L}\right], \tag{19}$$

where the first equality results from stationarity .

Now, the conditionally expected value of the normalized distribution of the starter particles selected from a realization of $\hat{S}^{(m)}(\vec{r})$ is

$$\frac{L\hat{S}^{(m)}(\vec{r})}{\int_D \hat{S}^{(m)}(\vec{r}')d^3r'}.$$

This implies that $\hat{S}^{(m+1)}(\vec{r})$ and $\hat{S}^{(m)}(\vec{r})$ are related as

$$\hat{S}^{(m+1)}(\vec{r}) = \int_D H(\vec{r}' \to \vec{r})\left[\frac{L\hat{S}^{(m)}(\vec{r}')}{\int_D \hat{S}^{(m)}(\vec{r}'')d^3r''}\right]d^3r' + \sqrt{L}\hat{\epsilon}^{(m)}(\vec{r}), \tag{20}$$

where $\hat{\epsilon}^{(m)}(\vec{r})$ is the fluctuating component conditional on $\hat{S}^{(m)}(\vec{r})$, is scaled similary to $\hat{s}^{(m)}$, and satisfies

$$E[\hat{\epsilon}^{(m)}|\hat{S}^{(m)}] = E[\hat{\epsilon}^{(m)}|\hat{s}^{(m)}] = 0. \tag{21}$$

Note that Eq. (21) implies $E[\hat{\epsilon}^{(m)}] = 0$. Eqs. (20) and (21) accommodate a broad class of the source normalization procedures with the fixed total weight of history starter particles. The substitution of Eq. (17) into Eq. (20) yields:

$$\begin{aligned} & S(\vec{r}) + \frac{1}{\sqrt{L}}\hat{s}^{(m+1)}(\vec{r}) = \\ & \quad \frac{1}{k}\int_D H(\vec{r}\,' \to \vec{r})S(\vec{r}\,')d^3r' + \frac{1}{\sqrt{L}}\left[\int_D A(\vec{r}\,' \to \vec{r})\hat{s}^{(m)}(\vec{r}\,')d^3r' + \hat{\epsilon}^{(m)}(\vec{r})\right] \\ & \quad -\frac{1}{Lk}\int_D\int_D A(\vec{r}\,' \to \vec{r})\hat{s}^{(m)}(\vec{r}\,')\hat{s}^{(m)}(\vec{r}\,'')d^3r'd^3r'' + O(L^{-3/2}), \end{aligned} \tag{22}$$

where Eq. (19) has been used and $A(\vec{r}\,' \to \vec{r})$ is defined to be

$$A(\vec{r}\,' \to \vec{r}) = \frac{1}{k}\left[H(\vec{r}\,' \to \vec{r}) - \frac{1}{k}\int_D H(\vec{q} \to \vec{r})S(\vec{q})d^3q\right].$$

Taking the expected value of Eq. (22) and using Eqs. (18) and (21), one obtains:

$$\begin{aligned} S(\vec{r}) = & \frac{1}{k}\int_D H(\vec{r}\,' \to \vec{r})S(\vec{r}\,')d^3r' \\ & -\frac{1}{Lk}\int_D\int_D A(\vec{r}\,' \to \vec{r})E\left[\hat{s}^{(m)}(\vec{r}\,')\hat{s}^{(m)}(\vec{r}\,'')\right]d^3r'd^3r'' + O(L^{-3/2})\,. \end{aligned} \tag{23}$$

The subtraction of Eq. (23) from (22) yields

$$\begin{aligned} & \hat{s}^{(m+1)}(\vec{r}) = \\ & \quad \int_D A(\vec{r}\,' \to \vec{r})\hat{s}^{(m)}(\vec{r}\,')d^3r' + \hat{\epsilon}^{(m)}(\vec{r}) + O\left(\frac{1}{\sqrt{L}}\right)\,. \end{aligned} \tag{24}$$

Also, Eq. (21) yields:

$$\begin{aligned} & E[\hat{\epsilon}^{(n)}|\hat{s}^{(m')}] = E[\hat{\epsilon}^{(n)}|\hat{s}^{(m')},\hat{s}^{(m'-1)},\ldots] = E[E[\hat{\epsilon}^{(n)}|\hat{s}^{(n)},\hat{s}^{(n-1)},\ldots]|\hat{s}^{(m')},\hat{s}^{(m'-1)},\ldots] \\ & = E[E[\hat{\epsilon}^{(n)}|\hat{s}^{(n)}]|\hat{s}^{(m')},\hat{s}^{(m'-1)},\ldots] = 0,\; n \geq m', \end{aligned} \tag{25}$$

where the first and third equalities are due to the Markov property in a sense that conditioning depends on only the most recent previous generation, the fourth equality due to Eq. (21), and standard probability textbooks can be consulted for the second equality (Theorem 34.4 in Ref. 11). The expected value of $\hat{s}^{(m')}\hat{\epsilon}^{(n)}$ then vanishes for $n \geq m'$:

$$E[\hat{s}^{(m')}\hat{\epsilon}^{(n)}] = E[E[\hat{s}^{(m')}\hat{\epsilon}^{(n)}|\hat{s}^{(m')}]] = E[\hat{s}^{(m')}E[\hat{\epsilon}^{(n)}|\hat{s}^{(m')}]] = 0,\, n \geq m' \,. \tag{26}$$

Setting $m = n-1$ in Eq. (24), multiplying the resulting expression by $\hat{s}^{(m)}$, taking the expectation, and using Eq. (26) with $n$ and $m'$ replaced by $n-1$ and $m$, respectively, one obtains:

$$\begin{aligned} &E\left[\hat{s}^{(n)}(\vec{r})\hat{s}^{(m)}(\vec{q})\right] = \\ &\qquad \int_D A(\vec{r}\,' \to \vec{r})E\left[\hat{s}^{(n-1)}(\vec{r}\,')\hat{s}^{(m)}(\vec{q})\right] d^3r' + O\left(\frac{1}{\sqrt{L}}\right),\, n > m. \end{aligned} \tag{27}$$

The repeated use of Eq. (27) yields

$$\begin{aligned} E\left[\hat{s}^{(n)}(\vec{r})\hat{s}^{(m)}(\vec{q})\right] = \int_D\int_D \cdots \int_D & A(\vec{r}_1 \to \vec{r})A(\vec{r}_2 \to \vec{r}_1)\cdots A(\vec{r}_{n-m} \to \vec{r}_{n-m-1}) \\ & E\left[\hat{s}^{(m)}(\vec{r}_{n-m})\hat{s}^{(m)}(\vec{q})\right] d^3r_{n-m}\cdots d^3r_2 d^3r_1 \\ +O\left(\frac{1}{\sqrt{L}}\right)\,,\ n > m. & \end{aligned} \tag{28}$$

Combining (28) with (6), (17) and (19), one can express the lag-n covariance as

$$\begin{aligned} C_R(n) &= E\left[\,(\hat{k}^{(m+n)} - E[\hat{k}^{(m+n)}])(\hat{k}^{(m)} - E[\hat{k}^{(m)}])\,\right] \\ &= \frac{1}{L}\int_D\int_D E\left[\hat{s}^{(m+n)}(\vec{r})\hat{s}^{(m)}(\vec{q})\right] d^3r d^3q \\ &= \frac{1}{L}\int_D\int_D \{\int_D\int_D \cdots \int_D A(\vec{r}_1 \to \vec{r})A(\vec{r}_2 \to \vec{r}_1)\cdots A(\vec{r}_n \to \vec{r}_{n-1}) \\ &\qquad E\left[\hat{s}^{(m)}(\vec{r}_n)\hat{s}^{(m)}(\vec{q})\right] d^3r_n\cdots d^3r_2 d^3r_1\,\}\, d^3r d^3q \\ &+O\left(L^{-3/2}\right)\,,\ m > 0\,, n > 0. \end{aligned} \tag{29}$$

Now, one can introduce immediate importance, i.e., the expected number of source particles directly resulting from a history starter particle at $\vec{r}$:

$$H(\vec{r}) = \int_D H(\vec{r} \to \vec{r}\,')d^3r'.$$

$C_R(n)$ is then expressed as

$$\begin{aligned}
&C_R(n) = \\
&\quad \frac{1}{L}\int_D \{ \int_D \int_D \cdots \int_D \left[ \frac{H(\vec{r}_1)}{k} - \frac{1}{k^2}\int_D H(\vec{q})S(\vec{q})d^3q \right] A(\vec{r}_2 \to \vec{r}_1)\cdots A(\vec{r}_n \to \vec{r}_{n-1}) \\
&\qquad\qquad E\left[\hat{s}^{(m)}(\vec{r}_n)\hat{s}^{(m)}(\vec{q})\right] d^3r_n \cdots d^3r_2 d^3r_1 \ \} \ d^3q \\
&\quad +O\left(L^{-3/2}\right) \ , \ m > 0 \, , n > 0.
\end{aligned} \tag{30}$$

Since Eq. (23) implies

$$S(\vec{r}) - \frac{1}{k}\int H(\vec{q}, \to \vec{r})S(\vec{q})d^3q = O\left(\frac{1}{L}\right), \tag{31}$$

Eq. (30) combined with Eq. (19) and the integration of Eq. (31) over $D$ yields

$$\begin{aligned}
C_R(n) \ = \ & \frac{1}{L}\int_D \{ \int_D \int_D \cdots \int_D \left[ \frac{H(\vec{r}_1)}{k} - 1 \right] A(\vec{r}_2 \to \vec{r}_1)\cdots A(\vec{r}_n \to \vec{r}_{n-1}) \\
& \qquad E\left[\hat{s}^{(m)}(\vec{r}_n)\hat{s}^{(m)}(\vec{q})\right] d^3r_n \cdots d^3r_2 d^3r_1 \ \} \ d^3q \\
& +O\left(L^{-3/2}\right) \ , \ m > 0 \, , n > 0.
\end{aligned} \tag{32}$$

The biases of the k-eigenvalue estimate and its eigenfunction were proved to be the order of $O(1/L)$ for a discretized model.[6] The same is also the case for continuous models as implied in Eq. (23).[9] Moreover, the bias of the k-eigenvalue estimate was proved to be bounded by a $O(1/\sqrt{L})$ quantity.[10] Therefore, $C_R(n)$ can be rewritten as

$$\begin{aligned}
C_R(n) \ = \ & \frac{1}{L}\int_D \{ \int_D \int_D \cdots \int_D \left[ \frac{H(\vec{r}_1)}{k_0} - 1 \right] A(\vec{r}_2 \to \vec{r}_1)\cdots A(\vec{r}_n \to \vec{r}_{n-1}) \\
& \qquad E\left[\hat{s}^{(m)}(\vec{r}_n)\hat{s}^{(m)}(\vec{q})\right] d^3r_n \cdots d^3r_2 d^3r_1 \ \} \ d^3q \\
& +O\left(L^{-3/2}\right) \ , \ m > 0 \, , n > 0.
\end{aligned} \tag{33}$$

It is worth pointing out that when $H(\vec{r}) = k_0$, the intergenerational correlation of $k$-eigenvalue samples does not exist within the leading order approximation with respect to $L$. Since $k_0$ is the mean of $H(\vec{r})$ as implied in Eq. (15):

$$k_0 = \frac{\int_D S_0(\vec{r}\,')H(\vec{r}\,')d^3r'}{\int_D S_0(\vec{r})d^3r},$$

the intergenerational correlation is small when the spatial variation of $H(\vec{r})$ is small. For example, $(\sigma_R^2 - \sigma_A^2)/\sigma_A^2$ would be small for an infinite homogeneous slab reactor because according to Eq. (5), $(\sigma_R^2 - \sigma_A^2)/\sigma_A^2$ can be considered a measure of the correlation effect on variance estimation. Table 1 shows $(\sigma_R^2 - \sigma_A^2)/\sigma_A^2$ for problems in Figures 3 and 5. The results therein indicate that the flatter the immediate importance of fissionable domain is, the smaller $(\sigma_R^2 - \sigma_A^2)/\sigma_A^2$ is.

It is important to explore whether or not immediate importance can be made constantly equal to $k_0$ by the biasing of particle transport. Since the operator $\mathbf{F}$ and the multiplication by a spatial function are commutative, the spatial transform of $S_0$ is considered instead of the spatial transform of the angular flux $\psi$ in Eqs. (8)-(9):

$$\tilde{S}_0(\vec{r}) = S_0^*(\vec{r})S_0(\vec{r}).$$

Introducing the modified integral kernel defined as[12]

$$\tilde{H}(\vec{q} \to \vec{r}) = \frac{H(\vec{q} \to \vec{r})S_0^*(\vec{r})}{S_0^*(\vec{q})},$$

Eq. (15) is transformed into

$$\tilde{S}_0(\vec{r}) = \frac{1}{k_0}\int_D \tilde{H}(\vec{q} \to \vec{r})\tilde{S}_0(\vec{q})d^3q. \tag{34}$$

Suppose that immediate importance is constantly equal to $k_0$ for the particle transport under $\tilde{H}$. One then obtains

$$\int_D \tilde{H}(\vec{q} \to \vec{r}) d^3 r = k_0 \Longleftrightarrow S_0^*(\vec{q}) = \frac{1}{k_0} \int_D H(\vec{q} \to \vec{r}) S_0^*(\vec{r}) d^3 r. \tag{35}$$

This is an adjoint equation to Eq. (15). Its solution can be interpreted as the importance over all future generations for a particle born with the energy spectrum $\chi$. Therefore, one arrives at the following conclusion: The biasing of particle transport by the importance over all future generations eliminates the intergenerational correlation of $k$-eigenvalue samples within the leading order apporoximation with respect to the number of histories per generation.

Practical significance of the above conclusion becomes clear when one reviews the expressions for real and apparent variances. First, apparent variance in the definition in (3) is expressed as[3]

$$\begin{aligned}
\sigma_A^2 &= \frac{1}{N} E[(\hat{k}^{(j)} - E[\hat{k}^{(j)}])(\hat{k}^{(j)} - E[\hat{k}^{(j)}])] \\
&\quad - \frac{2}{N^2(N-1)} \sum_{m=1}^{N-1} \sum_{n=m+1}^{N} E[(\hat{k}^{(m)} - E[\hat{k}^{(m)}])(\hat{k}^{(n)} - E[\hat{k}^{(n)}])] \\
&= \frac{1}{LN} \int_D \int_D E\left[\hat{s}^{(j)}(\vec{r}) \hat{s}^{(j)}(\vec{q})\right] d^3 r d^3 q \\
&\quad - \frac{2}{LN^2(N-1)} \sum_{m=1}^{N-1} \sum_{n=1}^{N-m} \int_D \Big\{ \int_D \int_D \cdots \int_D \left[\frac{H(\vec{r}_1)}{k_0} - 1\right] A(\vec{r}_2 \to \vec{r}_1) \cdots A(\vec{r}_n \to \vec{r}_{n-1}) \\
&\qquad E\left[\hat{s}^{(m)}(\vec{r}_n) \hat{s}^{(m)}(\vec{q})\right] d^3 r_n \cdots d^3 r_2 d^3 r_1 \Big\} d^3 q \\
&\quad + O\left(L^{-3/2}\right),
\end{aligned}$$

where Eqs. (6) and (33) were used at the second equality. Second, the difference between real and apparent variances is expressed by Eqs. (5) and (33) as

$$\sigma_R^2 - \sigma_A^2 = \frac{2}{LN(N-1)} \sum_{n=1}^{N} (N-n) \int \{ \int \int \cdots \int \left[ \frac{H(\vec{r}_1)}{k_0} - 1 \right] A(\vec{r}_2 \to \vec{r}_1) \cdots A(\vec{r}_n \to \vec{r}_{n-1}) E\left[ \hat{s}^{(j)}(\vec{r}_n) \hat{s}^{(j)}(\vec{q}) \right] d^3r_n \cdots d^3r_2 d^3r_1 \} \, d^3q + O(L^{-3/2}).$$

Therefore, taking into account that $(\sigma_R^2 - \sigma_A^2)/\sigma_A^2 = [(\sigma_R - \sigma_A)/\sigma_A][(\sigma_R + \sigma_A)/\sigma_A]$, the error estimation bias $(\sigma_R - \sigma_A)/\sigma_A$ is generally an $O(1)$ quantity with respect to $L$:

$$\frac{\sigma_R - \sigma_A}{\sigma_A} \sim O(1) \text{ w.r.t. } L.$$

However, when $H(\vec{r}) = k_0$, the error estimation bias becomes an $O(1/\sqrt{L})$ quantity:

$$\frac{\sigma_R - \sigma_A}{\sigma_A} \sim O(L^{-1/2}) \text{ w.r.t. } L \text{ when } H(\vec{r}) = k_0.$$

In other words, when immediate importance is made constant, error estimation bias is eliminated for large values of the number of histories per generation.

## VI. CONCLUSION

This paper has shown that the intergenerational correlation of Monte Carlo $k$-eigenvalue samples vanishes within the leading order approximation with respect to the number of histories per generation when immediate importance is constant. It has been derived that the immediate importance under simulation is made constant when the biasing with the importance over all future generations is applied to particle transport. The practical consequence is that the error estimation bias in Monte Carlo k-eigenvalue calculation, which can not generally be eliminated by making the number of histories per generation ($L$) tend to infinity, becomes a $\mathrm{O}(L^{-1/2})$ quantity.

## ACKNOWLEDGMENT

Analysis in Sec. V was greatly inspired by unpublished work of T.M. Sutton and F.B. Brown.[9] Especially, integral expressions mathematically equivalent to Eq. (33) appeared in that work. The present author (T. Ueki) deeply appreciates the communication with T.M. Sutton.

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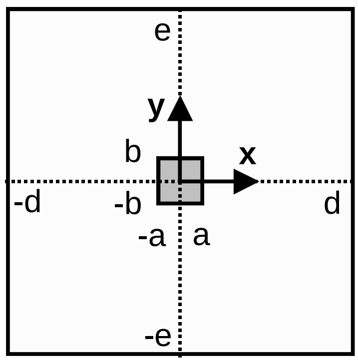
**LIST OF TABLE**

Table 1: $(\sigma_R^2 - \sigma_A^2)/\sigma_A^2$ for problems in Figures 3 and 5 (No exponential transform, 1000 histories per generation, 300 generations per replica, of which the first 100 generations were discarded)

| | Figure 3 | Figure 5 with no reflector | Figure 5 with reflector |
|---|---|---|---|
| $(\sigma_R^2 - \sigma_A^2)/\sigma_A^2$ | 2.5 | 0.4 | 0.2 |
| spatial shape of immediate importance | sharp | $\longleftrightarrow$ | flat |

**LIST OF FIGURES**




infinite square prism in vacuum with sides of 24 cm

$\Sigma_t$=1.0 cm$^{-1}$, $\Sigma_a$=0.3 cm$^{-1}$, $\nu\Sigma_f$=0.39 cm$^{-1}$ for the central region with sides of 3.0 cm

$\Sigma_t$=1.0 cm$^{-1}$, $\Sigma_a$=0.3 cm$^{-1}$, $\nu\Sigma_f$=0.24 cm$^{-1}$ for the surrounding region

a=b=1.5 cm, d=e=12 cm

Figure 1: Two dimensional heterogeneous problem

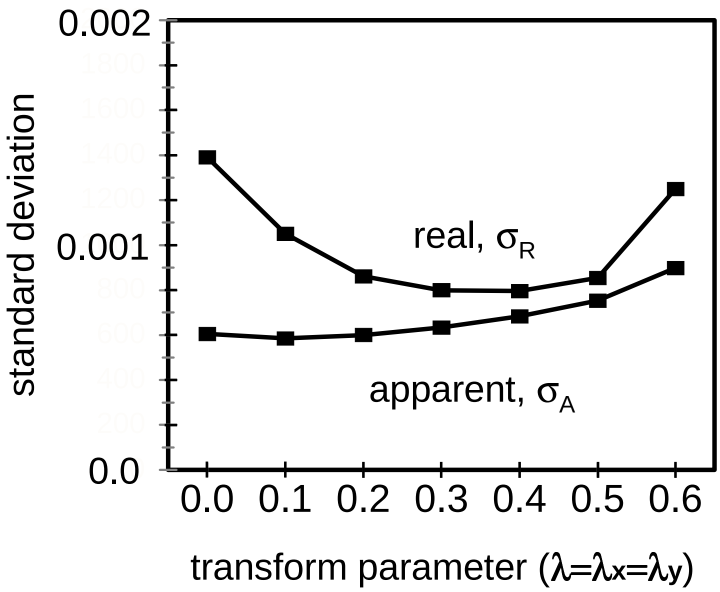
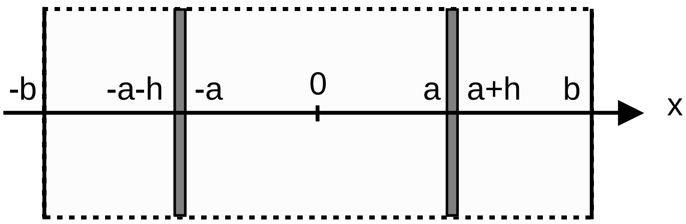



Figure 2: Real and apparent standard deviations for the two dimensional heterogeneous problem in Figure 1




Infinite slab in vacuum

a=14.4 cm, b=30 cm, h=1.2 cm

$\Sigma_t$=1.0 cm$^{-1}$, $\Sigma_a$=0.3 cm$^{-1}$, $\nu\Sigma_f$=0.39 cm$^{-1}$ for gray regions of thickness h
$\Sigma_t$=1.0 cm$^{-1}$, $\Sigma_a$=0.3 cm$^{-1}$, $\nu\Sigma_f$=0.24 cm$^{-1}$ for other regions

Figure 3: Plane-parallel heterogeneous problem

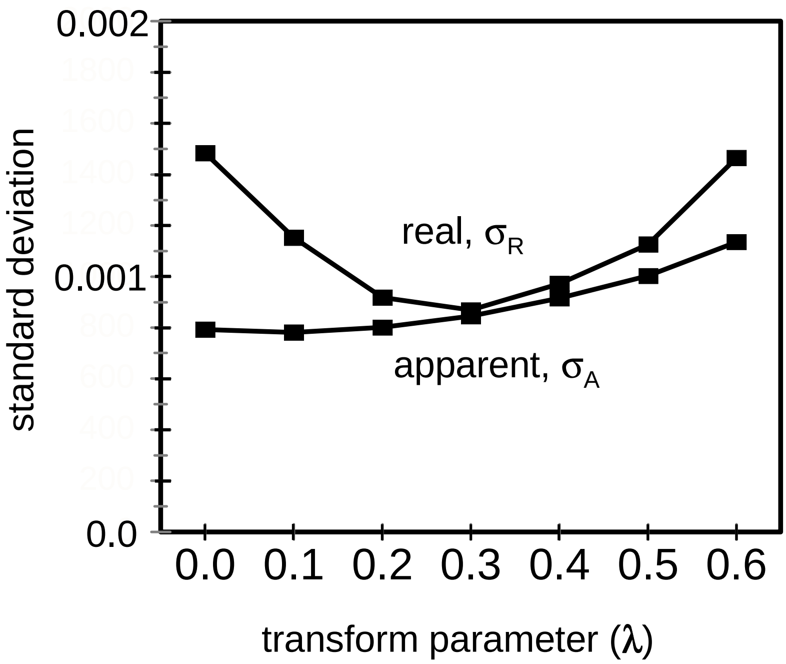



Figure 4: Real and apparent standard deviations for the plane-parallel heterogeneous problem in Figure 3

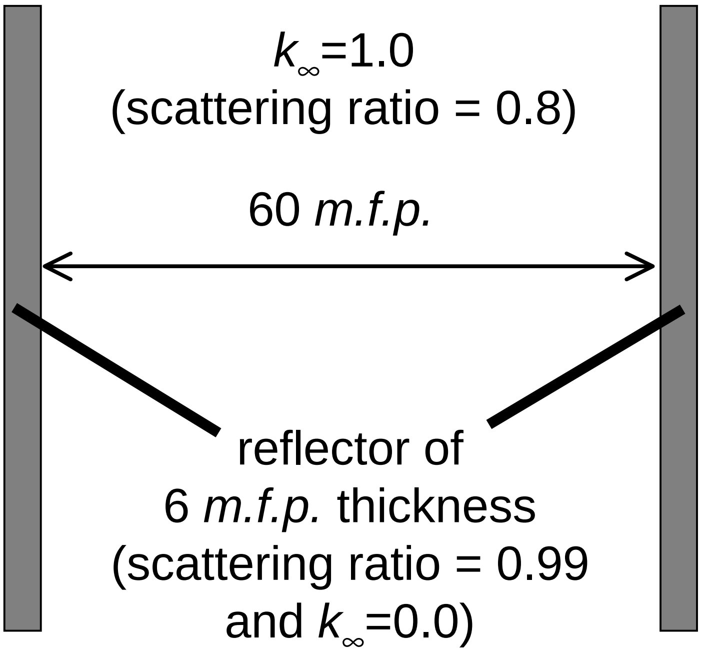



Figure 5: Energy-independent infinite slab reactor
($k_\infty = \nu\Sigma_f/\Sigma_a$=mean number of fission neutrons per absorption event)