Correlation diagnosis method for heterogeneous Monte Carlo eigenvalue simulations based on a diffusion approximation

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A B S T R A C T
This paper presents a predictive model of the correlation level present in tally regions of any mesh size without requiring extensive high accuracy discrete tallies. This model provides a quick indication of the accuracy of the variance estimated from uncorrelated statistics. The prediction is developed from the generalization of the Multitype Branching Processes (MBP) model to a continuous space and solving correlation coefficients (and thus variance correction factors) exactly in an equivalent homogeneous problem. The real heterogeneous problem is homogenized in a way that preserves neutron migration area. Correlation coefficients and the asymptotic variance underestimation ratio of the homogenized problem provide a rough estimate of the correlations observed in the real heterogeneous problem for a given tally region size.

1. Introduction

Limited approximations in nuclear data representation and system geometry make Monte Carlo methods a very common reference tool for neutron transport simulations. One essential component of Monte Carlo methods is that statistical uncertainty must be reported in addition to the expectation of any physical observable of interest. The default method to obtain the uncertainty of any tallied quantity in Monte Carlo simulation codes (OpenMC (Romano and Forget, 2013), MCNP (X-5 Monte Carlo, 2003) and MC21 (Kelly et al., 2002) is to divide the sample variance by the number of active generations. This variance estimator is based on the common assumption that neutron generations are independent. However, the correlation effects between tallies due to neutron multiplication primarily induced by fission reactions and the source update procedure while performing power iterations to evaluate eigenvalues violate the assumption of independent generations and lead to variance underestimation (Brissenden and Garlick, 1986; Dumonteil et al., 2014; Herman and Monte, 2014; Miao et al., 2016).

The magnitude of the variance underestimation due to the correlation effects can be significant for problems of high dominance ratio with large tally regions (Ueki et al., 2003). Previous studies address the uncertainty underestimation problem using three general approaches. The first approach tries to de-correlate tallies by combining contributing tallies from many generations into one neutron batch (Kelly et al., 2002). This method has been implemented in the above mentioned simulation codes (Romano and Forget, 2013; X-5 Monte Carlo, 2003; Kelly et al., 2002). Batching typically leads to higher computational costs since it requires a minimum number of batches that often exceeds common practice.

The second approach quantifies the underestimation by capturing the correlation from post-processing the tallied quantities (Demaret et al., 1999; Yamamoto et al., 2014). To resolve the extra required data storage issue of post-processing, fitting correlations on simulation output and extending the correlation to correct variance underestimation was investigated in Miao et al. (2016). The third approach investigates prediction of variance underestimation caused by correlated generations. The prediction methods approximate the Monte Carlo simulations by a surrogate model, directly compute covariance between the Monte Carlo generations for the corresponding model and use the correlation behavior of the model to correct variance estimators of the Monte Carlo simulations (Ueki, 2010; Sutton, 2017; Ueki, 2016; Miao et al., 2016; Miao et al., 2018). While accurate, this approach is often very costly.

Despite the ways of quantifying the correlation level in order to provide better variance estimates, in many problems, correlation levels are quite low thus not needing any correction to the typical variance estimator. This paper aims to provide a simple indicator of the potential impact of correlations on the problem at hand. To accomplish this, the derivation of the MBP method

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will be generalized to a continuous space and applied to a homogenized version of the problem.

Section 2 summarizes the results of the MBP method. Section 3 develops the theory of continuous model correlation prediction. Section 2.1 simplifies the derivation of the MBP model by assuming criticality of the system and stationarity of the neutron source distribution. Section 3.2 generalizes the MBP model to a continuous phase space and it is then applied to a homogeneous problem with reflective boundary conditions in Section 3.3 and Section 3.4 to verify this model with the analytic solution. This result demonstrates that the asymptotic variance underestimation ratio calculated from the correlation coefficients can be used as a numerical indicator of the correlation in the system. Section 3.3 investigates the criticality of the system and stationarity of the neutron source distribution. Section 3.3 simplifies the derivation of the MBP model by assuming the theory of continuous model correlation prediction. The model developed from multitype branching process discretizes the neutron phase space over all independent variables in a finite region and denotes the system state at generation $n$ with a vector $\mathbf{Z}(n)$ as in Eq. (2.1.1).

$$\mathbf{Z}(n) = (Z_1(n), \ldots, Z_i(n), \ldots, Z_q(n))$$

(2.1.1)

The $l^{th}$ component of the vector corresponds to the number of neutrons belonging to the discrete phase space l at generation $n$. A neutron in region $l$ is defined to be of type $l$ in the terminology of multitype branching processes.

$$X_i(n) = \frac{\sum_{j \in I} Z_{ij}(n)}{Z(n)}$$

(2.1.3)

Correlation coefficients of tally $X$ across generations $n$ and $n+k$ is defined in Eq. (2.1.4).

$$\rho(k) = \frac{\rho(n+k)}{\rho(n,n+k)} = \frac{\text{Cov}[X(n), X(n+k)]}{\sqrt{\text{Var}[X(n)] \text{Var}[X(n+k)]}}$$

(2.1.4)

The covariances of tally $X_i$ can be directly calculated from moments on finer discretized phase space regions as

$$\text{Cov}[X_i(n), X_j(n+k)] = \sum_{l \in I} \text{Cov}[X_{il}(n), X_{jl}(n+k)]$$

(2.1.5)

In addition, we care about the convergence rate of the variance of tally $X$ accumulated over $N$ active generations: $\sqrt{X(N)} = \frac{\sum_{i=0}^{N-1} X_{(n)}}{N}$. The variances of tally $X_i(n)$, $X_j(n+k)$ only depends on $k$.

$$\text{Var}[X(N)] = \frac{\text{Var}[X(N)]}{N^2} = 2 + \sum_{k=1}^{N-1} \left(1 - \frac{k}{N}\right) \rho(k)$$

(2.1.6)

where we assume $\sigma^2 = \text{Var}[X(N)]$, $\forall n$ and $\text{Cov}[X(n), X(n+k)]$ only depends on $k$.

2.2. Covariance of tallies

Determination of the correlation coefficients $\rho_{X_i}(k)$ requires the covariances in the form of $\text{Cov}[X_{il}(n), X_{j2}(n+k)]$ for each $n$ and $k$ and each comprising phase space regions $l \in I$. $\text{Cov}[X_{il}(n), X_{j2}(n+k)]$ were expressed in term of moments of $Z$ as Eq. (2.2.1) in Miao et al. (2016) and Miao et al. (2018).

$$\text{Cov}[X_{1l}(n), X_{2k}(n+k)] = \left(\frac{\delta_{l1} - \mu_{l1}(n)}{\mu(n)}\right) \left(\frac{\delta_{k2} - \mu_{k2}(n+k)}{\mu(n+k)}\right) \left[\text{E}[Z_l(n+k)] - \mu_l(n+k)\right] + \left(\frac{\delta_{l1} - \mu_{l1}(n)}{\mu(n)}\right) \left(\frac{\delta_{k2} - \mu_{k2}(n+k)}{\mu(n+k)}\right) \left[\text{E}[Z_l(n+k)] - \mu_l(n)\right] + \left(\frac{\delta_{l1} - \mu_{l1}(n)}{\mu(n)}\right) \left(\frac{\delta_{k2} - \mu_{k2}(n+k)}{\mu(n+k)}\right) \left[\text{E}[Z_l(n+k)] - \mu_l(n+k)\right] + \alpha(\text{E}^3),$$

(2.2.1)

The total number of neutrons of all phase space regions is the sum of all components of $\mathbf{Z}(n)$ and is denoted as $Z(n)$.

$$Z(n) = \sum_{l=1}^{M} Z_{l}(n)$$

(2.1.2)

The quantity of interest in most cases is the normalized tally $X_l(n)$ in a finite region $l$ comprising many discrete phase space regions.

$$\text{Var}[Z(n)] = \frac{\text{Var}[Z(n)]}{\mu(n)}$$

where $\mu_l(n)$ is the expectation of number of neutrons in region $l$ at generation $n$ and $\epsilon$ is the deviation of the number of neutrons in a discrete phase space region from its expectation value. Eq. (2.2.1) also introduced the Einstein tensor notation, where the sum is taken over all values when both subscript and superscript are the same, to facilitate notation.

We then simplify the covariance of a tally in region $l$ by performing the summation in Eq. (2.1.5) and using the properties of the Kronecker deltas in Eq. (2.2.1).
\[ \text{Cov}[X_i(n), X_i(n+k)] = \frac{\mu_i(n)}{\mu(n)} \mathbb{E} \left[ \left( \frac{Z_i(n)}{\mu(n)} \right) - \left( \frac{Z_i(n+k)}{\mu(n+k)} \right) \right] \]
\[ - \frac{\mu_i(n)}{\mu(n)} \mathbb{E} \left[ \left( \frac{Z_i(n+k)}{\mu(n+k)} \right) \left( \frac{Z_i(n)}{\mu(n)} \right) \right] \]
\[ = \frac{\mu_i(n)}{\mu(n)} \mathbb{E} \left[ \left( \frac{Z_i(n+k)}{\mu(n+k)} \right)^2 \right] - \frac{2}{\mu(n)} \mathbb{E} \left[ \frac{Z_i(n+k)}{\mu(n+k)} \right] \mathbb{E} \left[ \frac{Z_i(n)}{\mu(n)} \right] + o(\varepsilon^3) \]
\[ (2.2.2) \]

The detailed derivation is given in Eq. (A.3) and Eq. (A.8) (see Appendix A).

### 2.3. Recursive formulae for moments

What remains to be determined are the moments in the form of \( \mathbb{E} Z_i(n), \mathbb{E} Z_i(n)Z_j(n+k) \) and \( \mathbb{E} Z_i(n)Z_j(n)Z_k(n+k) \), which can be calculated recursively from deterministic initial conditions. Previous results (Miao et al., 2016, 2018) show that second order expansions give sufficiently accurate estimations of correlation coefficients. Therefore, we only need to evaluate the moments \( \mathbb{E} Z_i(n), \mathbb{E} Z_i(n)Z_j(n+k) \), which are denoted for simplification in Eq. (2.3.1).

\[ \mu_i(n) = \mathbb{E} Z_i(n) \]
\[ C_{ij}(n) = \mathbb{E} Z_i(n)Z_j(n) \]
\[ (2.3.1) \]

And the recursive formula are summarized in Eqs. (2.3.2–2.3.4).

The first response moments \( M_i^k \) is the expected number of neutrons found of type \( i \) after one generation given a source neutron of type \( i \). The second response moments \( V_{ij}^k \) is the covariance between the number of new neutrons of type \( i \) and type \( j \) after one generation given a neutron born of type \( i \). \( M^{k}\delta_{ij} \) is the expected number of neutrons found of type \( i \) and \( k \) generations after a source neutron of type \( i \) and is the \((l, i)\) element of the matrix \( M \) to the power of \( k \), \( M^{k} \delta_{ij} \) being the \( k^{th} \) power of the matrix \( M \).

\[ \mu_i(n+1) = \mu_i(n)M_i^1 \]
\[ C_{ij}(n+1) = M_{ij}^0 M_i^1 C_{ij}(n) + \mu_i(n)V_{ij}^1 \]
\[ \mathbb{E} Z_i(n)Z_j(n+k) = C_{ik}(n)M_{jk}^{(k)\delta_{ij}} \]
\[ (2.3.2–2.3.4) \]

### 2.4. Realization of response moments

If the probability of absorption and number of neutrons from fission, \( v_i \), in region \( i \) are assumed independent, we can relate \( M_i^k \) to \( P_i^k \), the probability that a neutron born in region \( i \) is absorbed in region \( i \).

\[ M_i^1 = P_i^0 v_i \]
\[ (2.4.1) \]

If energy and angle are not discretized, new neutrons must appear in the same region in which they were absorbed. The second order spatial moment responses \( V_{ij}^1 \) can thus be represented from fission-to-absorption probabilities and moments of new neutrons from fission as

\[ V_{ij}^1 = P_i^0 v_i^2 \delta_{ij} - P_i^0 P_j^0 v_i v_j \]
\[ (2.4.2) \]

### 3. Theory of correlation diagnosis on continuous models

#### 3.1. Simplification of covariance formula

Starting from the recursive formula for the spatial moments \( C_{ij}(n) \) (Eq. (2.3.3)), and shifting the focus to central moments

\[ \text{Cov}_{ij}(n) = C_{ij}(n) - \mu_i(n)\mu_j(n) \]
\[ (3.1.1) \]

where \( C_{ij}(n) \) is the expectation of the product of the number of neutrons in region \( j \) and \( i \) at generation \( n \), and \( \mu_i(n) \) is the expected number of neutrons in region \( i \) at generation \( n \) (Eq. (2.3.1)).

The recursive formula for \( C_{ij}(n) \) in Eq. (2.3.3) can be transformed to \( \text{Cov}_{ij}(n) \) as

\[ \text{Cov}_{ij}(n+1) = M_{ij}^{0} M_{ij}^{1} C_{ij}(n) + \mu_i(n)V_{ij}^1 - \mu_j(n+1)\mu_j(n+1) \]
\[ = M_{ij}^{0} M_{ij}^{1} C_{ij}(n) + \mu_i(n)V_{ij}^1 - \mu_j(n)M_{ij}^{0} \mu_i(n)M_{ij}^{1} \]
\[ = M_{ij}^{0} M_{ij}^{1} C_{ij}(n) - \mu_i(n)\mu_i(n) + \mu_i(n)V_{ij}^1 \]
\[ = M_{ij}^{0} M_{ij}^{1} \text{Cov}_{ij}(n) + \mu_i(n)V_{ij}^1 \]
\[ (3.1.2) \]

where the first equality uses the evolution of \( \mu_i(n) \) in Eq. (2.3.2), and the last equality defines \( \text{V}_{ij}(n) \equiv \). For convenience, Eq. (3.1.2) is rewritten in matrix form

\[ \text{Cov}(n+1) = M^{T} \text{Cov}(n)M + \text{V}(n). \]
\[ (3.1.3) \]

Suppose the initial source \( \mu_i(0) \) is identical to the fundamental eigenmode of the fission matrix \( M \), that is

\[ \mu_i(0)M_i^1 = \mu_i(0) \]
\[ (3.1.4) \]

Then the processes \( \mu_i(n) \) as function of \( n \) for each \( i \) are stationary

\[ \mu_i(n+1) = \mu_i(n)M_i^1 = \mu_i(n) \quad \forall n \]
\[ (3.1.5) \]

And the matrix \( \mu_i(n)V_{ij}^1 \) is stationary and defined as

\[ \text{V}_{ij}(n) = \mu_i(n)V_{ij}^1 \]
\[ (3.1.6) \]

For the fixed initial source, the spatial moment \( C(0) \) is deterministic and given by

\[ C_{ij}(0) = \mu_i(0)\mu_j(0) \]
\[ (3.1.7) \]

therefore the \( \text{Cov}_{ij}(0) = 0 \). Inserting in the recursive formula for \( \text{Cov}(n) \) leads to

\[ \text{Cov}(n) = \sum_{i=0}^{n} (M^{T})^{i-1} \text{V}^{i-1} M \]
\[ (3.1.8) \]

If we further assume that there is no branching processes within each generation and that the MBP model is critical, Eqs. (2.4.1) and (2.4.2) simplify \( V_{ij}^1 \) to

\[ V_{ij}^1 = \sigma_i^2 M_{ij}^1 \delta_{ij} - M_{ij}^1 M_{ij}^1 \]
\[ (3.1.9) \]

where \( \sigma_i^2 \equiv \mu_i^2 \). Multiplying \( V_{ij}^1 \) by eigendistribution \( \mu_i \) yields

\[ \text{V}_{ij} = \sigma_i^2 \mu_i \delta_{ij} - M_{ij}^1 M_{ij}^1 \]
\[ (3.1.10) \]

Inserting the explicit form of \( \text{V} \) (Eq. (3.1.10)) in the equation for \( \text{Cov}(n) \) (Eq. (3.1.8)) gives
\[ \text{Cov}(n)_{hk} = \sum_{n=0}^{\infty} \left( \left( (M^i)^{-1} \right)_h^{k+1} \sigma^2 \mu_h \delta_r \left( (M^i)^{-1} \right)_i^{k+1} - \left( (M^i)^{-1} \right)_h^{k+1} \mu_i M_i \left( (M^i)^{-1} \right)_i^{k+1} \right) \]  

(3.1.11)

### 3.2. Continuous space

This section will now focus on the generalization of first and second order moments into a continuous phase space. In a continuous phase space, the summations over the phase space region indices are replaced with integrals over the whole space composed of an infinite number of infinitesimal intervals. We can thus define \( \mu(x) \) such that \( \mu(r) dr \) is the expected number of neutrons in region \( dr \) around \( r \) which corresponds to the fundamental eigenmode.

It is worthwhile to note that in this section, \( dr \) (and similarly \( dr' \) and \( dr'' \)) denotes any infinitesimal volume in the neutron phase space. Let’s also define \( M^{(i)}(r, r') \) such that \( M(r, r') dr' \) is the expected number of neutrons in region \( dr' \) around \( r' \) induced by one source neutron at position \( r \) from the previous generation.

\[ \text{Cov}(\mathbf{x}_1(n), \mathbf{x}_1(n + d)) = \mu(n) \left[ \begin{array}{c} Z(n) \mu(n) \ Z_i(n) \mu(n) \ t(n + d) \mu(n + d) \ Z_i(n + d) \mu(n + d) \\ Z(n + d) \mu(n) - Z_i(n + d) \mu(n + d) \end{array} \right] + o(\varepsilon^2) \]

\[ = \mu(n) \left[ \begin{array}{c} \text{Cov}[Z_i(n), Z_i(n + d)] \mu(n + d) \mu(n + d) \end{array} \right] + o(\varepsilon^2) \]

(3.2.8)

For a critical system, \( M(r, r') dr' \) is equal to the probability that a source neutron from position \( x \) is absorbed in \( dr' \) around \( r' \) after one generation. Also, \( \mu(r) \) is the solution (fundamental eigenmode) of the integral equation corresponding to eigenvalue 1 (since our system is assumed critical).

\[ \mu(r) \equiv \int dr' \mu(r') M^{(i)}(r', r) \]

(3.2.1)

where the integral over the whole phase space is omitted. The \( g^{th} \) power of matrix \( M \) can be written as

\[ M^{(g)}(r, r') \equiv \int dr M^{(g-1)}(r, r') M^{(i)}(r, r') \]

(3.2.2)

where \( M^{(g)}(r, r') dr' \) represents the probability that a source neutron from position \( r \) is absorbed in \( dr' \) around \( r' \) after \( g \) generations.

We also define \( V(r, r', r) \) such that \( V(r, r', r') dr' dr'' \) is the covariance of the number of neutrons at region \( dr' \) and \( dr'' \) induced by one source neutron from position \( r \) from the last generation.

From Eq. (3.1.9), it can be explicitly written as

\[ V(r, r', r) = \sigma(r')^2 M^{(1)}(r, r') \delta(r' - r') - M^{(1)}(r, r') M^{(1)}(r, r') \]

(3.2.3)

\[ V(r', r, r'') \text{is then naturally defined as} \]

\[ V(r', r, r'') = \int dr'' \mu(r') V(r', r', r'') \]

\[ = \sigma(r')^2 \mu(r') \delta(r' - r'') - \int dr'' \mu(r') M^{(1)}(r', r'') M^{(1)}(r, r'') \]

\[ = \sigma(r')^2 \mu(r') \delta(r' - r'') - \int dr'' \mu(r') M^{(1)}(r', r'') M^{(1)}(r, r'') \]

(3.2.4)

Define \( V(n, r, r') \) such that \( V(n, r, r') dr'dr'' \) is the covariance of the number of neutrons in region \( dr \) around \( r \) and \( dr' \) around \( r' \) at generation \( n \). Similarly, define \( V^{(n)}(r, r') \) such that \( V^{(n)}(r, r') dr'dr'' \) is the covariance of the number of neutrons in region \( dr \) around \( r \) at generation \( n \) and in region \( dr' \) around \( r' \) at generation \( n + d \). Additionally, Eq. (3.2.4) that relates the spatial covariance within one generation and spatial covariance across different generations can be generalized to continuous phase space as

\[ \text{Cov}^{(n, n + d)}(r, r') = \int dr'' \text{Cov}^{(n)}(r, r'') M^{(d)}(r'', r') \]

(3.2.5)

The condensation equations for the neutron count in region \( l \) and covariance of the neutron count in region \( l_1 \) at generation \( n \) and region \( l_2 \) at generation \( n + d \) are given by

\[ \mu_i(n) = \int dr \mu(r) \]

(3.2.6)

\[ \text{Cov}[Z_i(n), Z_{jM}(n + d)] = \int dr \int dr' \text{Cov}^{(n, n + d)}(r, r') \]

(3.2.7)

The spatial covariance of a tally in a finite region, \( I \), at two different generations corresponds to the condensation equation (Eq. (2.2.2)). It suffices to only keep the \( O(\varepsilon^2) \) terms in Eq. (2.2.2).

### 3.3. Analysis of 1D homogeneous model

The above model is first tested on a continuous homogeneous problem. Let’s suppose that we have a 1D system of dimension \([-L, L]\) with reflective boundaries with a macroscopic absorption cross section \( c \). In this section, the infinitesimal volume \( dx \) is understood as an interval on the real line.

#### 3.3.1. Transition kernel and eigenmode

First, we evaluate \( M^{(1)}(x,x') \), the probability density for a neutron starting at \( x \) being absorbed around \( x' \). \( M^{(1)}(x,x') \) can be decomposed into all the components of a neutron reaching \( x' \) from \( x \) through all possible paths.

The probability that a neutron from \( x \) is absorbed in region \([x,x + dx']\) without any reflection at \( x = -L \) or \( x = L \) is proportional to \( e^{-\alpha x} dx' \). The corresponding probability for a neutron being absorbed after reflection once at \( x = L \) is proportional to \( e^{-\alpha(2L-x)} dx' \) because the source neutron can be equivalently viewed as starting from \( 2L - x \), the mirror image of \( x \) about the right boundary \( x = L \). Similarly, the probability for a neutron being absorbed after reflection once at \( x = -L \) is proportional to \( e^{-\alpha(2L-x)} dx' \) due to the image source at \(-2L - x\).

It can be shown by induction that if a neutron reaches \( x' \) from \( x \) after reflecting at \( x = -L \) for \( n \) times (number of reflections on left surface) and reflecting at \( x = L \) for \( n \) times (number of reflections on right surface), the coordinate of the equivalent image \( x_{img} \) satis-
\[
X_{\text{img}} = \begin{cases} (2(n + n_+L - x)(-1)^{n + n_+ + 1} & \text{if first reflected at } L \\ (2(n + n_+L + x)(-1)^{n + n_+} & \text{if first reflected at } -L \end{cases} \] (3.3.1)

X_{\text{img}} only depends on the initial direction and the total number of reflections.

The probability density \( M^1(x,x') \) can be calculated from all possible \( X_{\text{img}}(n,+) \)'s and \( X_{\text{img}}(n,-) \)'s.

\[
M^1(x,x') \propto e^{-c(x-x')} + \sum_{n=1} e^{-cX_{\text{img}}(n,+) - x'} + \sum_{n=1} e^{-cX_{\text{img}}(n,-) - x'} \] (3.3.2)

Then we insert the explicit form of \( X_{\text{img}} \), Eq. (3.3.1), into Eq. (3.3.2).

\[
M^1(x,x') \propto e^{-c(x-x')} + \sum_{n=1} e^{-c(4L - 2L-x)(-1)^{n+1} - x'} + \sum_{n=1} e^{-c(4L + 2L-x)(-1)^{n} - x'} \] (3.3.3)

Then separating the summation over index \( n \) into odd \( (n = 2k - 1) \) and even \( (n = 2k) \) integers simplifies Eq. (3.3.3) into Eq. (3.3.4).

\[
M^1(x,x') \propto e^{-c(x-x')} + \sum_{k=1} e^{-c(4L - 2L-x)(-1)^{2k-1} - x'} + \sum_{k=1} e^{-c(4L + 2L-x)(-1)^{2k} - x'} \] (3.3.4)

Realizing that \( x - x' \in [-L, L] \) and \( x + x' \in [-2L, 2L] \), the absolute value notation can be removed in the last four terms. Eq. (3.3.4) is then simplified to Eq. (3.3.5).

\[
M^1(x,x') \propto e^{-c(x-x')} + \sum_{k=1} e^{-c(4L - 2L-x)(-1)^{2k-1} - x'} + \sum_{k=1} e^{-c(4L + 2L-x)(-1)^{2k} - x'} \] (3.3.5)

Finally, we evaluate the geometric series indexed by \( k \) and obtain Eq. (3.3.6).

\[
M^1(x,x') \propto e^{-c(x-x')} + \left[ e^{2cL(x-x')} + e^{2cL(x+x')} \right] \sum_{k=1} e^{-4ck} = e^{-c(x-x')} + 2\cosh(c(x-x')) e^{2cL(x+x')} \sum_{k=1} e^{-4ck} \frac{e^{2ck}}{2ck} = e^{-c(x-x')} + \frac{e^{2cL(x+x')}}{\sinh[2cL]} \] (3.3.6)

Integrating Eq. (3.3.6) over \( x' \in [-L, L] \) is equal to \( \frac{1}{2} \), which allows to define the normalization constant and write

\[
M^1(x,x') = \frac{1}{2} \left[ e^{-c(x-x')} + \frac{e^{-2cL \cosh[c(x-x')]} + \sinh[c(x+x')]}{\sinh[2cL]} \right] \] which relies on the knowledge that the probability that a neutron starting from \( x \) ends between \([-L, L]\) is 1. It is worthwhile to note that in an infinite system,

\[
M^1_0(x,x') = \frac{1}{2} e^{-c(x-x')} \] (3.3.8)

The identical normalization factor in Eqs. (3.3.7) and (3.3.8) verifies that the contribution from reflection at boundaries has been treated correctly.

In order to predict the correlation (and the covariance) of a specific region of the domain, the power of the kernel as defined in Eq. (3.2.2) is needed. A simple closed form for the power of matrix \( M^1(x,x') \) evaluated in Eq. (3.3.7) does not exist. Alternatively, \( M^1(x,x') \) can be expanded using an orthonormal basis in region \([-L, L] \). The power of the kernel is then converted to the power of the corresponding matrix elements. For convenience, the bra-ket notation is used. For the basis set \( |x\rangle \), the matrix element is calculated as

\[
m_{x,\beta} = \langle x| M^1 |\beta \rangle = \langle x| x| M^1 |x' \rangle \langle x'| \beta \rangle = \int_{-L}^{L} dx \int_{-L}^{L} dx' \langle x|x | M^1 |x' \rangle \langle x' | \beta \rangle \] (3.3.10)

and the kernel \( M^1(x,x') \) can be reconstructed from the matrix elements as

\[
M^1(x,x') = \sum_{x,\beta} m_{x,\beta} |x\rangle \langle \beta | \] (3.3.11)

For the simple homogeneous problem in 1D, the eigenfunctions of the kernel can be calculated and normalized to form an orthonormal basis such that the corresponding matrix is diagonal.

Because the kernel \( M^1(x,x') \) is symmetric, the normalization condition directly shows that \( \mu(x) = 1 \) is an eigenfunction corresponding to an eigenvalue of 1.

\[
\int_{-L}^{L} M^1(x,x') \mu(x) = \mu(x) \] (3.3.12)

Additionally, reflective boundaries restrict the eigenfunctions to those with 0 derivative at \(-L \) and \( L \). The eigenfunctions are \( \sin(\frac{2k-1}{2} \pi x) \) and \( \cos(\frac{k}{2} \pi x) \) for \( k \in \mathbb{Z}^+ \). The corresponding eigenvalues can be found by

\[
\int_{-L}^{L} M^1(x,x') \sin \frac{2k-1}{2} \pi x = \frac{1}{2} \int_{-L}^{L} \sin \frac{2k-1}{2} \pi x \] (3.3.13)

\[
\int_{-L}^{L} M^1(x,x') \cos \frac{k}{2} \pi x = \frac{1}{2} \int_{-L}^{L} \cos \frac{k}{2} \pi x \] (3.3.14)

We index the eigenfunction \( \mu(x) = 1 \) as \( |0\rangle \), the sin functions as \( |1\rangle, |3\rangle \ldots \) and the cos functions as \( |2\rangle, |4\rangle, \ldots \). With appropriate normalization, the eigenfunctions of \( M^1(x,x') \) are

\[
|x0\rangle = \frac{1}{\sqrt{2}} \sin \frac{2k-1}{2} \pi x \] (3.3.15)

\[
|x2k-1\rangle = \frac{1}{\sqrt{2}} \sin \frac{2k-1}{2} \pi x \] (3.3.16)

From Eqs. (3.3.13) and (3.3.14), the corresponding eigenvalues are

\[
\lambda_k = \frac{1}{1 + (\frac{k}{2})^2} \] (3.3.17)

It can be shown that the basis in Eq. (3.3.15) is orthonormal.
\[ (\alpha \beta) = \delta_{\alpha, \beta} \]  
(Eq. (3.1.17))

Then, the matrix elements are defined as
\[ m_{ij} = \langle k | M^{(1)} | j \rangle = \lambda_i \delta_{ij} \]  
(Eq. (3.1.18))

According to Eq. (3.3.11),
\[ M^{(1)}(x,x') = \sum_k \lambda_k^2 \delta(k(x) k(x')) \]  
(Eq. (3.19))

Using the eigenfunctions in Eq. (3.3.15) and eigenvalues in Eq. (3.3.16), \( M^{(1)}(x,x') \) can be explicitly written as
\[ M^{(1)}(x,x') = \frac{1}{2L} \left[ \sum_{k=-\infty}^{\infty} \left( \frac{1}{1 + \left( \frac{k \pi x}{L} \right)^2} \right)^{\frac{1}{3}} \cos \left( \frac{k \pi x}{L} \right) \cos \left( \frac{k \pi x'}{L} \right) \right] \]
\[ + \frac{1}{L} \sum_{k=-1}^{\infty} \left( \frac{1}{1 + \left( \frac{2k-1}{2L} \right)^2} \right)^{\frac{1}{3}} \sin \left( \frac{(2k-1) \pi x}{2L} \right) \sin \left( \frac{(2k-1) \pi x'}{2L} \right) \]  
(Eq. (3.20))

\( M^{(1)}(x,x') \) is symmetric and all eigenvalues are positive.

### 3.3.2. Spatial covariance

The explicit form of the kernel \( M^{(1)}(x,x') \) for the homogeneous problem allows us to perform an analysis of the spatial correlations. Knowing that the eigenfunction corresponding to the largest eigenvalue 1 is constant, \( \mu(x) \) is chosen as
\[ \mu(x) = \frac{1}{2L} \]  
(Eq. (3.21))

such that \( \int dx \mu(x) = 1 \). With the \( \mu(x) \) above and the transition kernel being symmetric, \( \nu(x',x'') \) (Eq. (3.1.10)) is simplified to
\[ \nu(x',x'') = \frac{1}{2L} \left( \sigma_0 \delta(x' - x'') - M^{(2)}(x',x'') \right) \]  
(Eq. (3.22))

The spatial covariance in generation \( n \), \( \text{Cov}(n)_{ij} \) (Eq. (3.11)) becomes
\[ \text{Cov}^{(0)}(x,x') = \frac{1}{2L} \sum_{k=-\infty}^{\infty} \left\{ \sigma^2 \left[ M^{2(g-1)}(x,x') - M^{(2)}(x,x') \right] \right\} \]  
(Eq. (3.23))

where \( M^{(0)} \) is defined as
\[ M^{(0)}(x,x') \equiv \delta(x - x') \]  
(Eq. (3.24))

Then, relating the spatial covariances within one generation to the spatial covariances across different generations (Eq. (3.25)), we obtain
\[ \text{Cov}^{(n,n+1)}(x,x') = \frac{1}{2L} \sum_{k=-\infty}^{\infty} \left\{ \sigma^2 \left[ M^{2(g-1)+1}(x,x') - M^{(2g+1)}(x,x') \right] \right\} \]  
(Eq. (3.25))

From Eqs. (3.3.23) and (3.3.25) along with the explicit expressions of \( \mu(x) \) (Eq. (3.3.21)) and \( M^{(1)}(x,x') \) (Eq. (3.3.20)) enables explicit evaluation of spatial correlation \( \text{Cov}(x_i(x),x_i(x')) \) according to Eq. (3.28). This will require the integral over region \( I \times I \) of \( M^{(1)}(x,x') \).

\[ \text{Cov}(x_i(x),x_i(x')) = \frac{1}{2L} \sum_{k=-\infty}^{\infty} \left\{ \sigma^2 \left[ M^{2(g-1)+1}(x,x') - M^{(2g+1)}(x,x') \right] \right\} \]  
(Eq. (3.25))

Without loss of generality, let’s define
\[ I = [-a,a] \]  
(Eq. (3.26))

to investigate the correlation of the central tally region of width \( 2a \) and let’s define
\[ W = [-L,L] \]  
(Eq. (3.27))

The first order moments in Eq. (3.28) are simply
\[ \mu(n) = \mu(n + d) = 1 \]
\[ \mu_1(n) = \mu_1(n + d) = \frac{p}{g} \]  
(Eq. (3.28))

The integral of the matrix \( M^{(1)}(x,x') \) is calculated as
\[ \int_I dx \int_I dx' M^{(1)}(x,x') = \frac{1}{2L} \int_I dx \int_I dx' \]
\[ \times \cos \left( \frac{k \pi x}{L} \right) \int_I dx' \cos \left( \frac{k \pi x'}{L} \right) \]
\[ + \frac{1}{L} \sum_{k=1}^{\infty} \left( \frac{1}{1 + \left( \frac{2k-1}{2L} \right)^2} \right)^{\frac{1}{3}} \sin \left( \frac{(2k-1) \pi x}{2L} \right) \int_I dx' \]
\[ \times \sin \left( \frac{(2k-1) \pi x'}{2L} \right) \]
\[ \times \sin \left( \frac{(2k-1) \pi x''}{2L} \right) \]  
(Eq. (3.29))

Integration of the odd function \( \sin \left( \frac{(2k-1) \pi x''}{2L} \right) \) over the region \( I = [-a,a] \) symmetric about the origin vanishes. Only the integration of the cosine functions remain in Eq. (3.30). And they are evaluated explicitly in Eq. (3.31).
\[ \int_I dx \int_I dx' M^{(1)}(x,x') = \frac{2a^2}{L} + \frac{1}{L} \sum_{k=1}^{\infty} \left( \frac{1}{1 + \left( \frac{k \pi L}{a} \right)^2} \right)^{\frac{1}{3}} \sin \left( \frac{k \pi x}{L} \right) \]
\[ \times \int_I dx \cos \left( \frac{k \pi x}{L} \right) \int_I dx' \sin \left( \frac{k \pi x'}{L} \right) \]  
(Eq. (3.30))

\[ \text{Cov}(Z_i(n),Z_i(n + d)) = \frac{1}{\pi} \sum_{n=0}^{\infty} \left\{ \sigma^2 \int_I dx \int_I dy M^{2(g-1)+1}(x,x') - \int_I dx \int_I dx' M^{(2g+1)}(x,x') \right\} \]  
(Eq. (3.32))

We can then evaluate the \( \text{Cov}(Z_i(n),Z_i(n + d)) \) by first integrating the covariance density in Eq. (3.3.25) over region \( I \).
\[ \text{Cov}(Z_i(n),Z_i(n + d)) = \]
\[ \frac{1}{\pi} \sum_{n=0}^{\infty} \left\{ \sigma^2 \int_I dx \int_I dy \sin \left[ \frac{(2k-1) \pi x}{L} \right] \right\} \]
\[ \times \int_I dx \cos \left( \frac{k \pi x}{L} \right) \int_I dx' \sin \left( \frac{k \pi x'}{L} \right) \]  
(Eq. (3.31))

Then, we insert the explicit expression of \( M^{2(g-1)+1} \) and \( M^{(2g+1)} \).
Next, we change the order of the summation over basis index $k$ and the summation over generation index $g$ in Eq. (3.3.33) and evaluate the geometric series with index $g$.

\[
\text{Cov}[Z_i(n), Z_i(n + d)] = \frac{a_i^2}{L_i^2} (\sigma^2 - 1)n + \frac{2}{\pi^2} \sum_{k=1}^{\infty} \sigma^2 \left(1 - \left(\frac{1}{L_i^2}\right)^2 \right)^d \left(1 - \left(\frac{\sigma^2}{\sigma_i^2}\right)^{2k} \right) \times \frac{\sin^2 \left(\frac{2\pi k}{L_i^2}\right)}{k^2} \left(1 - \left(1 + \left(\frac{\sigma_i}{\sigma_i}\right)^{2k} \right)^d \right).
\]

Finally, we recognize $\beta_{2k}$ in Eq. (3.3.34) and with the assumption that stationarity was reached after sufficiently many generations $n, \beta_{2k} \sim 0$.

\[
\text{Cov}[Z_i(n), Z_i(n + d)] = \frac{a_i^2}{L_i^2} (\sigma^2 - 1)n + \frac{2}{\pi^2} \sum_{k=1}^{\infty} \sigma^2 - \beta_{2k}^2 \beta_{2k}^d \times \frac{\sin^2 \left(\frac{2\pi k}{L_i^2}\right)}{k^2} \left(1 - \left(\frac{1}{L_i^2}\right)^2 \right)^d \left(1 - \left(1 + \left(\frac{\sigma_i}{\sigma_i}\right)^{2k} \right)^d \right).
\]

Next, we can evaluate Cov($Z_i(n), Z_i(n + d)$). The $\langle x | k \rangle$ part of $M^{(i)}(x, x')$ for all components will be integrated over the whole region $W$ and the $\langle x' | k \rangle$ part will be integrated over the region of interest $I$. It can be seen that

\[
\int_W dx | x | k \rangle = \left\{ \begin{array}{ll} \frac{\sqrt{2L}}{k} & k = 0 \\ 0 & \text{otherwise} \end{array} \right. \quad \text{(3.3.36)}
\]

\[
\int_W dx | x | 0 \rangle = \frac{\pi^{1/2}}{L^{1/2}}. \quad \text{(3.3.37)}
\]

Therefore, only the $0^\text{th}$ term in the expansion of $M^{(i)}(x, x')$ contributes to the integral.

\[
\text{Cov}[Z_i(n), Z_i(n + d)] = \frac{1}{L^2} \left( \frac{\pi}{2} \right) (\sigma^2 - 1)n
\]

By symmetry:

\[
\text{Cov}[Z_i(n), Z_i(n + d)] = \frac{a_i^2}{L_i^2} (\sigma^2 - 1)n
\]

Similarly, only the $0^\text{th}$ term in the expansion of $M^{(i)}(x, x')$ contribute to the integral of Cov($Z_i(n), Z_i(n + d)$).

\[
\text{Cov}[Z_i(n), Z_i(n + d)] = \frac{1}{L^2} \left( \frac{\pi}{2} \right) (\sigma^2 - 1)n
\]

All the terms required to calculate Cov($X_1(n), X_1(n + d)$) in Eq. (3.2.8) are known (Eqs. (3.3.28), (3.3.35), (3.3.38), (3.3.39) and (3.3.40)). The covariance between normalized neutron tally in region $I$ across generation lag $d$ is thus

\[
\text{Cov}[X_1(n), X_1(n + d)] = \frac{a_i^2}{L^2} \left( \frac{\pi}{2} \right) (\sigma^2 - 1)n
\]

where Eq. (3.3.41) combines the $0^\text{th}$ term in Cov($Z_i(n), Z_i(n + d)$) (Eq. (3.3.35)) with the other covariance terms and cancels them out. Note that though the comprising covariances of $Z$ tallies are dependent on the generation number $n$, the approximated covariances of $X$ tallies are stationary. The covariances of $X$ tallies are function of generation lag $d$ only (besides the system and tally region parameters) and the covariances decay exponentially as a function of $d$.

3.3.3. Correlation coefficients

Similar calculations are performed for Var($X_1(n)$) which will allow us to obtain $\rho_d$ defined as Cov($X_1(n), X_1(n + d)$)/Var($X_1(n)$).

Var($X_1(n)$) is evaluated via Cov($X_1(n), X_1(n + d)$) with $d = 0$. Thus Cov($Z_i(n), Z_i(n)$), Cov($Z_i(n), Z_i(n^*)$) and Cov($Z_i(n), Z_i(n^*)$) are needed. One difference to note from the covariance terms evaluated in previous section, $d = 0$ leads to the appearance of $M^{(i)}(x, x') = \delta(x, x')$ in the summation indexed by generation number $g$. The following integrals of $\delta(x, x')$ are useful:

\[
\begin{align*}
\int dx \int dx' \delta(x - x') &= \int dx = 2a \\
\int dx \int dx' \delta(x - x') &= \int dx = 2a \\
\int dx \int dx' \delta(x - x') &= \int dx1_{\{x=g\}} = 2a \\
\int dx \int dx' \delta(x - x') &= 2L
\end{align*}
\]

where $1_{\{x=g\}}$ is the indicator function.

While integrating Cov($x^{(i)}(x, x')$) (Eq. (3.2.23)) into Cov($Z_i(n), Z_i(n^*)$, $g = 1$ and $g \gg 2$ should be treated separately.

\[
\begin{align*}
\text{Cov}[Z_i(n), Z_i(n)] &= \frac{1}{2L} \left( \frac{\pi}{2} \right) (\sigma^2 - 1)n \\
&= \frac{1}{2L} \left( \frac{\pi}{2} \right) (\sigma^2 - 1)n
\end{align*}
\]

Then Eq. (3.3.48) evaluates the geometric series indexed by $g$ in Eq. (3.3.47) in a similar way to Eq. (3.3.35).

\[
\begin{align*}
\text{Cov}[Z_i(n), Z_i(n)] &= \frac{a_i^2}{L^2} (\sigma^2 - (\frac{\alpha_i}{L})^2 + (\frac{\beta_i}{L})^2 (\sigma^2 - 1)(n - 1) \\
&- \frac{2}{\pi^2} \sum_{k=1}^{\infty} \sigma^2 - \beta_{2k}^2 \beta_{2k}^d \sin^2 \left(\frac{2\pi k}{L_i^2}\right) k^2 \\
&+ \frac{2}{\pi^2} \sum_{k=1}^{\infty} \sigma^2 - \beta_{2k}^2 \beta_{2k}^d \sin^2 \left(\frac{2\pi k}{L_i^2}\right) k^2
\end{align*}
\]

where Eq. (3.3.49) merges the two summations over index $k$ into one.

\[
\begin{align*}
\text{Cov}[Z_i(n), Z_i(n)] &= \frac{a_i^2}{L^2} (\sigma^2 - (\frac{\alpha_i}{L})^2 + (\frac{\beta_i}{L})^2 (\sigma^2 - 1)n \\
&+ \frac{2}{\pi^2} \sum_{k=1}^{\infty} \sigma^2 - \beta_{2k}^2 \beta_{2k}^d \sin^2 \left(\frac{2\pi k}{L_i^2}\right) k^2
\end{align*}
\]

Next, we evaluate Cov($Z_i(n), Z_i(n)$), which is similar to the previous expression for Cov($Z_i(n), Z_i(n + d)$).

\[
\text{Cov}[Z_i(n), Z_i(n)] = \frac{1}{L^2} \left( \frac{\pi}{2} \right) (\sigma^2 - 1)n
\]

\[
\begin{align*}
\text{Cov}[Z_i(n), Z_i(n)] &= \frac{a_i^2}{L_i^2} (\sigma^2 - (\frac{\alpha_i}{L_i})^2 + (\frac{\beta_i}{L_i})^2 (\sigma^2 - 1)n \\
&+ \frac{2}{\pi^2} \sum_{k=1}^{\infty} \sigma^2 - \beta_{2k}^2 \beta_{2k}^d \sin^2 \left(\frac{2\pi k}{L_i^2}\right) k^2
\end{align*}
\]
### 3.3.4. Test problem for numerical verification

A test problem, denoted as TC1 – 1D, is created to numerically verify the above derivations. The material properties of the problem are given in Table 1. In this problem, neutrons are transferred within the 1D continuous phase space with the transfer probability density for a collision from position $x$ to $x'$ being defined as

$$P(x,x') = \Sigma e^{-\Sigma |x-x'|}.$$  

Eq. (3.3.56) implies that the scattering is isotropic since the probability density at distance $|x-x'|$ on the left/right of position $x$ is equal.

We also need to specify the probability mass function of new neutrons after an absorption event at any position:

$$p_0 = \frac{x^5}{x^5}, \quad p_1 = 0, \quad p_2 = \frac{x^5}{x^5} 0.55, \quad p_3 = \frac{x^5}{x^5} 0.45$$

where $p_0$ is the probability of neutron capture, $p_2$ and $p_3$ represent a probability for producing a discrete number of neutrons from fission.

In the simple problem, only absorption events need to be sampled. $M^{\text{inv}}(x,x')$ (Eq. (3.3.7)) can be used to sample the first absorption site $x'$ for a neutron started at $x$. It is not straightforward to find the $\text{CDF}$ of $M^{\text{inv}}(x,x')$ and directly sample from it. However, $M^{\text{inv}}(x,x')$, the probability density for the first absorption site in an infinite system can easily be sampled to find the first absorption site $x'_0$ for a neutron started at $x$. It is thus not necessary within $[-L,L]$, but an equivalent image within the interval can be found. It can be shown by induction that $x'_0$ and $x'$ are related through

$$x' = (-1)^y \text{sgn}(x'_0) \left( |x'_0| - 2nL \right)$$

### Table 1

Parameters of demonstration problem.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Boundary Width(cm)</th>
<th>v</th>
<th>$\Sigma_c$(cm$^{-1}$)</th>
<th>$\Sigma_f$(cm$^{-1}$)</th>
<th>$\Sigma_r$(cm$^{-1}$)</th>
<th>$\Sigma$(cm$^{-1}$)</th>
<th>$k_{ef}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reflective</td>
<td>400</td>
<td>2.45</td>
<td>0.270</td>
<td>0.018</td>
<td>0.012</td>
<td>0.300</td>
<td>1</td>
</tr>
</tbody>
</table>

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<td>0.300</td>
<td>1</td>
</tr>
</tbody>
</table>

By symmetry,

$$\text{Cov}[Z_i(n),Z_i(n)] = \frac{a^2}{L} (\sigma^2 - 1)n$$

Similarly,

$$\text{Cov}[Z_i(n),Z_i(n)] = \frac{1}{L} \left( \sigma^2 \left( 2L + \sum_{k=1}^{\infty} \frac{\sqrt{2L}}{\sqrt{k}} \right) - \frac{1}{L} \sum_{k=1}^{\infty} \frac{\sqrt{2L}}{\sqrt{k}} \right)$$

where Eq. (3.3.53) combines the $0^\text{th}$ term of $\text{Cov}[Z_i(n),Z_i(n)]$ (Eq. (3.3.49)) with the other variance terms and cancels them out. Note that the covariances of $Z$ tallies are dependent on the generation number $n$ and that the approximated covariances of $X$ tallies are stationary.

With the covariances that are functions of only the generation lag and variances that are stationary, the correlation coefficients of a normalized tally in region $I$ are function of the generation lag $d$ only.

$$\rho_I(d) = \frac{\text{Cov}[X_I(n),X_I(n+d)]}{\text{Var}[X_I(n)] \text{Var}[X_I(n+d)]} = \frac{\sum_{k=1}^{\infty} \frac{\sqrt{2L}}{\sqrt{k}} \text{var}(Z_k)}{\frac{x^5}{x^5} \left( 1 - L \right) \sum_{k=1}^{\infty} \frac{\sqrt{2L}}{\sqrt{k}} \text{var}(Z_k)}$$

### Fig. 1

Correlation coefficients for central tally region with different sizes in TC1 – 1D. The tally size $a$ is in unit cm. The dots correspond to correlation coefficients estimated from independent simulations. The solid line curves correspond to correlation coefficients predicted from the continuous model. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this article.)

### Fig. 2

Variance convergence rate calculated from underestimation ratio for central tally region with different sizes in TC1 – 1D. The tally size $a$ is in unit cm. The dots correspond to $\frac{\Sigma}{\Sigma}$ estimated from independent simulations. The solid line curves correspond to predictions from the continuous model. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this article.)
where \( n \) satisfies
\[
\left\lceil \frac{|x_\text{in}|}{2L} \right\rceil + \frac{1}{2} \leq n + 1 \quad (3.3.59)
\]

After the first absorption site \( x_\text{in} \) is sampled according to \( M^0(x, x') \) and transformed to \( x' \). New neutrons are sampled at \( x' \). The distribution of new neutrons per absorption follows Eq. (3.3.57).

The simulation was performed with 100,000 neutrons per generation for 1000 active generations. Additionally, 200 independent simulations were performed to generate reference statistics.

3.3.5. Variance underestimation ratio and asymptotic behavior

The covariances of normalized \( X \) tallies can now be used to predict the variance of tallies averaged over the active generations, \( \text{Var} [X(N)] \), according to Eq. (2.1.6). Equivalently, the correlation coefficients can be converted to the variance underestimation ratio \( r(N) \) as defined in Eq. (2.1.7).

\[
r_i(N) = 1 + 2 \sum_{d=1}^{N+1} \rho_i(d) - 2 \sum_{d=1}^{N+1} \sigma_i(d) \quad (3.3.60)
\]

\[
r_i(N) = 1 + 2 \sum_{d=1}^{N+1} \rho_i(d) - 2 \sum_{d=1}^{N+1} \sigma_i(d) \quad (3.3.61)
\]

where Eq. (3.3.60) separates the summation in Eq. (2.1.7) over generation lag \( d \) into two parts that depend on \( d \) in different ways. Eq. (3.3.61) inserts the explicit form of \( \rho_i(d) \), switches the order of summation over expansion series and over generation lag, and separates the summands that depend on the generation lag. Eq. (3.3.62) evaluates the summation over the generation lag explicitly. \( \text{Var} [X_i] \) was written in Eq. (3.3.54) as \( \text{Var}[X_i(n)] \) and its generation independence is emphasized in Eq. (3.3.62).

In Fig. 2, numerical reference of the variance underestimation ratio from the independent simulations for the problem \( T = 1 \) is plotted with the numerical results of the derivation of \( r_l(N) \) above.

The variance underestimation ratio (Eq. (3.3.62)) also contains the real variance of the normalized tallies averaged over the active generations.

\[
\text{Var} [X_i(N)] = \text{Var} [X_i] r_l(N) \quad (3.3.63)
\]

Under the assumption that the estimators are unbiased, variance of a tally is equal to the expectation of corresponding square error. Then, the expectation of relative square error (RSE) can be calculated as

\[
\text{RSE}_l(N) = \frac{\text{Var}[X_i(N)]}{s^2} = \frac{\text{Var}[X_i]}{s} r_l(N) \frac{L^2}{\alpha^2} \quad (3.3.64)
\]

where \( s \) is the number of neutrons per generation. The normalized \( \mu(x) \) chosen above (Eq. (3.3.21)) corresponds to 1 neutron per gen-
The asymptotic $r_I$ values are plotted as a function of tally size in Fig. 5. The numerical reference is approximated by $r_I(1000)$.

Consistency between the predicted values and references (Fig. 1, 2 and 5) indicates that the continuous model generalized from the discrete model of Multitype Branching Processes can be applied to provide an approximate assessment of the correlation in a Monte Carlo simulation with generation-to-generation dependence and branching processes.

However, the values of the correlation coefficients and asymptotic variance underestimation ratios are much lower than those observed in a typical nuclear reactor (Herman and Monte, 2014; Miao et al., 2016). From a discrete point of view, as the dimension of the system increases, one phase space cell has exponentially more neighboring phase space regions to be correlated with, and thus contributes to much higher correlation level in the tally region containing these phase space cells. Negligible correlation level for tally region with width $2a$ in a 1D system with width $2L$ does not necessarily imply negligible correlations for a tally region with volume $(2a)^3$ in a 3D system with volume $(2L)^3$. The analysis in the 1D system must be extended to realistic 3D systems.

### 3.4. Analysis of 3D homogeneous model

Let’s now generalize the homogeneous 1D problem into 3D. Suppose the system is in the volume $[-L_x, L_x] \times [-L_y, L_y] \times [-L_z, L_z]$ with constant macroscopic cross sections and reflective boundaries. Denote any position in the system as $\mathbf{r} = (x, y, z)$.

#### 3.4.1. Transition kernel and diffusion approximation

For the 3D system, it is not easy to find the exact form of $M^1(x, \mathbf{r}, \mathbf{P})$ as was done for $M^1(x)$ in Eq. (3.3.7). Instead, this section builds a relation between the integral kernel $M^1(x, \mathbf{r}, \mathbf{P})$ and the diffusion operator in a 1D system and then generalize the relation as an approximation in 3D.

Recall that the one group diffusion approximation for the neutron transport equation in a homogeneous system reads as Reuss (2012)

\[
-D \nabla^2 \phi(x) + \Sigma_0 \phi(x) = \frac{v \Sigma_f}{k_{	ext{eff}}} \phi(x) \tag{3.4.1}
\]

Eq. (3.4.1) can be converted to an eigenvalue form of the Laplace operator

\[
\nabla^2 \phi(x) = \frac{1}{k_{	ext{eff}}} \phi(x) \tag{3.4.2}
\]

where $k_{\text{eff}}$ and the migration area $M^2$ are defined as

\[
k_{\text{eff}} = \frac{v \Sigma_f}{\Sigma_0} \tag{3.4.3}
\]

\[
M^2 = \frac{D}{\Sigma_0} \tag{3.4.4}
\]

where $v$ is the expected number of new neutron per fission.

If we assume that the problem is critical, which implies that $\Sigma = 1$, where $\xi$ denotes the number of new neutrons per absorption. The criticality condition is equivalent to

\[
1 = v \Sigma (\xi = 0) = \Sigma_0 \tag{3.4.5}
\]

where the second equality holds only if the probability that a fission produces no neutrons is identically zero. The eigenvalue problem of the Laplace operator is thus simplified to

\[
\nabla^2 \phi(x) = \frac{1}{M^2} \phi(x) \tag{3.4.6}
\]
The boundary conditions determine the eigenvalues of the Laplacian indexed by integer \( k \), as seen below

\[
\nabla^2 \phi(x) = \lambda_k \phi(x)
\]

(Eq. (3.4.7))

Eqs. (3.4.7) and (3.4.6) can be used to express the relation between the eigenvalues of the transport equation, \( \lambda_k \), and the eigenvalues of the Laplacian equation, \( \lambda_k \), as

\[
\lambda_k = \frac{\pi k}{2L} \quad (3.4.10)
\]

Comparing the eigenvalues of \( M^{(1)}(x,x') \), \( \lambda_k \), in Eq. (3.3.16) and the eigenvalues of the transport (diffusion) equation, \( \lambda_k \), in Eq. (3.4.11) and their corresponding eigenfunctions, it can be shown that the integral kernel \( M^{(1)}(x,x') \) and the diffusion equation have the same eigensystem as long as

\[
M^2 = \frac{\pi k}{2L} = \frac{\pi k}{2\ell}
\]

\[
\Rightarrow D = \frac{\pi k}{2\ell}
\]

The relation between \( \lambda_k \) and \( I_k \) (Eq. (3.4.11)) holds for any dimension.

\[
\lambda_k \equiv k_{\text{eff}} = \frac{1}{1 - \left( \frac{\pi k}{2\ell} \right)^2} \quad (3.4.17)
\]

From now on, \( \lambda_k \) instead of \( k_{\text{eff}} \) are used for consistency in notation with the previous sections.

The expansion of the transfer kernel \( M^{(1)}(x,x') \) can thus be approximated with the diffusion equation. What remains undetermined is the migration area \( M^2 \), which can often be approximated using classical models (Duderstadt and Hamilton, 1976) or the more rigorous cumulative migration method (Liu et al., 2018).

If we assume that the migration area can be approximated and knowing the eigensystem from diffusion theory, \( M^{(c)}(\vec{r}, \vec{r}') \) can be conceptually written as

\[
M^{(c)}(\vec{r}, \vec{r}') = \frac{1}{8L_xL_yL_z} + \frac{1}{L_xL_yL_z} \times \sum_{k=0}^\infty \left\{ \left( \frac{\pi k}{2L} \right)^2 \right\} \left( \frac{\pi k}{2L} \right)^2
\]

\[
\times \langle x | k_x \rangle \langle y | k_y \rangle \langle z | k_z \rangle \langle 0 | k_x \rangle \langle 0 | k_y \rangle \langle 0 | k_z \rangle \left( \frac{\pi k}{2L} \right)^2
\]

For convenience \( \sum_{k=0}^\infty \) is denoted as \( \sum_k \) from now on. With the approximated expansion series of the transfer kernel \( M^{(1)}(\vec{r}, \vec{r}') \), the derivations of spatial covariances, correlation coefficients and variance underestimation ratios are straightforward and in parallel with the development in Section 3.3.

3.4.2. Spatial covariance

In the homogeneous problem with reflective boundaries, the eigenfunction of the largest eigenvalue 1 is

\[
\mu(\vec{r}) = \frac{1}{8L_xL_yL_z}
\]

With the stationary \( \mu(\vec{r}) \) being constant in space and the transition kernel \( M^{(1)}(\vec{r}, \vec{r}') \) being symmetric in \( \vec{r} \) and \( \vec{r}' \) and \( \vec{r} \) and \( \vec{r}' \), \( \nu(\vec{r}, \vec{r}') \) (Eq. (3.1.10)) is simplified to

\[
\nu(\vec{r}, \vec{r}') = \frac{1}{8L_xL_yL_z} \left( \alpha^2 \delta^{(3)}(\vec{r}, \vec{r}') - M^{(c)}(\vec{r}, \vec{r}') \right)
\]

The continuous space version of the spatial correlation within generation \( n \), \( \text{Cov}(n) \), (Eq. (3.1.11)) becomes

\[
\text{Cov}(n-\delta) = \frac{1}{8L_xL_yL_z} \sum_{\delta=0}^{\infty} \left( \alpha^2 M^{(2g-s-1)}(\vec{r}, \vec{r}') - M^{(2g)}(\vec{r}, \vec{r}') \right)
\]

where \( M^{(2g)}(\vec{r}, \vec{r}') \) is defined as

\[
M^{(2g)}(\vec{r}, \vec{r}') \equiv \delta^{(3)}(\vec{r}, \vec{r}')
\]

Similarly, the continuous space version of the serial-spatial moments becomes

\[
\text{Cov}^{(s,n-d)} = \frac{1}{8L_xL_yL_z} \sum_{\delta=0}^{\infty} \left( \alpha^2 M^{(2g-s-d)}(\vec{r}, \vec{r}') - M^{(2g+d)}(\vec{r}, \vec{r}') \right)
\]
Symmetry makes the contribution from all eigenfunctions that are odd function of \( x \) to \( \text{Cov}[X_{i}(n), X_{i}(n + d)] \) and \( \text{Var}[X_{i}(n)] \) vanish, which simplifies calculation.

In the 3D problem, to make the prediction more challenging and expose the impact of the dominance ratio, whose contribution vanishes due to symmetry of the central region, the tally region is moved off-center, \( I \) is chosen to be a box with volume \( 8a_{a}a_{a}a_{a} \) but with one corner at \((0, 0, 0)\).

\[
I \equiv L_{x} \times L_{y} \times L_{z} = [0, 2a_{a}] \times [0, 2a_{a}] \times [0, 2a_{a}] \tag{3.4.24}
\]

In the 3D problem, the whole space is denoted as \( W \) for convenience.

\[
W = W_{x} \times W_{y} \times W_{z} = [-L_{x}, L_{x}] \times [-L_{y}, L_{y}] \times [-L_{z}, L_{z}] \tag{3.4.25}
\]

The first order moments in Eq. (3.2.8) are simply

\[
\mu(n) = \mu(n + d) = 0 \quad \mu_{l}(n + d) = \frac{\mu_{l}^{2}(n + d)R}{C_{2}} \tag{3.4.26}
\]

The following integrals will be useful and hold for any dimension.

\[
\int_{I_{x}} dx(x|k) = \frac{2a_{a}}{\sqrt{2L_{x}}} \quad k = 0 \tag{3.4.27}
\]

\[
\int_{I_{x}} dx(x|k) = \frac{1}{\sqrt{L_{x}}} \sin \left( \frac{\pi k x}{2L_{x}} \right) \quad k \text{ even} \tag{3.4.28}
\]

\[
\int_{I_{x}} dx(x|k) = \frac{2\sqrt{L_{x}}}{\pi} \sin \left( \frac{\pi k a_{a}}{L_{x}} \right) \quad k \text{ odd} \tag{3.4.29}
\]

\[
\int_{W_{x}} dx(x|k) = \left\{ \begin{array}{ll} \frac{2\sqrt{L_{x}}}{k} & k = 0 \\ 0 & \text{otherwise} \end{array} \right. \tag{3.4.30}
\]

Then we perform the integrals over region \( I \times I \) of \( M^{(e)}(\vec{r}, \vec{r}) \).

\[
j_{i} d^{3}r_{i} \int_{W} d^{3}P M^{(e)}(\vec{r}, \vec{r}) = \frac{\pi^{2} a_{a}^{6}}{6} \sum_{k} j_{l}^{2} d^{3}P \int_{W} d^{3}P \tag{3.4.31}
\]

\[
= \frac{2 a_{a}^{2} a_{a}^{2}}{L_{x}^{2} L_{y}^{2} L_{z}^{2}} + \sum_{k} \beta_{k}^{2} \left( \vec{k} \right) \tag{3.4.32}
\]

where Eq. (3.4.31) separates the integral over the tally region into a product of integrals along each dimension. Eq. (3.4.32) evaluates the component of \( k = \vec{0} \) since the explicit form of the leading term is useful in derivations below. The final form of the remaining integrals depends on the component of \( \vec{k} \neq \vec{0} \) since the corresponding dimension and the \( f(\vec{k})'s \) are written in Eqs. (3.4.27), (3.4.28), (3.4.29) and (3.4.30).

We then evaluate \( \text{Cov}[Z_{i}(n), Z_{i}(n + d)] \). First substitute the explicit form of kernel \( M \) into Eq. (3.1.8) and Eq. (3.1.8)

\[
\text{Cov}[Z_{i}(n), Z_{i}(n + d)] = \frac{1}{8L_{x}L_{y}L_{z}} \sum_{k} \left\{ \sigma^{2} \int d^{3}P d^{3}P M^{(e-1)(d)}(\vec{r}, \vec{r}) \right. \tag{3.4.33}
\]

Then substitute the integral of the matrix elements of the transfer kernel, Eq. (3.4.33) becomes Eq. (3.4.34)

\[
\text{Cov}[Z_{i}(n), Z_{i}(n + d)] = \frac{1}{8L_{x}L_{y}L_{z}} \left\{ \sigma^{2} \int d^{3}P d^{3}P M^{(2)(d)}(\vec{r}, \vec{r}) \right. \tag{3.4.34}
\]

Then switch the order of the summation over the eigenfunction expansion and the summation over the generation number \( g \) and separate the leading \( \vec{k} = \vec{0} \) term from the remaining \( \sum_{k} \) summation terms. Eq. (3.4.34) is simplified into Eq. (3.4.35).

\[
\text{Cov}[Z_{i}(n), Z_{i}(n + d)] = \frac{1}{8L_{x}L_{y}L_{z}} \left\{ 8a_{a}^{2} a_{a}^{2} \sigma^{2} - 1 \right. \tag{3.4.35}
\]

Then evaluate the geometric series of index \( g \) (Eq. (3.4.36)), and take the limit \( n \rightarrow \infty \) assuming that stationarity is reached after sufficiently many generations \( n \) and recognizes \( \vec{k}^{2n} \rightarrow 0 \) (Eq. (3.4.37)).

\[
\text{Cov}[Z_{i}(n), Z_{i}(n + d)] = \frac{1}{8L_{x}L_{y}L_{z}} \left\{ 8a_{a}^{2} a_{a}^{2} \sigma^{2} - 1 \right. \tag{3.4.36}
\]

Next, we can evaluate \( \text{Cov}[Z_{i}(n), Z_{i}(n + d)] \). The \( \langle x, y, z| k_{x}, k_{y}, k_{z} \rangle \) part of \( M^{(e)}(\vec{r}, \vec{r}) \) for all components will be integrated over the whole region \( W \) and the \( \langle k_{x}, k_{y}, k_{z}| x', y', z' \rangle \) part will be integrated over the region of interest \( I \). According to Eq. (3.30), only the leading \( \vec{k} = \vec{0} \) term contributes non-zero value to the integral \( \int d^{3}r_{i} d^{3}P \int_{W} d^{3}P \).

\[
\text{Cov}[Z_{i}(n), Z_{i}(n + d)] = \frac{1}{8L_{x}L_{y}L_{z}} \left\{ \sum_{k} \sigma^{2} \left( \sum_{n} \frac{2L_{x}}{\sqrt{2L_{x}}} \right)^{2} + 0 \right. \tag{3.4.38}
\]

\[
\text{Cov}[Z_{i}(n), Z_{i}(n + d)] = \frac{1}{8L_{x}L_{y}L_{z}} \left\{ \sum_{k} \sigma^{2} - 1 \right. \tag{3.4.39}
\]

By symmetry,

\[
\text{Cov}[Z_{i}(n), Z_{i}(n + d)] = \frac{1}{8L_{x}L_{y}L_{z}} \left( \sigma^{2} - 1 \right) \tag{3.4.40}
\]

Similarly, only the \( \vec{k} = \vec{0} \) term in the expansion of \( M^{(e)}(\vec{r}, \vec{r}) \) contribute to the integral of \( \text{Cov}[Z_{i}(n), Z_{i}(n + d)] \).

\[
\text{Cov}[Z_{i}(n), Z_{i}(n + d)] = \frac{1}{8L_{x}L_{y}L_{z}} \left\{ \left( \sum_{k} \frac{2L_{x}}{\sqrt{2L_{x}}} \right)^{2} + 0 \right. \tag{3.4.41}
\]

\[
\text{Cov}[Z_{i}(n), Z_{i}(n + d)] = \frac{1}{8L_{x}L_{y}L_{z}} \left( \sigma^{2} - 1 \right) \tag{3.4.42}
\]

where Eq. (3.4.41) is the same as Eq. (3.4.38) except that \( a_{i} \)’s are replaced with corresponding \( L_{i} \)’s.

All the terms required to calculate \( \text{Cov}[X_{i}(n), X_{i}(n + d)] \) in Eq. (3.2.8) are known (Eq. (3.2.6), (3.2.7), (3.2.8) and (3.4.2)). The covariance between the normalized neutron tally in region \( I \) across the generation lag \( d \) is
\[
\text{Cov}[X(n), X(n + d)] = \left(\frac{a_{\alpha} a_{\beta}}{Lx Ly Lz}\right)^2 \left(\frac{\sigma^2}{11}\right) - \frac{2 a_{\alpha} a_{\beta}}{Lx Ly Lz} \left(\frac{\sigma^2}{11}\right) + \frac{1}{6Lx Ly Lz} \sum_k \frac{\sigma^2 - 2\sigma f(k)}{1 - \sigma^2 f(k)} \tag{3.4.43}
\]
\[
\text{Cov}[Z(n), Z(n)] = \frac{1}{8Lx Ly Lz} \sum_k \frac{\sigma^2 - 2\sigma f(k)}{1 - \sigma^2 f(k)} \tag{3.4.44}
\]

where Eq. (3.4.43) combines the \(0\)th term in \(\text{Cov}[Z(n), Z(n + d)]\) (Eq. (3.4.37)) with the other covariance terms and cancels them out. Note that Eq. (3.4.44) is a complete analog to Eq. (3.3.42). The covariances of \(X\) tallies decay exponentially as a function of \(d\).

### 3.4.3. Correlation coefficients

Similar calculations are performed for \(\text{Var}[X(n)]\) to obtain \(\rho(d)\) as \(\text{Cov}[X(n), X(n + d)]/\text{Var}[X(n)]\). \(\text{Var}[X(n)]\) is evaluated via \(\text{Cov}[X(n), X(n + d)] \neq 0\). Thus \(\text{Cov}[Z(n), Z(n)], \text{Cov}[Z(n), Z(n)]\) and \(\text{Cov}[Z(n), Z(n)]\) are needed. One difference from the variance calculated from the covariance in the previous section, \(d = 0\) leads to the appearance of \(M^{(0)}(\vec{r}, \vec{r}) = \delta(\vec{r} - \vec{r})\) in the summation indexed by the generation number \(g\). The following integrals of \(\delta^{(3)}(\vec{r}, \vec{r})\) are useful in upcoming evaluations.

\[
\int d^3\vec{r} \int d^3\vec{r} \delta(\vec{r} - \vec{r}) = \int d^3\vec{r} = 8a_x a_y a_z \tag{3.4.45}
\]
\[
\int d^3\vec{r} \int d^3\vec{r} \delta(\vec{r} - \vec{r}) = \int d^3\vec{r} = 8a_x a_y a_z \tag{3.4.46}
\]
\[
\int d^3\vec{r} \int d^3\vec{r} \delta(\vec{r} - \vec{r}) = \int d^3\vec{r} = 8a_x a_y a_z \tag{3.4.47}
\]
\[
\int d^3\vec{r} \int d^3\vec{r} \delta(\vec{r} - \vec{r}) = 8Lx Ly Lz \tag{3.4.48}
\]

While integrating \(\text{Var}^{(3)}(x, y)\) (Eq. (3.3.23)), \(g = 1\) and \(g \geq 2\) should be treated separately. Where Eq. (3.4.49) separates the index \(g\) into \(g = 1\) and \(g \geq 2\). For the \(\sigma^2\text{Cov}^{(3)}(x, y)\) part, Eq. (3.4.50) combines the \(g = 1\) and \(g \geq 2\) terms. Eq. (3.4.51) switches the order of the summation over \(k\) and the summation over \(g\) and evaluates the geometric series of index \(g\) with \(n \rightarrow \infty\). Eq. (3.4.52) recognizes common factors in the two summations over index \(k\).

Next, we evaluate \(\text{Cov}[Z(n), Z(n)]\) which shows similarities to \(\text{Cov}[Z(n), Z(n + d)]\).

\[
\text{Cov}[Z(n), Z(n)] = \frac{1}{8Lx Ly Lz} \left[ \sigma^2 a_x a_y a_z \right] - \frac{2 a_x a_y a_z}{Lx Ly Lz} \left(\frac{\sigma^2}{11}\right) + \frac{1}{6Lx Ly Lz} \sum_k \frac{\sigma^2 - 2\sigma f(k)}{1 - \sigma^2 f(k)} \tag{3.4.49}
\]

By symmetry,

\[
\text{Cov}[Z(n), Z(n)] = \frac{a_x a_y a_z}{Lx Ly Lz} (\sigma^2 - 1) n \tag{3.4.50}
\]

Similarly,

\[
\text{Cov}[Z(n), Z(n)] = \frac{1}{8Lx Ly Lz} \sum_k \frac{\sigma^2 - 2\sigma f(k)}{1 - \sigma^2 f(k)} \tag{3.4.51}
\]

Then we combine the covariance of the neutron counts \(Z\) to the variance of relative counts \(X\) according to Eq. (3.2.8).

\[
\text{Cov}[X(n), X(n)] = \text{Cov}[X(n), X(n + d)]
\]

\[
= \left(\frac{a_x a_y a_z}{Lx Ly Lz}\right)^2 \left(\frac{\sigma^2}{11}\right) - \frac{2 a_x a_y a_z}{Lx Ly Lz} \left(\frac{\sigma^2}{11}\right) + \frac{1}{6Lx Ly Lz} \sum_k \frac{\sigma^2 - 2\sigma f(k)}{1 - \sigma^2 f(k)} \tag{3.4.52}
\]

where Eq. (3.4.56) combines the \(0\)th term in \(\text{Cov}[Z(n), Z(n)]\) (Eq. (3.5.2)) with the other variance terms and cancels them out. Note that Eq. (3.4.57) is a complete analog to Eq. (3.3.54), with the volume ratio \(\frac{g}{c}\) replaced by \(\frac{a_x a_y a_z}{Lx Ly Lz}\) and the absence of \(n\) in the final form indicates that Eq. (3.4.57) is stationary.

\[
\text{Cov}[Z(n), Z(n)] = \frac{1}{8Lx Ly Lz} \left[ \sigma^2 a_x a_y a_z \right] - \frac{2 a_x a_y a_z}{Lx Ly Lz} \left(\frac{\sigma^2}{11}\right) + \frac{1}{6Lx Ly Lz} \sum_k \frac{\sigma^2 - 2\sigma f(k)}{1 - \sigma^2 f(k)} \tag{3.4.53}
\]

With the covariances that are a function of the generation lag only and variances that are stationary, the correlation coefficients of the normalized tally in region \(l\) are a function of generation lag \(d\) only.

\[
\rho(d) = \frac{\text{Cov}[X(n), X(n + d)]}{\text{Var}[X(n)]} \tag{3.4.54}
\]

Eq. (3.4.58) also exhibits three important features of the correlation coefficients. Firstly, the dependence on \(n\) in the moments of the \(Z\) tallies disappeared after being transformed to \(X\) tallies and leads to the correlation coefficients being a function of the generation lag only. Secondly, the dependence on the eigenvalues and consequently the asymptotic dependence on the dominance ratio corresponds to the correlation due to the source dependence.
during the source update in consecutive generations and the dependence on $\sigma^2$ corresponds to the correlation due to the branching processes. Thirdly, the correlation coefficients do not depend on generation size.

### 3.4.4. Variance underestimation ratio and asymptotic behavior

Covariances of normalized $X$ tallies can now be used to predict the variance of a tally averaged over the active generations, $\text{Var}[X_t(N)]$, according to Eq. (2.1.6). Equivalently, the correlation coefficients can be converted to a variance underestimation ratio $r_t(N)$ as defined in Eq. (2.1.7).

\[
r_t(N) = 1 + 2 \sum_{d=1}^{N-1} \rho_1(d) \sum_{d=1}^{N-1} d \rho_1(d) \frac{1}{\text{Var}[X_t]} \sum_{d=1}^{N-1} \sum_{d=1}^{N-1} d \rho_1(d) \frac{1}{1+\frac{\sigma^2}{\rho_1(d)}} f(k) \tag{3.4.59}
\]

\[
= 1 + 2 \frac{1}{\text{Var}[X_t]} \sum_{d=1}^{N-1} \left( \frac{1}{1+\frac{\sigma^2}{\rho_1(d)}} \right) f(k) \tag{3.4.60}
\]

\[
= 1 + 2 \frac{1}{\text{Var}[X_t]} \sum_{d=1}^{N-1} \left( \frac{1}{1+\frac{\sigma^2}{\rho_1(d)}} \right) f(k) \tag{3.4.61}
\]

\[
= 1 + 2 \frac{\sigma^2 n(1-\frac{1}{2}) + \sum_{d=1}^{N-1} \sum_{d=1}^{N-1} d \rho_1(d) \frac{1}{1+\frac{\sigma^2}{\rho_1(d)}} f(k)}{\text{Var}[X_t]} \tag{3.4.62}
\]

where Eq. (3.4.59) separates the summation in Eq. (2.1.7) over generation lag $d$ into two parts that depends on $d$ in different ways. Eq. (3.4.60) inserts the explicit form of $\rho_1(d)$ and changes the order of summation over the eigenfunction expansion and generation lag, and separates the sums that depend on the generation lag. Eq. (3.4.61) evaluates the summation over the generation lag explicitly. $\text{Var}[X_t]$ was written in Eq. (3.4.57) as $\text{Var}[X_t(n)]$ and its generation independence is emphasized in Eq. (3.4.62). Eq. (3.4.62) inserts the explicit form of $\text{Var}[X_t]$ and recognizes volume of tally region $v$ and volume of the system $v$.

Finally, the asymptotic variance underestimation ratio can be obtained by taking the limit of $N \to \infty$ in $r_t(N)$ (Eq. (3.4.62)).

\[
r_t = \lim_{N \to \infty} r_t(N) = 1 + 2 \frac{\sigma^2 n(1-\frac{1}{2}) + \sum_{d=1}^{N-1} \sum_{d=1}^{N-1} d \rho_1(d) \frac{1}{1+\frac{\sigma^2}{\rho_1(d)}} f(k)}{\text{Var}[X_t]} \tag{3.4.63}
\]

The derivation of correlation coefficients $\rho_1(d)$, variance underestimation ratio $r_t(N)$ and its asymptotic value $r_t$ can be applied to many types of tallies by adjusting the values of $a_0$, $a_1$, $a_2$. For example, setting $a_0 = L$ and $a_1 = a_3 = \delta$, the tally region $l$ corresponds approximately to a nuclear fuel pin with cross section area $\delta^2$. And setting $a_2 = a_3 = L$ and $a_4 = \delta$, the tally region $l$ corresponds to a slab of width $\delta$. Note that, $f(k)$ depends on the tally region choice through the integrals in Eqs. (3.4.27), (3.4.28) and (3.4.29).

### 3.4.5. Numerical results

Simulations of a 3D test problem with the same material parameters as in Table 1 used to verify the previous derivations numerically. The test problem is denoted as TC1. As for geometry, TC1 corresponds to $L_x = L_y = L_z = 200cm$. The tally regions of interest are selected to be cubes of different sizes parameterized by $(2a)^3$. 1,000,000 neutrons per generation are simulated in the 3D system for 1000 active generations, and 200 such independent simulations are performed to generate reference results.

For the predictive mode, $M^2$ is approximated as $1/(3\Sigma\Sigma^2)$ since the diffusion coefficient is calculated assuming isotropic scattering in the LAB reference system

\[
D = \frac{1}{3\Sigma^2}
\]

The summation over $\sum_{k}$ in all of the eigenmode expansion equations such as Eqs. (3.4.58) and (3.4.62) can be written explicitly by separating the fundamental eigenmode, as well as the even and odd eigenmodes.

The correlation coefficients estimated from the independent simulation tallies are plotted along with the prediction from $\rho_1(d)$ in Eq. (3.4.58) in Fig. 6.

The reference autocorrelation coefficients at each state are calculated according to Eq. (2.1.4) by simply replacing the expectation...
operators with averages calculated over the independent simulations. Due to the stationarity of correlation coefficients, all \( \rho(n, n + d) \) of the same lag are combined to reduce statistical noise. Note that when \( a = 0.5 \text{cm} \), the volume of the tally region is only \( 1.5625 \times 10^{-8} \) of the total system volume. Even with 1000000 neutrons per generation simulated, for problem TC1, the expected number of neutron observed per generation in the tally region is 0.015625 or 1 neutron every 64 generations. This leads to 0 tally in many generations and thus 0 variance when estimated across many generations and thus 0 variance when estimated across many generations. Consequently, 0 in the denominator makes estimated correlation coefficients unavailable for tally region of size \( a = 0.5 \text{ cm} \).

As expected, the correlation coefficients are higher in larger tally regions. Additionally, it can be seen that when using the diffusion approximation, the predicted \( \rho_i(d) \) follows the correct trend of that calculated from independent simulations but the prediction is not exact as previously observed with the 1D problem in Section 3.3 (Fig. 1).

The numerical reference of the variance underestimation ratio from the independent simulations and the predicted values are plotted in Fig. 7. As expected, the underestimation ratio is larger as the tally size increases. For the same argument as above, the small tally region suffers from large statistical noise as observed in Fig. 7.

Similarly to the discussion related to the TC1 – 1D problem, the real variance of the normalized tally averaged over all active generations can also be extracted from the derivation of the variance underestimation ratio. The real variance can be used to predict the relative square error as expressed below

\[
\text{RSE}_i(N) = \frac{\text{Var}[X_i(N)]}{s^2} = \frac{\text{Var}[X_i]}{s} \frac{\langle N \rangle}{L^6} \tag{3.4.65}
\]

where \( s \) is the number of neutrons per generation.

The \( \text{RSE}_i \) derived above in Eq. (3.4.65) is plotted along with the relative square error obtained from independent simulations in Fig. 8.

Although smaller regions have lower correlation coefficients and thus their variance decreases closer to \( 1/N \), the relatively lower tally counts in the region lead to larger uncertainties.

Further, it can be seen from Fig. 8 that the relative square error monotonically decreases as tally region size increases. By the law of large numbers, the relative square error approaches its prediction, real variance divided by squared reference, which can be interpreted as the inverse of squared signal to noise ratio (SNR). SNR is higher for larger tally regions which explains the lower relative square error observed.

Quantitatively, it can be shown for the homogeneous problem that the real variance divided by the squared reference value in tally region \( i \) cannot be lower than the larger tally region \( I \) comprised of smaller regions which includes \( i \).

\[
\text{Var}[X_i(N)] = \sum_{n,n' \in N} \text{Cov}[X_i(n),X_i(n')] \\
= \sum_{n,n' \in N} \sum_{j \in I} \text{Cov}[X_i(n),X_j(n')] \\
= \sum_{i,j} \sum_{n \in N} \text{Cov}[X_i(n),X_j(n')] + \sum_{n \in N} \sum_{n' \in N} \text{Cov}[X_i(n),X_i(n')] \\
= \sum_{i,j} \text{Var}[X_i(N)] + \sum_{i,j} \sum_{n \in N} \text{Cov}[X_i(n),X_j(n')] \\
\tag{3.4.66}
\]
For \(i \neq j\), \(\text{Cov}[X_i(n), X_j(n')] < \text{Cov}[X_i(n), X_i(n')]\) since a tally in region \(i\) is more correlated with itself than with other regions.

\[
\text{Var}[X_i(n)] < \sum_{i \neq j} \text{Var}[X_i(n)] + \sum_{i \neq j} \sum_{n \neq n'} \text{Cov}[X_i(n), X_i(n')]
\]

\[
= \sum_{i \neq j} \text{Var}[X_i(n)] + \sum_{i \neq j} \text{Var}[X_i(n)]
\]

(3.4.67)

For a homogeneous problem, \(\text{Var}[X_i(n)] = \text{Var}[X_i(n)]\), then \(\text{Var}[X_i(n)] = \text{Var}[X_i(n)]\). Therefore,

\[
\text{Var}[X_i(n)] < I \text{Var}[X_i(n)] + (I - 1) \text{Var}[X_i(n)]
\]

\[
= I \text{Var}[X_i(n)]
\]

(3.4.68)

Since the system is reflective and homogeneous, \(E[X_i(n)] = E[X_i(n)]\), then \(E[X_i(N)] = E[X_i(n)]\) and \(E[X_i(n)] = E[X_i(n)]\). Finally,

\[
\frac{\text{Var}[X_i(n)]}{\langle X_i(n) \rangle^2} < \frac{I \text{Var}[X_i(n)]}{\langle X_i(n) \rangle^2} = \frac{\text{Var}[X_i(n)]}{\langle X_i(n) \rangle^2}
\]

(3.4.69)

which demonstrates that \(RMS_i < RMS\).

The asymptotic value \(r_I\) for different tally sizes are plotted explicitly as a function of the tally size in Fig. 9. The numerical reference values are approximated by using the value at \(r_I(1000)\).

Since the variance underestimation ratio measures the cumulative effect of correlation coefficients, the diffusion approximation can predict the asymptotic variance underestimation ratio with acceptable accuracy despite somewhat inaccurate correlation coefficients at each generation. Fig. 9 also shows that using the lowest truncation of the kernel expansion (single higher mode) gives unsatisfactory predictions of the underestimation ratio. However, as long as the homogenization is performed appropriately, the evaluation of the eigenfunctions of the homogeneous diffusion problem is not very costly.

### 4. Application to the 2D BEAVRS benchmark

Section 3.3 solves for the correlation exactly in a homogeneous 1D system, while Section 3.4 shows that the correlations can be reasonably estimated using diffusion theory in a homogeneous 3D system. It was shown that a good indicator in determining situations where correlations can become an issue is the asymptotic variance underestimation ratio \(r_I\).

![Fig. 11. Variance convergence rate for central tally region with different sizes in 2D BEAVRS. The tally size \(a\) is in unit cm. The dots correspond to \(\frac{\text{RMS}}{\text{RMS}_0}\) estimated from independent simulations. The solid line curves correspond to predictions from the continuous model. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this article.)](image)

Fig. 11. Variance convergence rate for central tally region with different sizes in 2D BEAVRS. The tally size \(a\) is in unit cm. The dots correspond to \(\frac{\text{RMS}}{\text{RMS}_0}\) estimated from independent simulations. The solid line curves correspond to predictions from the continuous model. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this article.)

This section will demonstrate how the \(r_I\) of a realistic problem can be used to identify tally sizes where the usual variance estimator fail. The 2D BEAVRS benchmark is used, which is represented by a 10 cm axial slice at mid-height of the 3D BEAVRS benchmark Horelik et al., 2013 with reflective top and bottom boundary conditions. In the notation of this work, the geometry parameters of the problem are

\[L_x = L_y = 182.78 \text{ cm}\]

\[L_z = 5.0 \text{ cm}\]

(4.0.1)

The cumulative migration area method (Liu et al., 2018) was used to estimate the migration area of the core as

\[M^2 = 55.06 \text{ cm}^2\]

(4.0.2)

The assemblies including the inter-assembly gaps are of size 21.5 cm \(\times\) 21.5 cm which in the notation of the previous section corresponds to \(a_x = a_y = 10.75 \text{ cm}\) and \(a_z = L_z = 5.0 \text{ cm}\). Correlations were investigated on four different tally sizes and reference values were obtained from 450 independent simulations.

With the migration area, system geometry and tally region geometry, the correlation coefficients can be evaluated immediately following Eqs. (3.4.58) and 3.4.17. The reference and predicted correlation coefficients are plotted in Fig. 10. As expected, the diffusion approximation does not match exactly the reference values, but does follow similar trends for all tally sizes. Consequentially, a similar behavior can be observed for the variance underestimation ratio \(r_I(n)\) as shown in Fig. 11.

The asymptotic value \(r_I\) for different tally sizes \(|0.2a_x| \times |0.2a_y| \times |L_z - L_z|\) is illustrated in Fig. 12. The reference values correspond to the value of \(r_I\) after 1000 generations. While not exact, especially for larger tallies, the diffusion approximation follows the appropriate trend and can provide a very simple way of deciding if independent simulations are needed or an alternative strategy to reduce or estimate the correlations should be used.

### 5. Conclusion

Previous work developed an approach to predict the underestimation of variance often seen in full core nuclear reactor simulations prior to performing a detailed simulation by discretizing the phase space. Knowing this underestimation allows for more
efficient simulations with truly quantifiable error estimates and stopping criteria. In many cases, however, the correlation effects are quite small (e.g. small system or small tally in large system) and it becomes unnecessary to develop an MBP model that can become somewhat costly. Therefore, this paper provides a simple metric to determine whether significant variance underestimate is expected in a given problem with a given tally size. This task was accomplished by developing a continuous space model that can predict correlation coefficients on a homogeneous problem, where correlation coefficients can be simply written as function of system geometry, migration area and tally region geometry. Results of the correlation coefficients and variance underestimate on tally region of different sizes were shown to be very accurate for 1D and 3D homogeneous problems. Additionally, this simple model provided a simple predictive way of determining which tally size would suffer from large variance underestimate on the heterogeneous 2D BEAVRS benchmark.

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### Appendix A. Simplification of covariance condition

This section simplifies Eq. (2.1.5) with Eq. (2.2.1). The simplification is performed for the $\mathcal{O}(\varepsilon^2)$ terms and the $\mathcal{O}(\varepsilon^3)$ terms separately. That is

$$
\text{Cov}[ Y_i(n), Y_j(n+k) ] = \text{Cov}^2[ Y_i(n), Y_j(n+k) ] + \text{Cov}^3[ Y_i(n), Y_j(n+k) ] + o(\varepsilon^2) \quad (A.1)
$$

First sum out the dummy index $i$ and $j$ in Cov$^2[ Y_i(n), Y_j(n+k) ]$ in all phase space regions,

$$
\text{Cov}^2[ Y_i(n), Y_j(n+k) ] = \sum_{l,j} \left( \frac{ \delta^l_j }{ \mu(n) } - \frac{ \mu_i(n+k) }{ \mu(n+k)^2 } \right) \left( \frac{ \delta^l_j }{ \mu(n+k) } - \frac{ \mu_i(n+k) }{ \mu(n+k)^2 } \right)
$$

$$
= \sum_{l,j} \left( \frac{ \delta^l_j }{ \mu(n) } - \frac{ \mu_i(n+k) }{ \mu(n+k)^2 } \right) \left( \frac{ \delta^l_j }{ \mu(n+k) } - \frac{ \mu_i(n+k) }{ \mu(n+k)^2 } \right)
$$

$$
= \sum_{l,j} \frac{ 1 }{ \mu(n) } \left( \delta^l_j \right) \left( \delta^l_j \right)
$$

$$
= \sum_{l,j} \frac{ 1 }{ \mu(n) } \left( \delta^l_j \right) \left( \delta^l_j \right)
$$

where any term indexed with $i$ is changed to index $l_i$, after being summed with $\delta^l_i$, any term indexed with $j$ is changed to index $l_j$ after being summed with $\delta^l_j$, and other summations count the total number of neutrons in the system from the count in all phase space regions using Eq. (2.2.1) \( \mu(n) = \sum_{l=1}^{N} \mu_i(n) \). Then sum out the index $l_i$ and $l_j$ through the range \( \{ l_i l_j \in l \} \).

$$
\text{Cov}^2[ Y_i(n), Y_j(n+k) ] = \frac{ \mu_i(n) }{ \mu(n) } \left( \frac{ \delta^l_j }{ \mu(n+k) } \right) \left( \frac{ \delta^l_j }{ \mu(n+k) } \right)
$$

$$
= \frac{ \mu_i(n) }{ \mu(n) } \left( \frac{ \delta^l_j }{ \mu(n+k) } \right) \left( \frac{ \delta^l_j }{ \mu(n+k) } \right)
$$

where the summation in $l$ adds the number of neutrons in region phase space region contained within region $l$ into the count of region $l$ according to $Z_l(n) = \sum_{l=1}^{N} Z_{l_i}(n)$ and its expectation.

$$
\text{Cov}^2[ Y_i(n), Y_j(n+k) ] = \sum_{l,j} \frac{ \mu_i(n) }{ \mu(n) } \left( \frac{ \delta^l_j }{ \mu(n+k) } \right) \left( \frac{ \delta^l_j }{ \mu(n+k) } \right)
$$

$$
= \sum_{l,j} \frac{ \mu_i(n) }{ \mu(n) } \left( \frac{ \delta^l_j }{ \mu(n+k) } \right) \left( \frac{ \delta^l_j }{ \mu(n+k) } \right)
$$

$$
= \sum_{l,j} \frac{ \mu_i(n) }{ \mu(n) } \left( \frac{ \delta^l_j }{ \mu(n+k) } \right) \left( \frac{ \delta^l_j }{ \mu(n+k) } \right)
$$

(A.3)
Identical terms are recognized in Eq. ([2.2.1]) and

\[
\text{Cov}_i^{(3)}[Y_i(n), Y_i(n+k)]
\]

\[
= \sum_{l_i = i}^{l_i = i} \frac{1}{\mu(n)} \frac{1}{\mu(n+k)} E \left( Z_i(n) - \mu_i(n) \right) \times \left( Z_i(n+k) - \mu(n+k) \right) + \frac{1}{\mu_i(n)} \frac{1}{\mu(n+k)} E \left( Z_i(n) - \mu_i(n) \right) \times \left( Z_i(n+k) - \mu(n+k) \right) + \frac{1}{\mu(n)} \frac{1}{\mu(n+k)} E \left( Z_i(n) - \mu_i(n) \right) \times \left( Z_i(n+k) - \mu(n+k) \right) + \frac{1}{\mu(n)} \frac{1}{\mu(n+k)} E \left( Z_i(n) - \mu_i(n) \right) \times \left( Z_i(n+k) - \mu(n+k) \right)
\]

Then sum out the index \( i \) and \( l_i \) through the range \( \{i, l_i \in I\} \).

\[
\text{Cov}_i^{(3)}[Y_i(n), Y_i(n+k)]
\]

\[
= \sum_{l_i = i}^{l_i = i} \frac{1}{\mu(n)} \frac{1}{\mu(n+k)} E \left( Z_i(n) - \mu_i(n) \right) \times \left( Z_i(n+k) - \mu(n+k) \right) + \frac{1}{\mu_i(n)} \frac{1}{\mu(n+k)} E \left( Z_i(n) - \mu_i(n) \right) \times \left( Z_i(n+k) - \mu(n+k) \right) + \frac{1}{\mu(n)} \frac{1}{\mu(n+k)} E \left( Z_i(n) - \mu_i(n) \right) \times \left( Z_i(n+k) - \mu(n+k) \right) + \frac{1}{\mu(n)} \frac{1}{\mu(n+k)} E \left( Z_i(n) - \mu_i(n) \right) \times \left( Z_i(n+k) - \mu(n+k) \right)
\]

The second term in \( \text{Cov}_i^{(3)}[Y_i(n), Y_i(n+k)] \) can be achieved by interchanging \( n \rightarrow (n+k) \).

\[
\text{Cov}_i^{(3)}[Y_i(n), Y_i(n+k)] = - E \left( \frac{Z(n+k)}{\mu(n+k)} \frac{\mu_i(n+k)}{\mu_i(n)} \frac{Z_i(n)}{\mu(n)} \frac{\mu(n)}{\mu(n+k)} \right) \times \left( \frac{Z_i(n)}{\mu(n)} - 1 \right) \left( \frac{Z_i(n)}{\mu(n)} - 1 \right)
\]

Eqs. ([2.2.2]) and ([A.7]) leads to

\[
\text{Cov}_i^{(3)}[Y_i(n), Y_i(n+k)] = - \frac{\mu_i(n)}{\mu(n)} \frac{1}{\mu(n+k)} E \left( \frac{Z(n+k)}{\mu(n+k)} \frac{\mu_i(n+k)}{\mu_i(n)} \frac{Z_i(n)}{\mu(n)} \frac{\mu(n)}{\mu(n+k)} \right) \times \left( \frac{Z_i(n)}{\mu(n)} - 1 \right) \left( \frac{Z_i(n)}{\mu(n)} - 1 \right)
\]

**Appendix B. Supplementary data**

Supplementary data associated with this article can be found in the online version, at [https://doi.org/10.1016/j.anucene.2019.02.048](https://doi.org/10.1016/j.anucene.2019.02.048).

**References**


