Predicting correlation coefficients for Monte Carlo eigenvalue simulations with multitype branching process

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Abstract

This paper provides a prediction method of the generation-to-generation correlations as observed when solving large scale eigenvalue problems such as full core nuclear reactor simulations. Knowing the correlations enables correction of the variance underestimation that occurs when assuming that the active generations are independent. The Monte Carlo power iteration is cast in the Multitype Branching Process (MBP) framework by discretizing the neutron phase space which allows calculation of spatial and temporal moments. These moments can then provide auto-correlation coefficients between the generations of MBP and are shown to accurately predict the auto-correlation coefficients of the original Monte Carlo simulation. This prediction capability was demonstrated on the full core 2D PWR BEAVRS benchmark and compared successfully with variance estimates from independent simulations.

1. Introduction

Monte Carlo methods are most often considered as a reference for neutron transport simulations since very limited approximations are made about nuclear data and system geometry. Uncertainty of any tallied quantity is commonly represented by taking the sample variance over the active generations, which is based on the assumption that the neutron generations are independent. Correlation effects between neutrons in multiplying systems, particularly when performing power iteration to evaluate eigenvalues have been observed and quantified in previous work (Brissenden and Garlick, 1986; Dumonteil et al., 2014; Herman et al., 2014; Miao et al., 2016). Neglecting this correlation effect results in an underestimate of uncertainty reported by Monte Carlo calculations, the magnitude of which depends on the dominance ratio of the problem and the size of the phase space being tallied (Ueki et al., 2003). Many studies have quantified this underestimation using post-processing techniques of the tallied quantities or by de-correlating batches using many generations per batch, both of which can become costly in either memory or runtime (Miao et al., 2016; Wilson et al., 2012).

Previous work has also proposed methods to predict the underestimation ratio between the correlated and uncorrelated estimates. The actively investigated methods are classified into two categories. The first performs data fitting on simulation outputs to capture the correlation. The second directly compute covariance between the Monte Carlo generations based on corresponding approximations of the Monte Carlo simulation (Ueki, 2010). Demaret et al. (1999) fitted AR (auto-regressive) and MA (Moving Average) models to the results of Monte Carlo eigenvalue calculations and used the AR and MA models to give variance estimator of $k_{eff}$. Yamamoto et al. (2014) expanded the fission source distribution with diffusion equation modes, performed numerical simulation of the AR process of the expansion coefficients and used the correlation of the AR process to predict the Monte Carlo eigenvalue simulation. Approximating the original neutron transport problem with a diffusion problem lead to a non-negligible lost in accuracy. Sutton (2015) applied the discretized phase space (DPS) approach to predict the underestimation ratio but the method cannot predict the ratio when one neutron generates offspring in different phase space regions or generates a random number of offspring. Ueki et al. (2016) developed variance estimator with orthonormally weighted standardized time series (OWSTS). The estimator is based on the convergence of step-wise interpolation of standardized tallies (SIST) to Brownian bridge. SIST weighted by a trigonometric family of weighting functions gives a new statistical estimator for the variance. Asymptotic behavior of expectation of the new static leads to a variance estimator that is not affected by the correlation effect thus converging at a 1/N rate. Numerical results showed that the variance can be accurately estimated.
estimated after approximately 5000 ~ 10000 active generations for problems with non-negligible autocorrelation up to 100 generation lags. A convergence diagnosis is also necessary to determine when the asymptotic behavior is reached. However, the convergence diagnosis cannot be implemented on-the-fly.

This paper presents a method to predict the correlation effect based on the model of multitype branching processes (MBP) (Mode, 1971).

This method uses tallies from Monte Carlo simulation to construct a Multitype Branching Processes model, evaluates the correlation effect of the MBP model analytically and can then predict the underestimation ratio for the original Monte Carlo simulation. The kernel to construct the MBP model is the transfer probabilities between the multi-types, which are the discretized phase space regions of the original problem. If phase space regions are discretized so fine that every region can be viewed as a flat source region, the transfer probabilities can be tallied from a fixed source calculation of uniformly sampled neutron sources. More practically, phase space regions need to be slightly finer than the tally regions but not as fine as when a flat source approximation would yield a satisfactory spatial convergence of the flux. Under this circumstance, transfer probabilities can be tallied from a few active generations right after the source becomes stationary.

Section 2 will present the theoretical derivation of autocorrelation of active generation tallies from multitype branching processes. In Section 2.1, a recursive relation between moment generating functions of neutron sources will be derived and used to derive various moments of neutron sources. Section 2.2 approximates the Monte Carlo power iteration by the multitype branching process and uses covariance expansion to relate the derived moments of the multitype branching process to the autocorrelation of the power iteration. Section 3 discusses how to construct the multitype branching process from unconverged tallies. Numerical results on applying the methods developed in this paper to the BEAVRS benchmark will be found in Section 4. This section will show that auto-correlation and thus variance can be accurately predicted from the constructed multitype branching process model.

2. Theory

Suppose generation $n$ yields tally $X_l(n)$ for tally region $l$, the simulation typically reports the average $X_l(N) = \sum_{n=1}^{N} X_l(n)/N$ and $\sigma_{X_l}^2 = \sum_{n=1}^{N} X_l(n)/N$ as an approximation of $\sigma_{X_l}^2$. Due to the correlation between generations in the power iteration process, $\sigma_{X_l}^2/\sqrt{N}$ underestimates $\sigma_{X_l}^2$. The $\text{Cov}(X_i(t), X_j(t))$, where $i, j$ are the active generation indexes, is required to correctly evaluate the uncertainty.

These correlations across generations result from the fission site update process where the source of generation $n + 1$ come from the fission sites created during generation $n$. The correlation of any tallied quantity can be calculated from the correlation of the fission source distribution Shim, 2015. The auto-correlation coefficient of $X_l$ between generation $n$ and $n + k$ is defined as

$$\rho_{nk} = \frac{\text{Cov}(X_l(n), X_l(n + k))}{\sqrt{\text{Var}(X_l(n))\text{Var}(X_l(n + k))}} \tag{2.1}$$

The theory of MBP model is developed to predict the autocorrelation coefficients (ACC) of the fission source distribution.

2.1. Theory of multitype branching processes

A branching process describes a population of individuals where each individual produces offsprings independently with identical distributions. Multitype branching process extends the model to a population of finite types of individuals, such as spatial position, energy, angle. An MBP model can approximate the Monte Carlo power iteration if the neutron phase space is discretized where each cell is treated as a unique type.

This subsection first defines the moment generating function (MGF) related to the MBP model. Then the MGF is used to extract the serial-spatial moments which can then be related to the ACCs.

2.1.1. Moment generating functions

The model of multitype branching process discretizes the neutron phase space over all independent variables into $m$ discrete regions and denotes the system state at generation $n$ with a vector $\tilde{Z}(n)$ (Eq. (2.2)). 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 $l$.

$$\tilde{Z}(n) = (Z_1(n), \ldots, Z_l(n), \ldots, Z_m(n)) \tag{2.2}$$

The total number of neutrons of all phase space regions is the sum of all components of $\tilde{Z}(n)$ and is denoted as $Z(n)$ (Eq. (2.3))

$$Z(n) = \sum_{l=1}^{m} Z_l(n). \tag{2.3}$$

The state vector at generation $n$ is related to generation $n - 1$ through

$$\tilde{Z}(n) = \sum_{l=1}^{m} \sum_{j=1}^{m} \tilde{Y}_{lj} Z_l(n-1), \tag{2.4}$$

where $\tilde{Y}_{lj}$ is the state vector generated by the $j$th neutron of type $l$ at generation $n - 1$.

The moment generating function of $\tilde{Z}(n)$ is defined as

$$F_s(\tilde{r}_0, \tilde{s}) \equiv \mathbb{E}\left[ \prod_{l=1}^{m} Z_l^n(0) \mid \tilde{Z}(0) = \tilde{r}_0 \right] \tag{2.5}$$

$$= \sum_{l=1}^{m} \mathbb{P}(\tilde{Z}(n) = \tilde{r}_0 \mid \tilde{Z}(0) = \tilde{r}_0) \prod_{l=1}^{m} \tilde{S}_l^{r_l}, \tag{2.5}$$

where $\tilde{r}_0$ denotes the initial configuration of neutrons in the discretized phase space and $\tilde{s}$ is the argument of the moment generating function. If $\tilde{r}_0$ is a point source of type $i$ ($\tilde{r}_0 = \tilde{e}_i$, $\tilde{r}_0 = \tilde{r}_i$), we denote $F_s(\tilde{r}_0, \tilde{s})$ as $F_s(i, \tilde{s})$. The random vector $\tilde{Z}(n)$ initiated by $\tilde{Z}(0)$ is the sum of the random vectors initiated by the $Z(0)$ neutrons represented by the vector $\tilde{Z}(0) = \tilde{r}_0$.

$$\tilde{Z}(n) \mid \tilde{Z}(0) = \tilde{r}_0 = \sum_{l=1}^{m} \sum_{j=1}^{m} \tilde{Z}_l(n) \mid \tilde{Z}(0) = \tilde{r}_0 \tag{2.6}$$

Eq. (2.6) expresses $\tilde{Z}(n)$ as sum of contributions from all neutrons in the 0th generation. Since the $Z(0)$ random vectors are independent, the moment generating function of the state vector $\tilde{Z}(n) \mid \tilde{Z}(0) = \tilde{r}_0$ is written as the product of the moment generating function of the state vectors of the $Z(0)$ components $\tilde{Z}(n) \mid \tilde{Z}(0) = \tilde{r}_0$.

Therefore, $F_s(\tilde{r}_0, \tilde{s})$ and $F_s(i, \tilde{s})$ are related by

$$F_s(\tilde{r}_0, \tilde{s}) = \prod_{i=1}^{m} F_s(i, \tilde{s})^{r_i}. \tag{2.7}$$

$F_s(i, \tilde{s})$ can be evaluated from $F_s(i, \tilde{s})$ recursively according to its definition in Eq. (2.5).
\[ F_n(i, S) = E \left[ \prod_{j=1}^{m} Z_{ij}^{(n)} \left| \tilde{Z}(0) = \tilde{e}_i \right. \right] \]
\[ = E \left[ \prod_{j=1}^{m} Z_{ij}^{(n-1)} \left| \tilde{Z}(n-1) = \tilde{e}_i \right. \right] \]
where the second equality in Eq. (2.8) is based on the Markov property of process \( \tilde{Z}(n) \). Substituting the relation between \( \tilde{Z}(n) \) and \( \tilde{Z}(n-1) \) (Eq. (2.4)) into the conditional expectation yields
\[
E \left[ \prod_{j=1}^{m} s_j^{(n-1)} \tilde{Z}(n-1) \right] = E \left[ \prod_{j=1}^{m} s_j^{(n-1)} \tilde{Z}(n-1) \right]
\]
\[
= E \left[ \prod_{j=1}^{m} s_j^{(n-1)} \right] \tilde{Z}(n-1)
\]
\[
= \prod_{k=1}^{m} E \left[ s_k^{(n-1)} \right] \tilde{Z}(n-1)
\]
Because the neutrons at generation \( n-1 \) reproduce independently, the product over \( k \) and \( j \) on the second line of Eq. (2.9) can be pulled out of the expectation operator. By the definition of \( Y_{ij} \),
\[
E \left[ \prod_{j=1}^{m} s_j^{(n-1)} \tilde{Z}(n-1) \right] = F_1(k, S).
\]
Combining the conditional expectation and Eq. (2.8) gives
\[
F_n(i, S) = E \left[ \prod_{j=1}^{m} F_1(k, S) s_j^{(n-1)} \tilde{Z}(0) = \tilde{e}_i \right]
\]
which is the moment generating function of \( \tilde{Z}(n-1) \) with \( \tilde{f}(1, S) \) as the argument, where the vector \( \tilde{f}(1, S) \) is defined with \( F_1(k, S) \) as its \( k \)th component:
\[
\tilde{f}(1, S) = (F_1(1, S), \ldots, F_1(m, S)).
\]
Therefore the recursive relation between \( F_n(i, S) \) and \( F_{n-1}(i, S) \) reads
\[
F_n(i, S) = F_{n-1}(i, \tilde{f}(1, S))
\]
This equivalence can be demonstrated by induction on the above equation which gives
\[
F_n(i, S) = F_{n-1}(i, \tilde{f}(1, S))
\]
\[
= F_{n-2}(i, \tilde{f}(1, \tilde{f}(2, S)))
\]
\[
= F_{n-2}(i, \tilde{f}(2, S))
\]
\[
= \cdots
\]
\[
= F_1(i, \tilde{f}(n-1, S))
\]
where \( \tilde{f}(n, S) \) is naturally defined as:
\[
\tilde{f}(n, S) = \tilde{f}(n-1, \tilde{f}(1, S)), n \geq 2
\]
Combining the definitions of \( \tilde{f}(n, S) \) (Eq. (2.12), Eq. (2.15)) and the last recursive evaluation of \( F_n(i, S) \) (Eq. (2.14)) yields
\[
F_n(i, S) = \tilde{f}(n, S)_i
\]
which means \( F_n(i, S) \) is the \( i \)th element of the vector function \( \tilde{f}(n, S) \).

2.1.2. Spatial Moments
The spatial moments of \( Z_i(n) \) defined in Eq. (2.17) can be evaluated by taking derivatives of \( F_n(r_0, S) \).
\[
\mu_i(n) = E[Z_i(n)]
\]
\[
C_{ij}(n) = E[Z_i(n)Z_j(n)]
\]
(2.17)
\[
T_{ijk}(n) = E[Z_i(n)Z_j(n)Z_k(n)]
\]
This would involve commuting the derivatives into the recursive definition of \( \tilde{f}(n, S) \) (Eq. (2.15)) which can be quite lengthy. A simpler way is to evaluate the expectations at generation \( n+1 \) conditional on \( \tilde{Z}(n) \). For simplicity, \( E[X|Y] \) is denoted as \( E[X]|_Y \) in the following. The moment generating function at generation \( n+1 \) can be written as
\[
F_{n+1}(r_0, S)|_{Z(n)} = F_1(\tilde{Z}(n), S)
\]
\[
= \prod_{k=1}^{m} F_1(k, S) Z_{k}(n).
\]
From the moment generating function in Eq. (2.18), \( \mu_i(n+1) \) is first evaluated as a conditional expectation on \( \tilde{Z}(n) \) and then expressed as a function of \( \mu_i(n) \).
\[
\mu_i(n+1)|_{Z(n)} = \frac{\partial}{\partial S_i} \prod_{i=1}^{m} F_1(k, S) Z_k(n) 
\]
\[
= \sum_{i=1}^{m} F_1(k, S) Z_k(n) \frac{\partial}{\partial S_i} F_1(k, S) Z_k(n) 
\]
\[
= \sum_{i=1}^{m} Z_i(n) M^f_i(n)
\]
(2.19)
where in the second to last line, the identity \( F_1(l, S)|_{l-1} = 1 \) is used. \( M^f_i(n) \) is used to denote \( \frac{\partial}{\partial S_i} F_1(l, S)|_{l-1} \), which by definition is the expected number of neutrons found of type \( i \) after one generation given a source neutron of type \( l \). It will be referred as the first spatial moment response and denoted as:
\[
M_i^f = E[Z_i(1)|r_0 = \tilde{e}_i].
\]
Evaluating the expected value of Eq. (2.19) removes the dependence on \( \tilde{Z}(n) \) and yields
\[
\mu_i(n+1) = \mu_i(n) M_i^f.
\]
where the Einstein tensor notation is used (the sum is taken over all values of the index whenever the same symbol appears as a subscript and superscript in the same term) and will be used throughout this paper.
A similar procedure will provide the second order factorial moments, \( \tilde{C}_{ij}(n) \), which can eventually be related to \( C_{ij}(n) \) (Eq. (2.17)) through Eq. (2.22).
\[
\tilde{C}_{ij}(n) = \frac{\partial}{\partial S_i} F_1(r_0, S) = \frac{\partial}{\partial S_i} E[Z_i(n)Z_j(n) - \delta_{ij} Z_k(n)]
\]
(2.22)
\[
\tilde{C}_{ij}(n+1) \text{ is first evaluated conditional on } \tilde{Z}(n) \text{ and then expressed as a function of } \tilde{C}_{ij}(n).
the dependence of $Z(n)$ on $(l, S, R^{(i)})$ and type $(l, S, R^{(i)})$ is the third spatial (central) moment response to a point $l$.\]

\[
F_1(l, S, R^{(i)}) = \sum_{k=1}^{m} F_1(k, S, R^{(i)}) \prod_{k=1}^{m} F_1(k, S, R^{(i)}) \bigg|_{l=1}^{m}
\]

\[
= \frac{\partial}{\partial S} \left( \sum_{l=1}^{m} Z(l, S, R^{(i)}) \frac{\partial}{\partial S} F_1(l, S) \right) \prod_{k=1}^{m} F_1(k, S, R^{(i)}) \bigg|_{l=1}^{m}
\]

\[
= \frac{\partial}{\partial S} \left( \sum_{l=1}^{m} Z(l, S, R^{(i)}) \frac{\partial}{\partial S} F_1(l, S) \right) \prod_{k=1}^{m} F_1(k, S, R^{(i)}) \bigg|_{l=1}^{m}
\]

\[
+ F_1(l, S, R^{(i)}) \sum_{l=1}^{m} Z(l, S, R^{(i)}) \frac{\partial}{\partial S} F_1(l, S) \prod_{k=1}^{m} F_1(k, S, R^{(i)}) \bigg|_{l=1}^{m}
\]

\[
= \sum_{l=1}^{m} Z(l) \left( Z(l) - 1 \right) \frac{\partial}{\partial S} F_1(l, S) \prod_{k=1}^{m} F_1(k, S, R^{(i)}) \bigg|_{l=1}^{m}
\]

\[
+ \frac{\partial}{\partial S} \left( \sum_{l=1}^{m} Z(l, S, R^{(i)}) \frac{\partial}{\partial S} F_1(l, S) \right) \prod_{k=1}^{m} F_1(k, S, R^{(i)}) \bigg|_{l=1}^{m}
\]

\[
\left( \prod_{l=1}^{m} F_1(l, S, R^{(i)}) \right) \bigg|_{l=1}^{m}
\]

\[
= \sum_{l=1}^{m} Z(l) \left( Z(l) - 1 \right) M^{1}(M^{1} + C^{11}(1))
\]

\[
+ Z(l) M^{1} \sum_{b=1}^{h} Z_{b}(n) M^{1} + Z^{1}(n) M^{1} \sum_{b=1}^{h} Z_{b}(n) M^{1}
\]

\[
+ Z(n) (C^{11}(1) - M^{1}) M^{1}
\]

\[
= \sum_{l=1}^{m} \sum_{b=1}^{h} Z(l) Z_{b}(n) M^{1} M^{1} + Z(n) C^{11}(1) - M^{1} M^{1}
\]

\[
(2.23)
\]

Taking the expected value of $\tilde{C}_{ij}(n+1)|_{Z(n)}$ (Eq. (2.23)) removes the dependence of $Z(n)$ and yields

\[
\tilde{C}_{ij}(n+1) = M^{1} M^{1} C_{ij}(n) + \mu_{i}(n) (C^{11}(1) - M^{1} M^{1})
\]

(2.24)

Substituting the relation between $\tilde{C}_{ij}$ and $C_{ij}$ (Eq. (2.22)) simplifies Eq. (2.24) to

\[
\tilde{C}_{ij}(n+1) = M^{1} M^{1} C_{ij}(n) + \mu_{i}(n) \tilde{C}_{ij}(1) - M^{1} M^{1}
\]

(2.25)

where

\[
V_{ij} = E[(Z_{i}(1) - \mu_{i}(1))(Z_{j}(1) - \mu_{j}(1))|\tilde{Z}_{l} = \tilde{Z}]
\]

(2.26)

with $V_{ij}$ being the covariance between the number of new neutrons of type $i$ and type $j$ after one generation given a neutron born of type $l$. It will be referred as the second spatial (central) moment response.

Following a similar but more lengthy derivation (Appendix A), the third order spatial moments can be given as

\[
T_{ijkl}(n+1) = T_{ijkl}(n) M^{1} M^{1} M^{1} + V_{ij} M^{1} M^{1} C_{ij}(n) + V_{ik} M^{1} M^{1} C_{ik}(n) + W_{ijk} M^{1} M^{1} M^{1}
\]

(2.27)

where $W_{ijk}$ is the third spatial (central) moment response to a point source of type $l$:

\[
W_{ijk} = E[(Z_{i}(1) - \mu_{i}(1))(Z_{j}(1) - \mu_{j}(1))(Z_{k}(1) - \mu_{k}(1))|\tilde{Z}_{l} = \tilde{Z}]
\]

(2.28)

2.1.3. Serial moments

To calculate the generation-to-generation correlation, the spatial moments in the form of $E[Z(n)]$, $E[Z(n)Z(n)]$, $E[Z(n)Z(n)Z(n)]$, are not sufficient, the serial-spatial moments in the form of $E[Z(n)Z(n)Z(n)Z(n)]$, are also required. Therefore, the joint moment generating function of $Z(n)$ and $Z(n+k)$ is needed (where $k$ is the generation lag):

\[
F_{n,n+k} (\tilde{F}_{0}, \tilde{S}, \tilde{F}) = E[Z(n)Z(n+k)|\tilde{Z}(0) = \tilde{F}_{0}]
\]

(2.29)

The relation between the moment generating function $F_{n,n+k} (\tilde{F}_{0}, \tilde{S})$ of $Z(n)$ and the joint moment generating function $(F_{n,n+k}(\tilde{F}_{0}, \tilde{S}, \tilde{F}))$ of $Z(n)$ and $Z(n+k)$ can be found:

\[
F_{n,n+k} (\tilde{F}_{0}, \tilde{S}, \tilde{F}) = \sum_{i,q} F_{i,n+k} (\tilde{F}_{0}, \tilde{S}, \tilde{F}) = \tilde{F}_{n+k} (\tilde{F}_{0}, \tilde{S}, \tilde{F})
\]

(2.30)

2.2. Approximating the ACCs

Section 2.1 derived various moments to evaluate the ACCs of an MBP model. This subsection shows the modifications of an MBP model to fit the Monte Carlo power iteration and explicitly writes ACC in term of the spatial and serial moments.

2.2.1. Expansion of fission source distribution

Before specifying the serial-spatial moments to be evaluated from the moment generating functions $F_{n}(\tilde{F}_{0}, \tilde{S})$ and $F_{n,n+k}(\tilde{F}_{0}, \tilde{S}, \tilde{F})$, ACCs must be expressed in the form of such moments. Since the Multitype Branching Processes does not include neutron population normalization, the ACC’s are defined over a normalized fission source distribution $X_{i}(n)$ (defined in Eq. (2.32)), rather than the unnormalized fission source $Z_{i}(n)$.

\[
X_{i}(n) = \frac{Z_{i}(n)}{Z(n)}
\]

(2.32)

The ACC of $X_{i}$ between generation $n$ and $n+k$ is defined in Eq. (2.1).

Taking derivatives of moment generating functions in Eqs. (2.5) and (2.29) gives expectation of products of $Z(n)$ such as $E[Z(n)]$, $E[Z(n)Z(n)]$ and $E[Z(n)Z(n+1)]$. However, to evaluate
the variance and covariance terms in Eq. (2.1), expectations in the form of $\mathbb{E}[X_i(n)]$ and $\mathbb{E}[X_i(n)X_j(n+k)]$ are required.

To perform the transformation, the definition of $X_i(n)$ (Eq. (2.32)) is viewed as a function of $\tilde{Z}(n)$ and expanded around $\mathbb{E}[\tilde{Z}(n)] (\equiv \mu_i(n))$:

$$X_i(n) = g_i(\tilde{Z}(n)) = g_i(\mu_i(n)) + \sum_{i=1}^{m} \frac{\partial g_i(\tilde{Z}(n))}{\partial Z_i(n)} (\tilde{Z}_i(n) - \mu_i(n)) + \frac{\partial^2 g_i(\tilde{Z}(n))}{\partial Z_i(n)\partial Z_j(n)} (\tilde{Z}_i(n) - \mu_i(n))(\tilde{Z}_j(n) - \mu_j(n)) + \cdots$$

(2.33)

where the derivatives of $g_i(\tilde{Z}(n))$ can be calculated explicitly from Eq. (2.32) as

$$\frac{\partial g_i(\tilde{Z}(n))}{\partial Z_i(n)} \bigg|_{\tilde{Z}(n) = \mu_i(n)} = g_i'(n) = \frac{\delta_{ij}}{\mu_i(n)} - \frac{\mu_i(n)}{\mu_i(n)^2} \frac{\partial g_i(\tilde{Z}(n))}{\partial Z_i(n)} \bigg|_{\tilde{Z}(n) = \mu_i(n)}$$

(2.34)

$$\frac{\partial^2 g_i(\tilde{Z}(n))}{\partial Z_i(n)\partial Z_j(n)} \bigg|_{\tilde{Z}(n) = \mu_i(n)} = \frac{\delta_{ij}}{\mu_i(n)^2} + 2 \frac{\mu_i(n)}{\mu_i(n)^3}$$

(2.35)

where $\mu_i(n) \equiv \sum_{i=1}^{m} \mu_i(n)$.

The covariance terms required to evaluate $\rho_{h,k}(X_i)$ (Eq. (2.1)) are of the form $\mathbb{E}[X_i(n)X_j(n+k)]$. Therefore $X_i$ and $X_j$ must preserve terms of the same order following an expansion. $g_i(\tilde{Z}(n))$ (corresponding to $X_i$) and $\tilde{g}_i(\tilde{Z}(n))$ (corresponding to $X_j$) will be expressed explicitly below to obtain consistent expansion orders. Also for simplicity, the dependence on generation $n$ and neutron type $i$ is suppressed and the first and second order derivatives of $g(\tilde{Z}(n))$ evaluated at $\mu_i(n)$ are denoted as $g_i'$ and $g_i''$, respectively.

Eqs. (2.34) and (2.35) show that $g_i'$ is of order $\frac{1}{\mu_i(n)}$, and $g_i''$ is of order $\frac{1}{\mu_i(n)^2}$. And $g_i'$ and $g_i''$ are coefficients of $Z_i - \mu_i \equiv \Delta Z_i$, and $(Z_i - \mu_i)(Z_j - \mu_j) \equiv \Delta Z_i \Delta Z_j$, respectively. Therefore, as long as the system has a large number of $\mu_i(n)$ of expected neutrons, the expansion in Eq. (2.33) is justified. Eq. (2.33) can be conceptually written as Eq. (2.37):

$$g(\tilde{Z}) = g(\mu) + \frac{\Delta \tilde{Z}}{\mu} + \left( \frac{\Delta \tilde{Z}}{\mu} \right)^2 + o(\epsilon^2)$$

(2.37)

where $\epsilon$ denotes $\frac{\Delta \tilde{Z}}{\mu}$. It is worthwhile to note that if a function of $\tilde{Z}(n)$ is defined as

$$h(\tilde{Z}(n)) = \sum_{i=1}^{m} \frac{Z_i(n)}{m}$$

(2.38)

MBP methodology can be applied to analyze correlation and variance underestimate of $k_{eff}$ eigenvalue tallies.

2.2.2. Variance terms

From the expansion of fission source distribution

$$g(\tilde{Z}) = g(\bar{\mu}) + g(\tilde{Z} - \mu) + \frac{1}{2} \sigma^2 \mathbb{E}[\tilde{Z}^2] + o(\epsilon^2)$$

its expectation is given by

$$\mathbb{E}[g(\tilde{Z})] = g(\bar{\mu}) + \frac{1}{2} \sigma^2 \mathbb{E}[\tilde{Z}^2] + o(\epsilon^2).$$

(2.39)

From Eqs. (2.39) and (2.40), an expression for $\text{Var}[g(\tilde{Z})]$ can be obtained

$$\text{Var}[g(\tilde{Z})] = \mathbb{E} \left[ g(\tilde{Z} - \mu)^2 \right] - g(\bar{\mu})^2 = \frac{1}{2} \sigma^4 \mathbb{E}[\tilde{Z}^4] + o(\epsilon^4)$$

(2.41)

Since the lowest order of $g(\tilde{Z}) - \mathbb{E}[g(\tilde{Z})]$ is $O(\epsilon)$, a second order expansion of $g(\tilde{Z})$ is sufficient to provide the third order expansion of $\text{Var}[g(\tilde{Z})]$. Otherwise, third order expansion is required to comprise all third order terms in $\text{Var}[g(\tilde{Z})]$ with the leading constant term in $g(\tilde{Z})$. The third order terms of the form $g_i'\sigma^2(\tilde{Z} - \mu)\mathbb{E}[\tilde{Z}^2\tilde{Z}]$ vanish because $\text{var} = \mu^2$.

Inserting the expansion coefficients (Eqs. (2.34), (2.35)) and spatial moments, (Eq. (2.17)) and restoring the neutron type and generation dependence, the variance can be explicitly expressed as

$$\text{Var}[g_i(\tilde{Z}(n))] = \left( \frac{\delta_{ij}}{\mu_i(n)} - \frac{\mu_i(n)}{\mu_i(n)^2} \right) \mathbb{E}[C_{ij}(\mu_i(n) - \mu_i(n))^2] + \left( \frac{\delta_{ij}}{\mu_i(n)} - \frac{\mu_i(n)}{\mu_i(n)^2} \right)^2 + \frac{\mu_i(n)}{\mu_i(n)^2}$$

(2.42)

2.2.3. Covariance terms

The expansion of $g(\tilde{Z}(n))$ (Eq. (2.39)) and $\mathbb{E}[g(\tilde{Z}(n))]$ (Eq. (2.40)) can also be used to evaluate the covariance terms. Since the dependence on generation is suppressed, $g_i$ and $g_i'$ are used to denote $g(\tilde{Z}(n))$ and $g(\tilde{Z}(n+k))$, $\mu_1, \mu_2, \mu_3$ and $\mu_2$ are introduced similarly.

$$\mathbb{E}[g_i(\tilde{Z}(n))g_j(\tilde{Z}(n+k))] = \mathbb{E} \left[ \left( g_i(\tilde{Z} - \mu_i) + \frac{1}{2} \sigma^2 \mathbb{E}[\tilde{Z}^2] \right) \left( g_j(\tilde{Z} - \mu_j) + \frac{1}{2} \sigma^2 \mathbb{E}[\tilde{Z}^2] \right) + o(\epsilon^2) \right]$$

(2.43)

Inserting the expansion coefficients (Eqs. (2.34), (2.35)) and reintroducing the neutron type and generation dependence, the covariance can be explicitly written as

=$g_i'g_j'\mathbb{E}[\tilde{Z}^2] + \frac{1}{2} \sigma^4 \mathbb{E}[\tilde{Z}^4] + o(\epsilon^4)$
Due to two parts: (1) neutrons from a given cell remain or re-enter another cell enters a given cell at a later generation. The first part is determined by the diagonal elements of the spatial covariance matrix. Contributions from neighboring cells is determined by the off-diagonal elements of the spatial covariance matrix.

After a more lengthy but similar procedure, the third order serial-spatial moments are found as:

\[ \mathbb{E}[Z_n(n)Z_i(n+k)] = \mathbb{E}[Z_n(n)Z_i(n+k)] - \mathbb{E}[Z_n(n)Z_i(n)] \mathbb{E}[Z_i(n+k)] + \mathbb{E}[Z_n(n)] \mathbb{E}[Z_i(n)] \mathbb{E}[Z_i(n+k)] \]  

Similarly, \( \mathcal{C}^\ell_{ij}(n) \) is defined as the same way as \( \mathcal{C}^\ell_{ij}(n) \) except that \( \mathcal{C}^\ell_{ij}(n) \) is a conditional expectation on \( \bar{r}_0 = \bar{c}_0 \).

2.2.4. Auto-correlation \( \rho_{n,k} \) of Coarse tally regions

In realistic simulations, auto-correlation might be needed on discretized regions of different size (e.g. pin vs assembly size tallies in a reaction simulation). To avoid recomputing multiple moments on varying mesh sizes, a condensation process is proposed allowing to evaluate ACCs on coarser meshes. Suppose tally region \( I \) contains phase space cells \( l_1, \ldots, l_i, \ldots \), the number of neutrons in region \( I \) (denoted by \( N_I(n) \)) is the sum of neutrons in the phase space cells, \( Y_I(n) \) is defined in Eq. (2.51).

\[ Y_I(n) = \sum_{i=1}^{n} Z_{A_i}(n) \]  

The covariance terms of tally region \( I \) can be directly written as

\[ \text{Var}[Y_I(n)] = \sum_{i=1}^{n} \text{Cov}[Z_{A_i}(n), Z_{A_j}(n)] \]  

\[ \text{Cov}[Y_I(n), Y_I(n+k)] = \sum_{i=1}^{n} \text{Cov}[Z_{A_i}(n), Z_{A_j}(n+k)] \]  

All the terms on the right hand side of equations in Eq. (2.53) have already been explicitly written in Eq. (2.44). Though Eq. (2.44) only evaluates \( \text{Cov}[Z_{A_i}(n), Z_{A_j}(n+k)] \), it is straightforward to substitute subscripts \( i \) and \( j \) at generation \( n \) with \( I \) and \( J \) at generation \( n+1 \) with \( J \), therefore the condensation process can be easily done.

2.3. Procedure to calculate \( \rho_{n,k} \)

In summary, knowing the spatial moments, serial-spatial moments, evolution equations and expansions of \( X_i(n) \), generation-to-generation correlation coefficients, \( \rho_{n,k}(X_i) \), can be calculated following the steps below:

1. Calculate the spatial moment responses \( M_i^1, V_i^1 \) and \( W_i^1 \) given in Eqs. (2.20), (2.26) and (2.28).
2. Evolve the spatial moments \( \mu_i(n), C_{ij}(n) \) and \( T_{ijk}(n) \) according to Eqs. (2.21), (2.25) and (2.27).
3. Combine the spatial moments of different generations to evaluate the serial-spatial moments according to Eqs. (2.48), (2.49) and (2.50).
4. Condense the covariances of discretized phase space cells into concerned tally regions with Eq. (2.53).
5. Substitute the moments into expansion of \( \text{Var}[Y_I(n)] \) and \( \text{Cov}[Y_I(n), Y_I(n+k)] \) to evaluate \( \rho_{n,k}(Y_I) \).

The above procedure yields \( \rho_{n,k} \) after evolving the MBP for \( n \) generations.
It should be noted that the above procedure starts before performing a full converged simulation. If the moment responses \( M_i^j, V_{ij} \) are affordable with all phase space cells being finely discretized into flat source regions, they can be tallied from fixed source calculation of uniformly sampled neutron sources. Since such a fine mesh can be costly, the moment responses can be tallied from a stationary source on a mesh slightly finer than the tallied quantities. Generation-to-generation correlation of a tally region is captured by the generation-to-generation and spatial correlation among the comprising phase space cells. Prediction should be accurate if the migration distance of neutrons between generations is on the same order or larger than the MBP phase space cells for a given tally region.

Following the above procedure, evolving the constructed MBP model for \( k \) generations gives ACC of generation lag \( k \) and thus correction for variance estimator after \( k \) active generations. In order to predict termination of Monte Carlo simulation to a given user determined variance criterion, very long calculation of MBP is required to evaluate ACC’s up to arbitrary generation lag \( k \). Alternatively, the method of fitting ACC to a sum of exponentially decaying terms can be applied on the ACC’s found from MBP instead of the noisy estimated value as in Miao et al. (2016). With data fitting, the MBP model can be evolved for a fixed number of generations and the fit can be used to predict ACC and variance underestimation to any arbitrary number of generations. Results from MBP also verifies the data fitting method where ACC’s are fitted to a sum of exponentially decaying terms. If ACC’s predicted from MBP are written explicitly, a quadratic form of the response matrices appears, whose dominant eigenvalues are equivalent to the exponential terms used in data fitting.

### 3. Application

#### 3.1. Evaluate spatial moment responses

With the procedure given in Section 2.3, the spatial moment responses are needed to initialize the calculation of ACC’s. Based on their definition, spatial moment responses are just spatial moments except that they specify the starting phase space region and are one generation away from the source. Therefore, these spatial moment responses can be tallied from a single generation of a Monte Carlo simulation. Due to computational cost, it is unreasonable to tally directly higher order spatial moments. For example, the moment response \( V_{ij} \) of second order spatial moments is a third order tensor that depends on three phase space regions and would require many neutrons per generation to accurately resolve. We propose instead to tally the fission-to-absorption probability for each region pair and moments of new neutrons (from fission) for each region and use these to construct the spatial moment responses. The feasibility of constructing the spatial moment responses is limited to cases where only spatial (excluding energy, angle) correlation effects are of concern.

Assuming that the probability of absorption and the number of neutrons born from fission are independent, we can denote the probability that a neutron born at phase space region \( l \) is absorbed at phase space region \( i \) as \( P_{il} \). Defining the random variable \( v_i \) as the number of new neutrons out of absorption at phase space region \( i \), then by definition of \( M_i^j \):

\[
M_i^j = P_{ij}E_{V_i}
\]

As for the second order spatial moment responses, Eq. (2.26) can be rearranged as

\[
V_{ij} = E(Z_iZ_j) - M_i^jM_j^i
\]

Since energy and angle are not considered, new neutrons out of absorption cannot appear at different phase space regions, \( Z_i(1)Z_j(1) = v_i^2\delta_{ij} \) (3.3) Therefore the second order spatial moment responses \( V_{ij} \) can be constructed from fission-to-absorption probabilities and moments of new neutrons from fission as

\[
V_{ij} = P_{ij}v_i^2\delta_{ij} - P_{ij}E_{V_i}E_{V_j}
\]

Although \( V_{ij} \) is a third order tensor, it can be constructed from a matrix \( P_{ij} \) and a vector \( E_{V_i} \). The matrix \( P_{ij} \) and vectors \( E_{V_i} \) and \( E_{V_j} \) can be either computed from the unconverged or converged fission source. If unconverged fission source is used, a fine mesh is needed such that the flat source approximation yields a suitable approximation of the Monte Carlo eigenvalue problem. Under this circumstance, the distribution of fission source does not alter \( P_{ij}, E_{V_i} \) and \( E_{V_j} \). If starting from a converged fission source, \( P_{ij}, E_{V_i} \) and \( E_{V_j} \) can be tallied directly on a mesh as coarse as the tally regions to be analyzed and used to construct an MBP model.

The above construction of spatial moment responses \( M_i^j \) and \( V_{ij} \) are based on the reasonable assumption that the occurrence of branching defines the concept of generation. However, in Monte Carlo simulations, other branching processes like \( (n,xn) \) are treated within a generation (Romano and Forget, 2013). To describe such processes exactly, a more detailed structure of transfer is required which can be shown to require 3 additional matrices and 2 additional vectors. The detailed derivation is given in Appendix B, but results were shown unnecessary for capturing the bulk correlation behavior in nuclear systems and were thus omitted.

#### 3.2. Approximating source normalization

Another difference between the Multitype Branching Processes (MBP) presented previously and realistic Monte Carlo simulations is the normalization of neutron population. This problem can be mitigated by making the corresponding MBP critical. In OpenMC (Romano and Forget, 2013), the number of new neutrons for each fission event is normalized by the estimated \( k_{en} \) to maintain the neutron population near constant with subsequent normalization steps to enforce a constant fission bank. Correspondingly, with the tallied fission-to-absorption matrix \( P_{ij} \) and the expected number of new neutrons for each cell \( E_{V_i} \), a fission matrix can be constructed and the vector \( E_{V_i} \) normalized by the estimated eigenvalue of the fission matrix.

### 4. Results and analysis

The MBP model was implemented in OpenMC and its predictive capability was compared on assembly size tallies using the 2D BEAVRS benchmark (Horelik et al., 2013) at Hot Zero Power conditions. The 2D model is represented by a 10 cm axial slice at mid-height with reflective top and bottom boundary conditions. To serve as a reference for the variance and prediction of ACCs, 300 independent simulations were performed. Each simulation contains 100 inactive generations and 1000 active generations. Each generation tracks \( 4 \times 10^6 \) neutrons. These independent simulations provide a true measure of variance at each generation. To limit the amount of tally data while still exploring the spatial dependency of the predicted quantities, three representative assemblies were selected as shown in Fig. 1. Among the three fuel assemblies selected, one is at the edge, one is at the center and the
last one is in the middle. U235 enrichment of Assembly 1, 2, 3 are 3.1%, 1.6% and 1.6% respectively. The correlation level decreases from the boundary to the center. The MBP model’s transfer matrix \( P_i \) was computed on a quarter-assembly mesh using the first 8 active generations.

4.1. Application of the predicted ACC’s

The predictive capability of the MBP model is shown on three quantities:

- ACCs as function of generation lag: \( \rho_k \)
- Bias of the estimator of sample variance as function of active generations: \( b(N) \)
- Underestimation ratio of the variance of the estimator (tally averaged over active generations) as function of active generations: \( r(N) \)

The underestimation ratio, \( r(N) \), is the ratio between the real variance of the estimator accumulated up to \( N \)th active generation and the variance of the estimator at any generation divided by \( N \).

\[
r(N) = \frac{\sigma^2_{\hat{\lambda}_i}}{\sigma^2_{\hat{\lambda}_i}/N} \quad (4.1)
\]

The relation between the underestimation ratio (\( r(N) \)) and the ACCs is shown in Eq. (4.2) (Miao et al., 2016).

\[
r(N) = 1 + 2 \sum_{k=1}^{N-1} \left( 1 - \frac{k}{N} \right) \rho_k \quad (4.2)
\]

\[
\hat{\rho}_k(l) = \frac{1}{N - K} \sum_{n=1}^{N-K} \sqrt{\frac{s\sum_{p=1}^{s} X^{(o)}_1(n)}{\left( \sum_{p=1}^{s} X^{(o)}_1(n) \right)^2} - \left( \sum_{p=1}^{s} X^{(o)}_1(n) \right)^2 \left( N - k \right)}
\]

However, finding \( r(N) \) is only part of the problem in estimating \( \sigma^2_{\hat{\lambda}_i} \). The ratio \( r(N) \) corrects the convergence rate from 1/\( N \) to \( r(N)/N \), but the leading term \( \sigma^2_{\hat{\lambda}_i} \) is biased from the correlation. Instead of estimating \( \sigma^2_{\hat{\lambda}_i} \) with

\[
\hat{\sigma}^2_{\hat{\lambda}_i} = \frac{1}{N - 1} \sum_{l=1}^{N} (X_l(i) - \bar{X}_i(N))^2 \quad (4.3)
\]

the unbiased estimator is defined as (Miao et al., 2016)

\[
\overline{\hat{\sigma}^2_{\hat{\lambda}_i}} = \frac{1}{N - r(N)} \sum_{l=1}^{N} (X_l(i) - \bar{X}_i(N))^2 \quad (4.4)
\]

where \( r(N) < N \) unless \( \rho(k) = 1 \) for all \( k \). Therefore, a correction term can be defined as

\[
b(N) = \frac{N - 1}{N - r(N)} \quad (4.5)
\]

4.2. Comparing to reference

The above three quantities, \( \rho_k, r(N) \) and \( b(N) \) can be solved analytically using the MBP model and thus used as a prediction for the 2D BEAVRS benchmark. These three quantities can be also estimated directly from the \( s \) independent simulations using the following definitions.

The ACC, \( \rho_{ak} \), can be estimated by first calculating \( \rho_{ak} \) as the Pearson correlation coefficient of the two samples, \( \{X^{(a)}_1(n), \ldots, X^{(a)}_1(n)\} \) and \( \{X^{(a)}_1(n + k), \ldots, X^{(a)}_1(n + k)\} \) and then taking the average of all \( n \)‘s using the fact that \( \rho_{ak} \) is stationary. \( X^{(a)}_1 \) uses the same notation as Section 2 with a superscript (a) to identify the independent simulations from \( a = 1 \) to \( a = s \).

Eq. (4.6) is equivalent to the definition in Eq. (2.1) by simply replacing the expectation operator in Eq. (2.1) with average over the independent simulations:

\[
\hat{\rho}_k(l) = \frac{1}{N - K} \sum_{n=1}^{N-K} \sqrt{\frac{s\sum_{p=1}^{s} X^{(o)}_1(n)X^{(o)}_1(n + k) - \sum_{p=2}^{s} X^{(o)}_1(n)\sum_{p=2}^{s} X^{(o)}_1(n + k)}{s\sum_{p=1}^{s} X^{(o)}_1(n)^2 - \left( \sum_{p=1}^{s} X^{(o)}_1(n) \right)^2}} \quad (4.6)
\]

where \( l \) denotes the location, \( s \) denotes the number of simulations, \( n \) denotes the number of generations in each of the \( s \) simulations. The outermost sum exploits the stationary feature of correlation coefficients and averages over the \( N - k \) active generations.
The reference of \( r(N) \) can be obtained by calculating \( \text{Var}[X_i(N)] \) directly. For any generation \( N \), each of the \( s \) independent simulations gives an estimate of \( X_i(N) \). The variance of the \( s \) of them is an estimate of \( \text{Var}[X_i(N)] \) and is denoted as \( \text{Var}[X_i(N)] \).

\[
\text{Var}[X_i(N)] = \frac{1}{s} \sum_{n=0}^{s-1} \left( X_i^{(n)}(N) - \left( \sum_{n=1}^{s} X_i^{(n)}(N) \right) / s \right)^2
\]

\( \text{(4.7)} \)

Eq. (4.7) forms a sample of \( X_i(N) \) from each independent simulation \( a \) and then calculates the variance over the \( s \) independent simulations. Since the \( s \) simulations are independent, \( \text{Var}[X_i(N)] \) estimated by Eq. (4.7) is not underestimated. To view the convergence rate, predicted \( \frac{\Delta_{\text{MC}}}{\Delta} \) will be compared with \( \frac{\Delta_{\text{MC}}}{\Delta} \) calculated from \( \text{Var}[X_i(N)] \).

\[
\frac{\Delta_{\text{MC}}}{\Delta} = \frac{\text{Var}[X_i(N)]}{\text{Var}[X_i(1)]}
\]

Similarly, the reference of \( b(N) \) can be obtained by estimating \( \text{Var}[X_j] \) directly.

\[
\text{Var}[X_j] = \frac{1}{N} \sum_{n=1}^{N} \sum_{n=1}^{s} \left( X_j^{(n)}(n) - \left( \sum_{n=1}^{s} X_j^{(n)}(n) \right) / s \right)^2
\]

\( \text{(4.9)} \)

The ratio between the variance calculated from Eq. (4.9) and the variance calculated from Eq. (4.3) is the reference expression for \( b(N) \).

\[
\frac{b(N)}{b_0} = \frac{\frac{1}{s} \sum_{n=1}^{s} \left( X_j^{(n)}(n) - \left( \sum_{n=1}^{s} X_j^{(n)}(n) \right) / s \right)^2}{\frac{1}{s} \sum_{n=1}^{s} \left( X_j^{(n)}(n) - \left( \sum_{n=1}^{s} X_j^{(n)}(n) \right) / s \right)^2}
\]

\( \text{(4.10)} \)

4.2.1. ACC prediction

The predicted and reference ACCs for the three assemblies as a function of the generation lag are shown in Fig. 2. The fitted to prediction ACCs are also given. To show the stability of the MBP methodology, the prediction is performed for each of the 300 independent simulations. In Fig. 2, the black curves correspond to average of the 300 independent predictions, the black shaded regions correspond to one standard deviation of the 300 predictions, the green curves correspond to average of the 300 independent ACC fittings, the green shaded regions correspond to one standard deviation of the 300 ACC fittings. The fitted ACC curve agrees well with the predicted values as expected from the analysis in Section 2.3. The deviation of the predicted curves is negligible, which implies that estimation of the moments \( M_l \) and \( V_{ij} \) from first 8 active generations is accurate enough to capture the ACC of the system. The greater deviation of the fitted curves is due to the instability of data fitting to sum of exponential terms (Acton, 1990).

4.2.2. Underestimation ratio prediction

The ACCs are then used to correct the underestimation ratio. The real convergence rates from independent simulations according to Eq. (4.7) are shown in Fig. 3 with the convergence rates predicted from the MBP model and from the fitted ACC of MBP. As mentioned in Section 4.2, \( \text{Var}[X_i(N)] \) is renormalized to give \( r(N) / N \) (Eq. (4.8)). In the peripheral assembly with the highest correlation level among the three, real variance deviates from 1/N by a factor of 7. In the central assembly with lowest correlation level, this factor is around 4.

4.2.3. Variance bias prediction

The impact of the correlation coefficients on bias of the estimator of \( \text{Var}[X_i(N)] \) is shown in Fig. 4. In the peripheral assembly with high correlation, the variance for each generation is underestimated by a factor of 2 if 10 active generations are simulated for statistics. In the central assembly with lower correlation, the factor is around 1.6. In comparison with the deviation from 1/N, which remains constant asymptotically, the underestimation of leading variance becomes negligible as more active generations are simulated.

Fig. 5 plots the variance after incorporating both correction from bias ratio and underestimation of 1/N.

4.3. Cost of the prediction method

Theoretical predictions above are based a MBP model (resulting from discretizing the BEAVRS 2D benchmark into \( m = 34 \times 34 = 1156 \) cells) and the second order expansion of fission source distributions (Section 2.2.1). The 1156 cells are actually quarter-assembly cells because a 17 discretization exactly matches the boundary of assemblies (Fig. 1). To perform the second order calculation, moment responses \( M_l \) and \( V_{ij} \) and moments \( \mu_l(n), \mu_l(k) \) and \( C_{ij}(n) \) are needed. \( M_l \) and \( V_{ij} \) can be constructed from the fission to absorption matrix \( (P)^i \) and first \( (E)^j \) and second \( (E)^{1/2} \) order moments of \( v_i \), where \( v_i \) is the number of neutrons born from absorption in phase space region \( i \). The quantities \( P_i, (E)^j \) and \( (E)^{1/2} \) are tallied during the first few active generations. These correspond to one \( m \times m \) matrix and two length \( m \) vectors, respectively. \( M_l \) and \( V_{ij} \) are used to find the stationary distribution of \( \mu_l(n) \) and spatial covariance \( C_{ij}(n) \).

Then \( M_l \) is used to evolve the first order point response moment \( \mu_l(k) \) with \( \mu_l(0) = \delta_l^k \). According to Eqs. (2.53) and (2.44), \( \mu_l(n), C_{ij}(n) \) and \( \mu_l(k) \) are sufficient to evaluate \( p_{h_{nl}}(X_i) \).

Fig. 2. Predicted and Reference ACC for the three selected assemblies. The black curves correspond to average of the 300 predictions. The black shaded regions correspond to one standard deviation of the 300 predictions. The green curves correspond to average of the 300 fittings. The green shaded regions correspond to one standard deviation of the 300 fittings. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this article.)
To provide a better variance estimate, $r(N)$ rather than $\rho(k)$ is required for each tally region. According to Eq. (4.2), two accumulated summation of $\text{ACC}'s$ for each tally region should be maintained:

$$P_{N/C0}^{1k} = q_k$$

and

$$P_{N/C0}^{1k} = q_k(X_i)$$

thus needing to store two vectors of length $m$. In total, the minimal memory requirement of a second order MBP calculation is four $m$ length vectors $(M_l, C_{ij}(l), \mu_l^i(k))$ and three $m \times m$ matrices $(M_l, C_{ij}(l), \mu_l^i(k))$. For the BEAVRS 2D benchmark discretized to $34 \times 34 = 1156$ cells with all matrix element represented as double precision numbers, the memory requirements are approximately 30 MB.

However, once the $\text{ACC}'s$ for each tally region have been calculated for enough MBP generations ($\approx 100$) to perform exponential fitting, only $2 \sim 3$ coefficients per tally are needed to provide a better variance estimate.

5. Conclusion

This work proposes an approach for predicting the underestimation of variance often seen in full core nuclear reactor simulations prior to performing a detailed simulation. Knowing this underestimation will allow for more efficient simulations with truly quantifiable error estimates and stopping criteria. By discretizing the phase space, the Multitype Branching Process was used to explicitly write the spatial and temporal moments which were then related to the auto-correlation coefficients. The discretization process introduces an approximation of the true transport process that can be used to efficiently approximate the variance. The discretization must be finer than the tally regions of interest. The more stationary the fission source used to compute the moments, the coarser the MBP mesh can be.
Numerical results compared to 300 independent simulations have shown to accurately predict assembly auto-correlation coefficients and variance estimates in various spatial location of the 2D full core PWR BEAVRS benchmark. This paper used a mesh 4-times finer than the assembly-sized tally regions needed for the MBP process with moments computed in the first 8 active batches. MBP tallies were performed to compute the fission to absorption matrix and moments of $v_i$ (new neutrons produced from an absorption site at each phase space cells). Evolution of the MBP model by moment responses $M$ and $V$ can be related to the ACCs for any coarser tally region at any generation lag. For efficiency, the ACCs can be exponentially fitted using 2 ~ 3 parameters which can then be used in calculating the variance underestimation. This predictive capability can help us calculate the number of active generations needed to achieve a target variance.

Presently, the prediction method requires memory $\propto m^2$, where $m$ measures the fineness of the discretized mesh on which MBP is applied. Future work will investigate further approximations that can be made to reduce memory requirement and identify ways of using the moment estimates to de-correlate the fission bank and reduce the variance.

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**Appendix A. Derivation of third order spatial moments**

This section derives Eq. (2.27). Third order derivatives of the moment generating function will provide the third order factorial moments, $\tilde{T}_{kij}(n)$, which can eventually be related to $T_{ij}(n)$ through Eq. (A.1).

$$
\tilde{T}_{kij}(n) = \frac{\partial^3}{\partial x_i \partial y_j \partial z_k} F_k(\bar{0}, \bar{\sigma})
$$

$$= E[Z_k(n)Z_j(n)Z_i(n) - Z_k(n)Z_i(n)\delta_{ij} - Z_i(n)Z_j(n)\delta_{ik} - Z_j(n)Z_i(n)\delta_{ik} + 2\mu_k(n)\delta_{ij}\delta_{ik}]
$$

(A.1)

$\tilde{T}_{kij}(n+1)$ is first evaluated conditional on $\tilde{Z}(n)$ and then expressed as a function of $\tilde{T}_{kij}(n)$. The conditional expectation is evaluated as,
Evaluating Eq. (A.2) at $\tilde{s} = \tilde{t}$, the moment generating functions become 1, the derivates become factorial moments.

\[
\tilde{T}_{k_i,j}(n + 1)|_{\tilde{s} = \tilde{t}} = \sum_{l=1}^{m} \left( Z_l(n)(Z_l(n) - 1)(Z_l(n) - 2)M_{k_l}^2M_{j_l}^2 + Z_l(n)Z_l(n) - 1 \right) \left( \tilde{C}_{k_l,j_l}(1)M_{k_l}^1 + M_{k_l}^2\tilde{C}_{k_l,j_l}(1) + M_{j_l}^2\tilde{C}_{k_l,j_l}(1) \right) + Z_l(n)\tilde{T}_{k_i,j}(1) \\
+ \sum_{l=1}^{m} \left( Z_l(n)(Z_l(n) - 2)M_{k_l}^1M_{j_l}^1 + Z_l(n)Z_l(n) - 1 \right) \times \sum_{s=l}^{m} Z_s(n)M_{s}^0 + \sum_{l=1}^{m} \left( Z_l(n)(Z_l(n) - 1)M_{k_l}^1M_{j_l}^1 + Z_l(n)Z_l(n) - 1 \right) \times \sum_{s=l}^{m} Z_s(n)M_{s}^0 \\
+ \sum_{l=1}^{m} Z_l(n)M_{k_l}^1 \times \sum_{s=l}^{m} \left[ Z_s(n)(Z_s(n) - 1)M_{k_s}^0\tilde{C}_{k_s,j_s}(1) + Z_s(n)\tilde{C}_{k_s,j_s}(1) + Z_s(n)M_{s}^0 \sum_{g=l} Z_g(n)M_{g}^0 \right] \\
= \sum_{l=1}^{m} \left( Z_l(n)(Z_l(n) - 1)(Z_l(n) - 2)M_{k_l}^2M_{j_l}^2 + Z_l(n)Z_l(n) - 1 \right) \left( \tilde{C}_{k_l,j_l}(1)M_{k_l}^1 + M_{k_l}^2\tilde{C}_{k_l,j_l}(1) + M_{j_l}^2\tilde{C}_{k_l,j_l}(1) \right) + Z_l(n)\tilde{T}_{k_i,j}(1) \\
+ \sum_{l=1}^{m} \left( Z_l(n)(Z_l(n) - 2)M_{k_l}^1M_{j_l}^1 + Z_l(n)Z_l(n) - 1 \right) \times \sum_{s=l}^{m} Z_s(n)M_{s}^0 + \sum_{l=1}^{m} \left( Z_l(n)(Z_l(n) - 1)M_{k_l}^1M_{j_l}^1 + Z_l(n)Z_l(n) - 1 \right) \times \sum_{s=l}^{m} Z_s(n)M_{s}^0 \\
+ \sum_{l=1}^{m} \left( Z_l(n)(Z_l(n) - 1)M_{k_l}^1 + Z_l(n)Z_l(n) - 1 \right) \times \sum_{s=l}^{m} Z_s(n)M_{s}^0 + \sum_{l=1}^{m} Z_l(n)M_{k_l}^1 \times \sum_{s=l}^{m} Z_s(n)M_{s}^0 \sum_{g=l} Z_g(n)M_{g}^0 \right] \\
\tag{A.3}
\]

Denote the 1st term, the 2nd to 4th terms and the last term in Eq. (A.3) as $T_1, T_2$ and $T_3$ respectively for simplification in the following derivations. $T_1$ can be simplified as Eq. (A.4).

\[
T_3 = \sum_{l=1}^{m} \left( Z_l(n)M_{l}^0\tilde{Z}_l(n)M_{k_l}^0\tilde{Z}_l(n)M_{j_l}^0 \right) \\
\tag{A.4}
\]

$T_1$ can be simplified as Eq. (A.5).

\[
T_1 = \sum_{l=1}^{m} Z_l(n) \times \left[ (Z_l(n) - 1)(Z_l(n) - 2)M_{k_l}^2M_{j_l}^2 + Z_l(n) - 1 \right] \times \left( \tilde{C}_{k_l,j_l}(1)M_{k_l}^1 + M_{k_l}^2\tilde{C}_{k_l,j_l}(1) + M_{j_l}^2\tilde{C}_{k_l,j_l}(1) \right) + \tilde{T}_{k_i,j}(1) \\
= \sum_{l=1}^{m} Z_l(n) \times \left[ (Z_l(n)^2 - 3Z_l(n))M_{k_l}^0M_{j_l}^0 \right] + Z_l(n) \left( \tilde{C}_{k_l,j_l}(1)M_{k_l}^1 + M_{k_l}^2\tilde{C}_{k_l,j_l}(1) + M_{j_l}^2\tilde{C}_{k_l,j_l}(1) \right) + 2M_{k_l}^1M_{j_l}^1 - \tilde{C}_{k_l,j_l}(1)M_{k_l}^1M_{j_l}^1 + \tilde{T}_{k_i,j}(1) \\
\tag{A.5}
\]

The third spatial (central) moment response to a point source of type $l$ (defined in Eq. (2.28)) can be expanded as Eq. (A.6).

\[
\tilde{W}_{k_i,j} = \tilde{E}(Z_1(n)Z_1(1)\tilde{Z}_1(n)\tilde{Z}_1(1)|\tilde{f}_0 = \tilde{e}_l) + 2\tilde{E}(Z_1(1)\tilde{Z}_1(1)|\tilde{f}_0 = \tilde{e}_l)\tilde{E}(Z_1(1)|\tilde{f}_0 = \tilde{e}_l) \\
\times \tilde{E}(Z_1(1)Z_1(1)|\tilde{f}_0 = \tilde{e}_l) - \tilde{E}(Z_1(1)|\tilde{f}_0 = \tilde{e}_l)\tilde{E}(Z_1(1)|\tilde{f}_0 = \tilde{e}_l) \\
- \tilde{E}(Z_1(1)|\tilde{f}_0 = \tilde{e}_l)\tilde{E}(Z_1(1)|\tilde{f}_0 = \tilde{e}_l) \\
- \tilde{E}(Z_1(1)|\tilde{f}_0 = \tilde{e}_l)\tilde{E}(Z_1(1)|\tilde{f}_0 = \tilde{e}_l) \\
= \tilde{T}_{k_i,j}(1) + 2M_{k_l}^1M_{j_l}^1 - \tilde{C}_{k_l,j_l}(1)M_{k_l}^1 - \tilde{C}_{k_l,j_l}(1)M_{j_l}^1 \tag{A.6}
\]

The third factorial moment response to a point source of type $l$ can be defined by replacing the moments in Eq. (A.6) with factorial moments.

\[
\tilde{W}_{k_i,j} = \tilde{T}_{k_i,j}(1) + 2M_{k_l}^1M_{j_l}^1 - \tilde{C}_{k_l,j_l}(1)M_{k_l}^1 - \tilde{C}_{k_l,j_l}(1)M_{j_l}^1 \tag{A.7}
\]

$\tilde{W}_{k_i,j}$ defined in Eq. (A.7) simplifies $T_1$ to

\[
T_1 = \sum_{l=1}^{m} \left( Z_l(n)(Z_l(n) - 3)M_{k_l}^1M_{j_l}^1 + \tilde{C}_{k_l,j_l}(1)M_{k_l}^1 + M_{j_l}^2\tilde{C}_{k_l,j_l}(1) \right) + \tilde{W}_{k_i,j} \tag{A.8}
\]

For simplification, the three terms in $T_2$ are defined as $T_{2,1}, T_{2,2}, T_{2,3}$, $T_{2,1}$ is simplified in Eq. (A.9).

\[
T_{2,1} = \sum_{l=1}^{m} Z_l(n) \left( \tilde{C}_{k_l,j_l}(1)M_{k_l}^1 + M_{j_l}^2\tilde{C}_{k_l,j_l}(1) + 2M_{k_l}^1M_{j_l}^1 - \tilde{C}_{k_l,j_l}(1)M_{k_l}^1M_{j_l}^1 \right) \times \sum_{s=l}^{m} Z_s(n)M_{s}^0 \\
= \sum_{l=1}^{m} Z_l(n) \left( \tilde{V}_{k_l,j_l}(1)M_{k_l}^1 + Z_l(n)M_{j_l}^1 \right) \times \sum_{s=l}^{m} Z_s(n)M_{s}^0 \\
= \sum_{l=1}^{m} Z_l(n) \left( \tilde{V}_{k_l,j_l}(1)Z_l(n)M_{j_l}^1 \right) \times Z_l(n)M_{j_l}^1 \\
= \sum_{l=1}^{m} Z_l(n) \left( \tilde{V}_{k_l,j_l}(1)Z_l(n)M_{j_l}^1 \right) \times Z_l(n)M_{j_l}^1 \tag{A.9}
\]

Simplifying $T_{2,2}$ and $T_{2,3}$ in the same way and combining them to $T_2$ lead to

\[
T_2 = \sum_{l=1}^{m} Z_l(n)Z_l(n) \left( \tilde{V}_{k_l,j_l}(1)Z_l(n)M_{j_l}^1 + \tilde{V}_{k_l,j_l}(1)M_{j_l}^1 \right) \\
+ Z_l(n)^2Z_l(n) \left( M_{k_l}^1M_{j_l}^1 + M_{k_l}^1M_{j_l}^1 + M_{j_l}^2M_{j_l}^1 \right) \tag{A.10}
\]

where $\tilde{V}_{k_l,j_l}$ is defined in a similar way to $\tilde{W}_{k_i,j}$ by replacing moments in Eq. (2.26) with factorial moments.

\[
\tilde{V}_{k_l,j_l} = \tilde{C}_{k_l,j_l}(1) - M_{k_l}^1 \tag{A.11}
\]
Combining $T_1$ (Eq. (A.8)), $T_2$ (Eq. (A.10)) and $T_3$ (Eq. (A.4)) simplifies $\tilde{T}_{kji}(n+1)$ (Eq. (A.3)) to Eq. (A.12)

$$
\tilde{T}_{kji}(n+1)
= 
\sum_{l=1}^{m} Z_l(n) W_{kji}^l + Z_l(n)^2 M_l^j M_l^i M_i^j
- 3Z_l(n)^2 M_l^j M_l^i M_i^j
+ \sum_{l=1}^{m} Z_l(n) Z_l(n) \left( \bar{V}_{ji} M_i^j + \bar{V}_{ki} M_k^i + \bar{V}_{ij} \right)
+ \sum_{l=1}^{m} Z_l(n) Z_l(n) \left( \bar{V}_{ij}^l M_i^j + \bar{V}_{ki} M_k^i + \bar{V}_{ij} M_i^j \right)
+ \sum_{l=1}^{m} Z_l(n) M_l^j Z_l(n) \left( \bar{V}_{ji} M_i^j + \bar{V}_{ki} M_k^i + \bar{V}_{ij} \right)
+ \sum_{l=1}^{m} Z_l(n) M_l^j Z_l(n) \left( \bar{V}_{ij}^l M_i^j + \bar{V}_{ki} M_k^i + \bar{V}_{ij} \right)
$$

(A.12)

Denote the sum of terms in the form of $Z^1M^i$ in Eq. (A.12) as $T_{z1}$.

$$
T_{z1} = 
\sum_{l=1}^{m} Z_l(n)^2 M_l^j M_l^i M_i^j
+ \sum_{l=1}^{m} Z_l(n) M_l^j Z_l(n) M_l^i Z_l(n) M_i^j
+ \sum_{l=1}^{m} Z_l(n) Z_l(n) M_l^j M_l^i M_i^j
$$

(A.13)

Denote the sum of terms in the form of $Z^2M^i$ or $Z^2M^j$ in Eq. (A.12) as $T_{z2}$.

$$
T_{z2} = 
\sum_{l=1}^{m} Z_l(n)^2 \left( \bar{C}_{ij}(1) M_i^j + \bar{C}_{ji}(1) M_j^i \right)
- 3Z_l(n)^2 M_l^j M_l^i M_i^j
+ \sum_{l=1}^{m} Z_l(n) \left( \bar{C}_{ij}(1) M_i^j - M_l^j M_l^i M_l^i \right)
+ \sum_{l=1}^{m} Z_l(n)^2 \left( \bar{V}_{ij}^l M_i^j + \bar{V}_{ki} M_k^i + \bar{V}_{ij} \right)
$$

(A.14)

where the last line uses the definition of $\bar{V}_{ij}$ in Eq. (A.11). Denote the sum of $T_{z2}$ (Eq. (A.14)) and terms in the form of $Z^2VM$ in Eq. (A.12) as $T_{z2}$.

$$
T_{z2} = 
\sum_{l=1}^{m} Z_l(n)^2 \left( M_l^j \bar{V}_{ij} + M_l^i \bar{V}_{ki} + M_l^i \bar{V}_{ij} \right)
+ \sum_{l=1}^{m} Z_l(n) Z_l(n) \left( \bar{V}_{ij} M_i^j + \bar{V}_{ki} M_k^i + \bar{V}_{ij} M_i^j \right)
+ \sum_{l=1}^{m} Z_l(n) M_l^j Z_l(n) \left( \bar{V}_{ij} M_i^j + \bar{V}_{ki} M_k^i + \bar{V}_{ij} M_i^j \right)
$$

(A.15)

$$
T_{z2} = T_{z1} + T_{z2}
$$

Then taking the expected value of $\tilde{T}_{kji}(n+1)|Z(n)$ removes the dependence of $\bar{Z}(n)$ and yields

$$
\tilde{T}_{kji}(n+1) = T_{lkh}(n) M_l^j M_l^i M_l^j
+ C_{ij}(n) \left( \bar{V}_{ij} M_i^j + \bar{V}_{ki} M_k^i + \bar{V}_{ij} M_i^j \right)
+ \mu_l(n) \bar{W}_{kji}^l
$$

(A.17)

Substituting the relation between $\tilde{T}_{kji}$ and $T_{kji}$ (Eq. (A.1)) simplifies Eqs. (A.17) to (2.27).

Appendix B. Branching processes within generations

To treat the $(n, xn)$ processes accurately, instead of one fission-to-absorption probability matrix, four matrices are needed.

1. $P_{ij}^n$: the probability of a neutron born from fission at region $i$ to being absorbed at region $i$
2. $Q_{ij}^n$: the probability of a neutron born from fission at region $i$ to inducing a $(n, xn)$ reaction at region $i$
3. $P_{ij}^n$: the probability of a neutron born from $(n, xn)$ at region $i$ to being absorbed at region $i$
4. $Q_{ij}^n$: the probability of a neutron born from $(n, xn)$ at region $i$ to inducing a $(n, xn)$ reaction at region $i$

Similarly, rather than one random variable $v$, moments of two random variables are needed.

1. $v_i$: number of fissioned neutrons from absorption at phase space region $i$, for simplicity, the moments of $v_i$ are denoted as below

$$
\mathbb{E} v_i = \lambda_i
$$

(B.1)

2. $\zeta_i$: number of new neutrons out of $(n, xn)$ at phase space region $i$, $\zeta_i \geq 2$, for simplicity, the moments of $\zeta_i$ are denoted as below

$$
\mathbb{E} \zeta_i = \zeta_i
$$

(B.2)

Similarly to the case without $(n, xn)$ processes discussed above, all the transport processes $P_f, Q_f, P_s, Q_s$ and the branching processes $v, \zeta$ are assumed to be independent of each other. In other
words, $v_i$ and $\zeta_i$ is assumed to be function of phase space region $i$ only (not dependent on whether the incoming neutron is born from fission or $(n,xn)$). Therefore, the expectation of the composite processes can be expressed as the product of the expectation of each process.

1st order moment response $M_i^l$

The lowest order component of $M_i^l$ corresponds to the process where a neutron is born at cell $i$ and finally fissioned at cell $i$ without any $(n,xn)$ processes in between. The expected number of new neutrons would be

$$M_i^{l(0)} = P_{l,i}^i$$

(B.3)

The next order component would come from the process where a neutron is born at cell $i$, then encounter $(n,xn)$ reaction at cell $j$, and finally fissioned at cell $i$. Since it is assumed branching and transport are independent and the neutrons out of $(n,xn)$ behave independently, the expected number of new neutrons of this process would be

$$M_i^{l(1)} = Q_j^i P_{l,j}^i + \zeta_i^l$$

(B.4)

The above process continues with infinitely higher order terms and can be conveniently written in matrix forms. Denote the moments of new neutrons from absorption and $(n,xn)$ in the diagonal of matrices $\Lambda$ and $X$ respectively.

$$\Lambda_{ij} = \delta_{ij} \delta_i$$

(B.5)

$$X_{ij} = \delta_{ij} \delta_i$$

(B.6)

$$\Lambda_{ij} = \sigma_i^2 \delta_i$$

(B.7)

Then, the moment response $M$ can be expressed as the series

$$M = M_0^l + M_1^l + M_2^l + \cdots$$

$$\equiv P_l \Lambda + Q_l X P_l \Lambda + Q_l X Q_l X P_l \Lambda + \cdots$$

(B.8)

$$= P_l \Lambda + Q_l X (P_l \Lambda + Q_l X (P_l \Lambda + Q_l X (\ldots )))$$

$$= P_l \Lambda + Q_l X (1 + Q_l X + (Q_l X)^2 + \cdots ) P_l \Lambda$$

The series of $Q_l X$ must converge and thus sums to $(1 - Q_l X)^{-1}$. Therefore the infinite contributions of $M$ sum to

$$M = P_l \Lambda + Q_l X (1 - Q_l X)^{-1} P_l \Lambda$$

(B.9)

2nd order moment response $V_{ij}^l$

By Eq. (3.2), the undetermined part of $V_{ij}^l$ so far is $\zeta_i^l \Lambda (1,1)$.

The lowest order contribution of $V_{ij}^l$ come from the neutrons that were born at phase space cell $i$ and fissioned into $i,j$ without $(n,xn)$ processes in between.

$$V_{ij}^{l(0)} = P_{l,i}^i \sigma_i^2 \delta_i$$

(B.10)

Higher order terms result from $(n,xn)$ neutrons. Define the number of fissioned neutrons at phase space cell $i$ induced by the $j^{th}$ neutron among the $\zeta_i$ neutrons out of the $(n,xn)$ reaction at phase space cell $k$ as $\rho_{k,j}^i$. Then contribution from $(n,xn)$ neutrons in $V_{ij}^l$ can be written as

$$V_{ij}^{l(1)} = Q_{ij}^k \sum_{j=1}^{\zeta_i^l} \rho_{k,j}^i$$

(B.11)

The expectation part can be solved following the processes below

$$D_{ij}^l \equiv E \left( \sum_{j=1}^{\zeta_i^l} \rho_{k,j}^i \rho_{k,j}^i + \sum_{j=1}^{\zeta_i^l} \rho_{k,j}^i \rho_{k,j}^i \right)$$

$$= E \left( \zeta_i^l \rho_{k,j}^i \rho_{k,j}^i \right) + E \left( \zeta_i^l \rho_{k,j}^i \rho_{k,j}^i - \rho_{k,j}^i \rho_{k,j}^i \right)$$

$$= E \left( \zeta_i^l \rho_{k,j}^i \rho_{k,j}^i \right) + E \left( \zeta_i^l \rho_{k,j}^i \rho_{k,j}^i - \rho_{k,j}^i \rho_{k,j}^i \right)$$

(B.12)

where the $\zeta_i^l$ neutrons out of a $(n,xn)$ react are assumed to behave independently. For simplicity of below equations, expectations in Eq. (B.12) are denoted as

$$R_{ij}^l \equiv \rho_{k,j}^i \rho_{k,j}^i$$

(B.13)

$$F_{ij}^l \equiv \rho_{k,j}^i \rho_{k,j}^i$$

(B.14)

$$G_{ij}^l \equiv \chi_j^l F_{ij}^l$$

(B.15)

$$S_{ij}^l \equiv \tau^2 R_{ij}^l$$

(B.16)

$$D_{ij}^l \equiv R_{ij}^l + S_{ij}^l$$

(B.17)

The first order moment response of $(n,xn)$ reaction denoted as $R_{ij}^l$ (Eq. (B.13)) can be solved the same way as the above analysis for $M_i^l$ and turned out to be in a very similar form.

$$R = (1 - Q_l X)^{-1} P_l \Lambda$$

(B.18)

The second order moment response of $(n,xn)$ reaction denoted as $F_{ij}^l$ (Eq. (B.14)) can be solved recursively. Similarly to $V_{ij}^l$, decompose $F_{ij}^l$ into zeroth order contributions (neutrons out of $(n,xn)$ were absorbed before any $(n,xn)$ reactions) and high order terms (neutrons out of $(n,xn)$ were absorbed after some $(n,xn)$ reactions).

$$F_{ij}^l = P_{l,j}\sigma_i^2 \delta_i + Q_{ij}^k \sum_{j=1}^{\zeta_i^l} \rho_{k,j}^i$$

$$= P_{l,j}\sigma_i^2 \delta_i + Q_{ij}^k \chi_j^l D_{ij}^l$$

(B.19)

Plugging the solution of $D_{ij}^l$ in the form of $F_{ij}^l$ (Eq. (B.12)) into the above equation gives another equation where $F_{ij}^l$ is the only unknown term.

$$F_{ij}^l = P_{l,j}\sigma_i^2 \delta_i + Q_{ij}^k \chi_j^l D_{ij}^l$$

(B.20)

which can be easily converted to an equation of $D_{ij}^l$

$$D_{ij}^l = P_{l,j}\chi_j^l \sigma_i^2 \delta_i + S_{ij}^l + Q_{ij}^k \chi_j^l D_{ij}^l$$

(B.21)

and $D_{ij}^l$ is solved as

$$D_{ij}^l = \left( (1 - Q_l X)^{-1} \right) (P_{l,j}\chi_j^l \sigma_i^2 \delta_i + S_{ij}^l)$$

(B.22)

In summary, the 2nd order moment response $V_{ij}^l$ is found as

$$V_{ij}^l = V_{ij}^{l(0)} + V_{ij}^{l(1)} - M_i^l M_i^l$$

(V = $P_l \Lambda + Q_l (1 - Q_l X)^{-1} (P_l X \Lambda + S_l) - M_i^l M_i^l$)

(B.23)

where four types of tensor production are implied

$$\left( AB \right)_{ij}^l \equiv A_{ij}^l B_{ij}^l$$

(B.24)

$$\left( A + B \right)_{ij}^l \equiv A_{ij}^l + B_{ij}^l$$

(B.25)

$$\left( A \cdot B \right)_{ij}^l \equiv A_{ij}^l B_{ij}^l$$

(B.26)

$$\left( A \cdot B \right)_{ij}^l \equiv A_{ij}^l B_{ij}^l$$

(B.27)
References


