Annals of Nuclear Energy 112 (2018) 307–321

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

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

Jilang Miao *, Benoit Forget, Kord Smith

Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, MA 02139, United States

ARTICLE INFO

Article history:
Received 20 July 2017
Received in revised form 2 October 2017
Accepted 6 October 2017

Keywords:
Monte Carlo
Auto-correlation prediction
Variance estimate
Multitype Branching Processes

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 betwen 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

* Corresponding author.
E-mail addresses: jlmiao@mit.edu (J. Miao), bforget@mit.edu (B. Forget), kord@mit.edu (K. Smith).

https://doi.org/10.1016/j.anucene.2017.10.014
0306-4549/

estimated after approximately $5000 \sim 10000$ 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 auto-correlation of active generation tallies from multitype branching processes. In Section 2.1, a resursive 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 auto-correlation 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 $\bar{X}_l(N) = \sum_{n=1}^{N} X_l(N)/N$ and $\sigma^2_{X_l}/N$ as an approximation of $\sigma^2_{\bar{X}_l(N)}$. Due to the correlation between generations in the power iteration process, $\sigma_{X_l}/\sqrt{N}$ underestimates $\sigma_{\bar{X}_l(N)}$. The $Cov[X_l(i), X_l(j)]$, 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

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

The theory of MBP model is developed to predict the *auto-correlation 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 $\vec{Z}(n)$ (Eq. (2.2)). The lth 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.

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

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

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

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

$$\vec{Z}(n) = \sum_{i=1}^{m} \sum_{j=1}^{Z_i(n-1)} \vec{Y}_{ij}, \tag{2.4}$$

where $\vec{Y}_{ij}$ is the state vector generated by the j^{th} neutron of type i at generation $n-1$.

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

$$\begin{aligned} F_n(\vec{r}_0, \vec{s}) &\equiv \mathbb{E}\left[\prod_{i=1}^{m} s_i^{Z_i(n)} \middle| \vec{Z}(0) = \vec{r}_0\right] \\ &= \sum_{\vec{r}} \mathbb{P}\left(\vec{Z}(n) = \vec{r} \middle| \vec{Z}(0) = \vec{r}_0\right) \prod_{i=1}^{m} s_i^{r_i}, \end{aligned} \tag{2.5}$$

where $\vec{r}_0$ denotes the initial configuration of neutrons in the discretized phase space and $\vec{s}$ is the argument of the moment generating function. If $\vec{r}_0$ is a point source of type i ($\vec{r_0} \equiv \vec{e}_i, (r_0)_j = \delta^i_j$), we denote $F_n(\vec{r}_0, \vec{s})$ as $F_n(i, \vec{s})$. The random vector $\vec{Z}(n)$ initiated by $\vec{Z}(0)$ is the sum of the random vectors initiated by the $Z(0)$ neutrons represented by the vector $\vec{Z}(0) (= \vec{r_0})$

$$\vec{Z}(n)\Big|_{\vec{Z}(0)=\vec{r_0}} = \sum_{i=1}^{m} \sum_{j=1}^{r_0^i} \vec{Z}(n)\Big|_{\vec{Z}(0)=\vec{e}_i} \tag{2.6}$$

Eq. (2.6) expresses $\vec{Z}(n)$ as sum of contributions from all neutrons in the 0^{th} generation. Since the $Z(0)$ random vectors are independent, the moment generating function of the state vector $\vec{Z}(n)\Big|_{\vec{Z}(0)=\vec{r_0}}$ is written as the product of the moment generating function of the state vectors of the $Z(0)$ components $\vec{Z}(n)\Big|_{\vec{Z}(0)=\vec{e}_i}$. Therefore, $F_n(\vec{r}_0, \vec{s})$ and $F_n(i, \vec{s})$ are related by

$$F_n(\vec{r}_0, \vec{s}) = \prod_{i=1}^{m} F_n(i, \vec{s})^{r_0^i}. \tag{2.7}$$

$F_n(i, \vec{s})$ can be evaluated from $F_1(i, \vec{s})$ recursively according to its definition in Eq. (2.5),