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Analysis of correlations and their impact on convergence rates in Monte Carlo eigenvalue simulations

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ABSTRACT

This paper provides an analysis of the generation-to-generation correlations as observed when solving full core eigenvalue problems on PWR systems. Many studies have in the past looked at the impact of these correlations on reported variance and this paper extends the analysis to the observed convergence rate on the tallies, the effect of tally size and the effect of generation size. Since performing meaningful analysis on such a large problem is inherently difficult, a simple homogeneous reflective cube problem with analytical solution was developed that exhibits similar behavior to the full core PWR benchmark. The data in this problem was selected to match the dimensionality of the reactor problem and preserve the migration length travelled by neutrons. Results demonstrate that the variance will deviate significantly from the $1/N$ (N being the number of simulated particles) convergence rate associated with truly independent generations, but will eventually asymptote to $1/N$ after 1000's of generations regardless of the numbers of neutrons per generation. This indicates that optimal run strategies should emphasize lower number of active generations with greater number of neutrons per generation to produce the most accurate tally results. This paper also describes and compares three techniques to evaluate suitable confidence intervals in the presence of correlations, one based on using history statistics, one using generation statistics and one batching generations to reduce batch-to-batch correlation.

1. Introduction

Monte Carlo methods have long been considered a reference for neutron transport simulations since they make very limited approximations in simulating the random walk of neutrons in a system. Most often it is assumed that each neutron is independent of all others thus allowing for simple evaluation of unbiased means and uncorrelated variance. Previous work has observed correlation effects between neutrons in systems with fission, particularly when performing eigenvalue simulations based on the power iteration. Brissenden and Garlick (1986) demonstrated the existence of this bias in the Monte Carlo power iteration and suggested that this bias became quite small when a sufficient number of neutrons per generation were simulated. Dumonteil et al. (2014) further studied this issue and attributed the generation-to-generation correlation to spatial correlation of the fission process and ensuing asymmetry between neutron creation and annihilation in a stochastic branching process.

These works thus indicate that using a sufficiently large number of particles per generation will incur a negligible bias, but neglecting the correlations in the variance estimate will lead to an underestimation of that variance. Additionally, the existence of correlation impacts the convergence rate of the sample mean leading to the conundrum that additional generations of neutrons will only slightly improve the sample mean and may not be worth the additional run time. This has been demonstrated extensively in recent work by Herman on a realistic 2D full core PWR benchmark (Herman et al., 2014). The simple approach to avoid underestimation of the variance is to perform multiple independent simulations with different initial random seeds. This will lead to good variance estimates but requires lots of additional work since each independent simulation needs an independent fission source and will not improve convergence rates (Herman et al., 2014). Many studies over the years have been performed to evaluate the ratio between estimated and true variance. This eventually led to the concept of generations-per-batch (Kelly et al., 2012) that can provide a better estimate of the variance in a single simulation.

In recent years, more effort has been dedicated at evaluating the magnitude and lag of the autocorrelation coefficients observed in the eigenvalue mode of Monte Carlo simulations. Herman et al. (2014) calculated the autocorrelation coefficients and showed the

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dependency on the mesh size as well as the insensitivity to the number of neutrons per generation. Yamamoto et al. (2014, 2013) used the autoregressive (AR) model to predict underestimation of variance. In this method, the fission source distribution for each generation is expanded with eigenfunctions of the diffusion equation. Generation-to-generation correlation is represented by propagation of fluctuation of expansion coefficients. Sutton et al. (2015) explained and predicted underestimation of variance with a discretized phase space approach inspired by Brissenden and Garlick's work (Brissenden and Garlick, 1986).

In this paper, we will demonstrate the impact of the autocorrelation coefficients on the sample mean and its convergence rate during the power iteration process and seek to develop some intuition on how best to assign computational resources in evaluating problems with large correlations starting from a stationary fission source. This work will use a very simple problem with known solution to eliminate any uncertainties that can occur in evaluating convergence rates. Related work was performed by Tuttelberg and Dufek (2015) where they optimized the number of neutrons per generation for a fixed amount of total neutrons on both inactive and active generations to minimize bias and statistical error. However, their work did not account explicitly for the impact of correlation effects on statistical error and convergence rate. In this work, we will focus on determining optimal simulation parameters for the active generations only in the presence of strong correlations as observed in full core simulations. It will thus be assumed that acceleration methods can be used in the inactive region (Herman et al., 2014; Lee et al., 2014, 2012; Kelly Iii et al., 2013; Brown et al., 2013; Carney et al., 2013; Willert et al., 2013) to provide an initial unbiased stationary source. Section 2 will present the simple mono-energetic homogeneous cube problem with reflective boundary conditions used in the simulation and demonstrate its similarities with previous analysis on a full core PWR. Section 3 will present a review on statistical analysis in the presence of correlation. Section 4 will develop the theory behind the autocorrelation coefficients and the variance estimates. Section 5 will derive the optimal relation between generations and number of neutrons per generation, followed in Section 6 on the best practices to define interval estimates of tallied quantities. Concluding remarks and future work recommendations will follow in Section 7.

2. Homogeneous cube

Analyzing correlation coefficients on full core realistic problems becomes a very costly endeavor. Herman et al. (2014) were able to compute such coefficients on the 2D BEAVRS benchmark using extensive computational time making substantial analysis very impractical. In order to accelerate the process a simple benchmark was developed that preserves the correlation effects, reduces run time and has a simple analytical reference solution. Parameters of the homogenized cubic reactor are given in Table 1. The simple benchmark was chosen as a 400 cm reflective cube since it has dimensionality similar to a full core PWR, additionally the cross sections were selected such that the system is critical and preserves the migration length of neutrons.

Previous work relied on obtaining a suitable reference solution which was quite costly and introduced some amount of uncertainty in the analysis. The simple benchmark used in this work alleviates this issue since the reference solution is known analytically, thus eliminating any possible aberration that can be observed when computing RMS convergence rates.

The Relative Square Error (RSE) between accumulated tallies and the reference source distribution is defined for each tally region m as

$$RSE_m = \frac{\left(\widehat{X}_m - \langle X_m \rangle\right)^2}{\langle X_m \rangle^2} \tag{2.1}$$

where $\widehat{X}_m$ is the generation averaged estimator (i.e. within a single generation) and $\langle X_m \rangle$ is the reference solution. *RSE* in Eq. (2.1) is then averaged over all M tally regions and taken square root. We define this as Root Mean Square error (RMS) in Eq. (2.2). *RMS* is essentially a spatial average using L_2 norm.

$$RMS = \sqrt{\frac{\sum_{m=1}^{M} RSE_m}{M}} \tag{2.2}$$

The fission source distribution in the simple benchmark can be evaluated analytically, as shown by Eq. (2.3), and used as a reference in the *RMS* calculation.

$$\langle X_m \rangle = \frac{\Sigma_f}{\Sigma_t - \Sigma_s} \frac{1}{(\Delta x)^3} \tag{2.3}$$

where Σ_t, Σ_f, Σ_s are the total cross section, fission cross section, scattering cross section of the cube respectively and $(\Delta x)^3$ is the volume of each tally region.

To analyze this benchmark a simple Monte Carlo code was developed on a GPU to accelerate the analysis. At each generation the number of neutrons is normalized to the number of threads to be launched. Each thread has a local collision tally in each spatial bin and a reduction algorithm is performed after each generation to obtain the global tally. When the generation size (number of neutrons per generation) exceeds the number of threads on the GPU, kernels are launched sequentially. Generation sizes are selected to the power of 2 for more efficient use of the GPU hardware. The fission source distribution is then obtained by correcting the collision source distribution by the constant factor $\frac{\Sigma_f}{\Sigma_t}$.

A mesh tally of $16 \times 16 \times 16$ was selected since it is representative of an assembly size tally in a PWR. Figs. 1(a) and 2(a) illustrate the similarities in autocorrelation coefficients (ACC) between the 2D BEAVRS with assembly size tallies and the simple cube with 25 cm size tallies. The simple benchmark also illustrates an important feature of the problem, that of lower autocorrelation coefficients with smaller tally regions, as seen in the BEAVRS benchmark from Fig. 1(a) and (b) and illustrated in the benchmark by Fig. 2(a) and (b). Additionally, Figs. 1(c) and 2(c) present similar deviations from the ideal convergence rate which is directly caused by the presence of correlations.

3. Background

3.1. Variance of correlated sample average

In Monte Carlo eigenvalue simulations, quantities of interests are usually estimated as an average over many generations once

Table 1
Parameters of demonstration problem.

Geometry		ν	Macro cross-section				k_{eff}	Meshes
			$\Sigma_s(cm^{-1})$	$\Sigma_c(cm^{-1})$	$\Sigma_f(cm^{-1})$	$\Sigma_t(cm^{-1})$		
Reflective	400	2.45	0.270	0.018	0.012	0.300	1	$16 \times 16 \times 16$