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NOISE ANALYSIS OF SMOOTHED RESIDUAL ACCELERATION, A MONTE CARLO NEUTRON SOURCE CONVERGENCE ALGORITHM

Bryan E. Toth and William R. Martin
Department of Nuclear Engineering and Radiological Sciences
University of Michigan
2355 Bonisteel Boulevard
Ann Arbor, MI 48109
betoth@umich.edu; wrm@umich.edu

ABSTRACT

A detailed noise analysis is presented for linear extrapolation, an eigenfunction convergence acceleration technique, when it is applied to a general stochastic power method eigenfunction convergence algorithm. To the author's knowledge, such a noise analysis has not been published. If the variance of the cycle noise per mode is known, the noise analysis can predict the unavoidable level of poisoning from non-fundamental modes, which persist in the converged fission distribution because of noise inherent in the stochastic process. The analysis also indicates that extrapolation amplifies the iteration noise; therefore, a cutoff cycle is necessary to realize any gains from using extrapolation. Implications of this analysis on the Smoothed Residual Acceleration (SRA) algorithm are presented. Results from a 1-D slab test simulation using a coarse mesh to approximate SRA filtering are presented. The results show that a 70% reduction in the number of iterations needed to converge the source is achievable. Using a more conservative level of extrapolation for stability can still yield impressive gains of 44% with ease. The Monte Carlo results from the slab problem verify the accuracy of the noise analysis model.

Key Words: power method, extrapolation, acceleration, Monte Carlo, criticality

1. INTRODUCTION

Monte Carlo based criticality calculations are an important tool in nuclear design and safety analysis. The Monte Carlo method is especially well-suited for working with complex geometries commonly found in criticality safety problems. During criticality calculations, Monte Carlo transport codes use an iterative method to converge to the correct multiplication factor (eigenvalue) and fission source distribution (eigenfunction) for the system of interest. For problems with large dominance ratios, this iterative method can converge very slowly, requiring many batches of discarded neutrons before a stationary source distribution is achieved. The topics of fission source convergence [1-3] and stationarity [4] have been widely studied over the years. SRA was proposed as a method for reducing the number of discarded neutron histories necessary to achieve a converged source distribution [5]. This was demonstrated to successfully accelerate some problems with several modifications to the algorithm [6], but the influence of noise was not systematically addressed.

2. BACKGROUND

2.1. Power Method Iteration

First, let us consider a deterministic operator A which has the eigenfunctions $u_n(R)$ with corresponding eigenvalues λ_n, i.e.

$$Au_n(R) = \lambda_n u_n(R) \tag{1}$$

where n ranges from 0 to infinity, and R denotes the spatial dependence of the function. Suppose that the eigenvalues can be ordered such that $\lambda_0 > \lambda_1 \geq ... \geq \lambda_\infty \geq 0$. The power method is a well-known iterative scheme to estimate the fundamental eigenmode of an operator, and can be expressed succinctly as

$$u^{(m+1)}(R) = k^{-1} A u^{(m)}(R) \tag{2}$$

where $u^{(m)}(R)$ is the m^{th} iteration eigenfunction estimate, k is a normalization constant, and $u^{(0)}(R)$ is the initial guess such that

$$u^{(0)}(R) \equiv \sum_{n=0}^{\infty} \gamma_n u_n(R) \tag{3}$$

where γ_n are the eigenfunction expansion coefficients of the initial guess function. Selecting k to be λ_0 and by recursion, Eq. (2) becomes the familiar result,

$$u^{(m+1)}(R) = \sum_{n=0}^{\infty} \left(\lambda_n / \lambda_0 \right)^m \gamma_n u_n(R) . \tag{4}$$

The $n > 0$ modes decay or converge at the rate λ_n / λ_0 with mode 1 having the slowest decay rate because it has the second largest eigenvalue by virtue of the eigenvalue ordering. Often this decay rate can make numerical calculations prohibitively slow, so we seek a means to accelerate the convergence of the slowest converging mode.

2.1. Extrapolation Applied to the Power Method

Extrapolation is probably the simplest means to accelerate the convergence of the power method. In extrapolation, the change observed from one application of A is amplified to push the eigenfunction estimate further toward convergence. This extrapolation scheme can be expressed as

$$v^{(m+1)}(R) = k^{-1} A v^{(m)}(R) + \alpha \left(k^{-1} A v^{(m)}(R) - v^{(m)}(R) \right) \text{for } m \geq 0 \tag{5}$$

$$v^{(0)}(R) = u^{(0)}(R) \equiv \sum_{n=0}^{\infty} \gamma_n u_n(R) \tag{6}$$

where α is a specified extrapolation parameter that is greater than 0. Using λ_0 as the normalization constant and recursion, Eq. (5) can be expressed as

$$v^{(m)}(R) = \sum_{n=0}^{\infty} \left[\left((1+\alpha) \lambda_n / \lambda_0 - \alpha \right)^m \gamma_n u_n(R) \right] \text{ for } m > 0. \tag{7}$$

The extrapolation effectively shifts the convergence rate of all non-fundamental modes lower. This allows the low order modes to converge faster. The convergence rates of modes with lower eigenvalues are typically made negative by the shift, which can increase their magnitudes and slow their convergence. The gain from using extrapolation is that the slowest converging mode of the extrapolated power method will converge faster than the slowest converging mode of the standard power method, but only if α is chosen such that

$$\max\left\{ \left| (1+\alpha) \lambda_n / \lambda_0 - \alpha \right| : n > 0 \right\} < \max\left\{ \left| \lambda_n / \lambda_0 \right| : n > 0 \right\}. \tag{8}$$

If $\lambda_\infty = 0$, then the optimal choice for α has been shown [11] to be

$$\alpha_{opt} = \frac{\lambda_1}{2\lambda_0 - \lambda_1}. \tag{9}$$

3. NOISE ANALYSIS

3.1. Power Method

For some systems, the deterministic operator may be difficult to define without making unwanted approximations; therefore, one may choose to construct a stochastic analog $\tilde{A}$ for the deterministic operator, such that

$$E[\tilde{A}u_n(R)] = Au_n(R) \tag{10}$$

where $E[*]$ denotes the expectation value of *. This implies that

$$\tilde{A}u_n(R) = Au_n(R) + \xi(R) \tag{11}$$

$$E[\xi(R)] = 0 \tag{12}$$

The stochastic analog can be combined with the power method to construct an iterative scheme that can solve for the fundamental eigenmode $u_0(R)$ as follows

$$u^{(m+1)}(R) = k^{-1} \tilde{A} u^{(m)}(R) = k^{-1} A u^{(m)}(R) + \xi^{(m+1)}(R) \tag{13}$$

where $u^{(m)}(R)$ is the m^{th} iteration eigenfunction estimate, k is a normalization constant, $\xi^{(m)}(R)$ is the noise distribution in the m^{th} iteration after absorbing k, and $u^{(0)}(R)$ is the initially sampled guess such that

$$u^{(0)}(R) \equiv \sum_{n=0}^{\infty} \gamma_n u_n(R) + \sum_{n=0}^{\infty} \xi_n^{(0)} u_n(R) \equiv \sum_{n=0}^{\infty} u_n^{(0)} u_n(R) \tag{14}$$

Where γ_n are the eigenvector expansion coefficients of the initial guess function, and $\xi_n^{(0)}$ are the expansion coefficients of the noise that arises in sampling the initial guess function, and $u_n^{(0)}$ is the sum of these coefficients for the n^{th} mode. The choice of k is not significant in this abstract context; however, to ease understanding, this work will choose k to be λ_0., which would be the asymptotic value necessary to keep the eigenfunction estimate from decaying or growing exponentially. The cycle eigenvector estimates in Eq. (13) can be decomposed into the eigenfunctions of A such that

$$u^{(m+1)}(R) \equiv \sum_{n=0}^{\infty} u_n^{(m+1)} u_n(R) = \sum_{n=0}^{\infty} \left(\lambda_0^{-1} A u_n^{(m)} + \xi_n^{(m+1)} \right) u_n(R) \tag{15}$$

where $u_n^{(m)}$ are defined as the eigenfunction expansion coefficients for mode n of the fundamental mode estimate at cycle m of the iteration. Using Eq. (1) and successive applications of Eq. (15), one finds that

$$u_n^{(m)} = \left(\lambda_n / \lambda_0 \right)^m \gamma_n + \sum_{k=0}^{m} \left(\lambda_n / \lambda_0 \right)^k \xi_n^{(m-k)} . \tag{16}$$

3.2 Extrapolated Power Method

Replacing the true operator in Eq. (5) with the stochastic operator, the noise can be explicitly represented in the extrapolation iteration as

$$v^{(m)}(R) = (1+\alpha)\left(\lambda_0^{-1} A v^{(m-1)}(R) + \xi^{(m)}(R) \right) - \alpha \cdot v^{(m-1)}(R) \text{ for } m > 0 \tag{17}$$

$$v^{(0)}(R) = u^{(0)}(R) \equiv \sum_{n=0}^{\infty} \gamma_n u_n(R) + \sum_{n=0}^{\infty} \xi_n^{(0)} u_n(R) \equiv \sum_{n=0}^{\infty} u_n^{(0)} u_n(R) . \tag{18}$$

After applying the relation in Eq. (1) and expressing the result as an eigenfunction decomposition, Eq. (17) simplifies to

$$v^{(m)}(R) = \sum_{n=0}^{\infty} \left[\left((1+\alpha) \lambda_n / \lambda_0 - \alpha \right) v_n^{(m-1)} + (1+\alpha) \xi_n^{(m)} \right] u_n(R) \tag{19}$$

where the coefficients of the expansion are

$$v_n^{(m)} = \left((1+\alpha) \lambda_n / \lambda_0 - \alpha \right) v_n^{(m-1)} + (1+\alpha) \xi_n^{(m)} \tag{20}$$

With successive applications of Eq. 20, the coefficients can be simplified to

$$v_n^{(m)} = \left[(1+\alpha) \lambda_n / \lambda_0 - \alpha \right]^m \gamma_n + \sum_{k=0}^{m} \left[(1+\alpha) \lambda_n / \lambda_0 - \alpha \right]^k (1+\alpha) \xi_n^{(m-k)} \tag{21}$$

Defining the modal cycle multipliers, β_n, as

$$\beta_n \equiv (1+\alpha) \lambda_n / \lambda_0 - \alpha \quad \text{for all } n \geq 0, \tag{22}$$

$v^{(m)}(R)$ will only converge to the fundamental mode if the cycle multipliers are bounded by one, i.e.

$$\left| (1+\alpha) \lambda_n / \lambda_0 - \alpha \right| < 1 \quad \text{for all } n > 0. \tag{23}$$

Previous work [1] has shown that Eq. (22) is satisfied for all n such that $0 < n < N$ when

$$-1 < \alpha < \frac{\lambda_0 + \lambda_N}{\lambda_0 - \lambda_N} \tag{24}$$

Because of the monotonically non-increasing nature of the eigenvalues, β_n is also monotonically non-increasing. Therefore, the maximum value of $|\beta_n|$ for $0 < n < N$ is equal to the larger value of the terms $|\beta_1|$ and $|\beta_{N-1}|$. Convergence of the iteration is fastest when $|\beta_n|$ is minimized. Because $|\beta_1|$ and $|\beta_{N-1}|$ move in opposite directions when α changes, they are simultaneously minimized when they are equal. Therefore, the optimal value of α for minimizing the modal cycle multipliers over all n such that $0 < n < N$ is

$$\alpha = \frac{\lambda_1 + \lambda_{N-1}}{2\lambda_0 - \lambda_1 - \lambda_{N-1}}. \tag{25}$$

3.3 Method Comparison

In the deterministic case, i.e. $\xi_n^{(m)} = 0$ for all m, we see that equations (16) and (21) are identical to the well-known results presented in the background section. In the absence of noise, a properly selected extrapolation parameter serves to reduce the coefficients of the lower order modes, which hastens the rate at which the slowest converging modes decay. However, the higher modes will persist longer because the magnitudes of their cycle multipliers increase. The

net effect allows one to obtain an accurate approximation to the true fundamental mode with less iterations.

When noise is present from a stochastic implementation, the accelerated algorithm is no longer guaranteed to outperform the standard algorithm even when the optimal acceleration parameter is chosen. This can be shown by assuming $\xi_n^{(m-k)}$ are normally distributed random variables with mean 0 and standard deviation σ. Then the summation in Eq. (16) can be reduced to a single normally distributed random variable with mean 0 and standard deviation of $a_n^{(m)}\sigma$ [7] where

$$a_n^{(m)} = \sqrt{\sum_{k=0}^{m}\left(\lambda_n/\lambda_0\right)^{2k}} = \sqrt{\frac{1-\left(\lambda_n/\lambda_0\right)^{2(m+1)}}{1-\left(\lambda_n/\lambda_0\right)^{2}}}. \tag{26}$$

And the summation in Eq. (21) reduces to a different normally distributed random variable with mean 0 and standard deviation of $b_n^{(m)}\sigma$ where

$$b_n^{(m)} = \sqrt{\frac{1-\left((1+\alpha)\lambda_n/\lambda_0-\alpha\right)^{2(m+1)}}{1-\left(\lambda_n/\lambda_0\right)^{2}-\frac{2\alpha}{1+\alpha}\left(1-\lambda_n/\lambda_0\right)}} \tag{27}$$

Therefore, if the initial guess is close to the fundamental mode, i.e. $\gamma_n \approx 0$ for $n > 0$, one can expect the error in the n^{th} mode at iteration m to be

$$E[\left|u_n^{(m)}\right|] = a_n^{(m)}\sigma\sqrt{2/\pi} \tag{28}$$

for the standard power method, and

$$E[\left|v_n^{(m)}\right|] = b_n^{(m)}\sigma\sqrt{2/\pi}. \tag{29}$$

for the extrapolated power method, respectively. In the infinite cycle limit,

$$\lim_{m\to\infty} a_n^{(m)} = \sqrt{\frac{1}{1-\left(\lambda_n/\lambda_0\right)^{2}}}, \tag{30}$$

and

$$\lim_{m\to\infty} b_n^{(m)} = \sqrt{\frac{1}{1-\left(\lambda_n/\lambda_0\right)^2 - \frac{2\alpha}{1+\alpha}\left(1-\lambda_n/\lambda_0\right)}}. \tag{31}$$

Since $0 \le \lambda_n/\lambda_0 < 1$,

$$\lim_{m\to\infty} a_n^{(m)} \le \lim_{m\to\infty} b_n^{(m)}, \tag{32}$$

and the limits are only equal when α is zero. This implies that the effectiveness of the extrapolation will depend upon the accuracy of the initial guess and the noise inherent in the stochastic operator because a gain from extrapolation can only be realized when the initial guess is not close to the fundamental mode, and noise has the potential to wash away those gains as the iteration progresses.

3.4 Smoothed Residual Acceleration

In SRA, the user carefully selects an ideal cutoff filter such that only the lower order modes are extrapolated while the rest are left to decay according to the standard power method. Therefore, the stochastic SRA is simply a combination of Eqs. (16) and (21) as follows.

$$s^{(m)}(R) = \sum_{n=0}^{N-1} v_n^{(m)} u_n(R) + \sum_{n=N}^{\infty} u_n^{(m)} u_n(R) \tag{33}$$

where N is the cutoff mode number, and $s^{(m)}(R)$ is the fundamental eigenfunction estimate from SRA at iteration m.

4. NUMERICAL EXPLORATION OF EXTRAPOLATION

For numerical comparison, the gain, G, at cycle m from extrapolation will be defined as the smallest difference between the iteration numbers when the average magnitudes of the decomposition coefficients are equivalent, i.e.

$$\left|\overline{u}_n^{(m+G)}\right| = \left|\overline{v}_n^{(m)}\right| \text{ for } n > 0. \tag{34}$$

The modal gain, G_n, will be similarly defined such that G_n satisfies

$$\left|u_n^{(m+G_n)}\right| = \left|v_n^{(m)}\right| \text{ for } n > 0. \tag{35}$$

An increasing gain should indicate that the extrapolation is accelerating the convergence of the guess to the solution. A decrease in gain indicates that the extrapolated power method is approaching convergence or the extrapolation parameter is poor. Negative gain indicates that the extrapolation hurts the simulation in that the standard method has a lower error at the cycle for which the gain was calculated. In the absence of noise, the gain asymptotically approaches a linearly increasing function with respect to iteration number.

The first mode has the slowest decay rate and will therefore persist the longest. Because of that, consideration of the first mode is paramount over the other faster decaying modes. Fig. 1 is a plot of 100 realizations of the first mode coefficient magnitude, i.e. $\left|v_1^{(m)}\right|$ or $\left|u_1^{(m)}\right|$, for a system with 101 equally spaced eigenvalues on the interval [1 0]. The initial guess consisted of an equally weighted sum of all modes. The realizations were generated by replacing ξ with a Gaussian random variable with mean 0, whose standard deviation is indicated in the legend of the figures. For the same system, Fig. 2 is a plot of the modal gain, G_1, averaged over 100 realizations. For the first mode, the maximum modal gain of 237 cycles occurred at cycle 245 for the higher noise simulation, and a maximum modal gain of 339 cycles occurred at iteration 353 for the low noise simulation. These represent a cycle savings of 49% for both simulations. From Fig. 1, one can see that the iteration noise does not have a significant effect on the first mode convergence rate because the slow decay rate of the initial guess keeps the noise insignificant throughout most of the simulation. Only when the estimate approaches its asymptotic error level does the higher noise simulation diverge from the lower noise simulation.

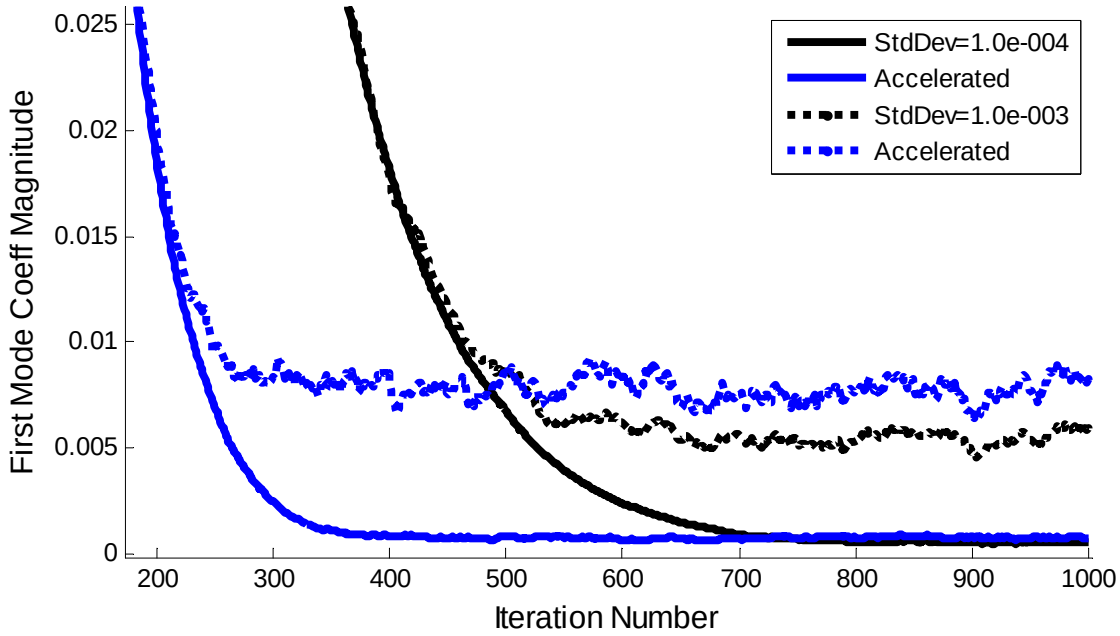

Figure 1. Plot of first mode decomposition coefficient versus iteration for a system with dominance ratio 0.99 and γ_n = 1.0 using α = 0.98 with two noise levels.

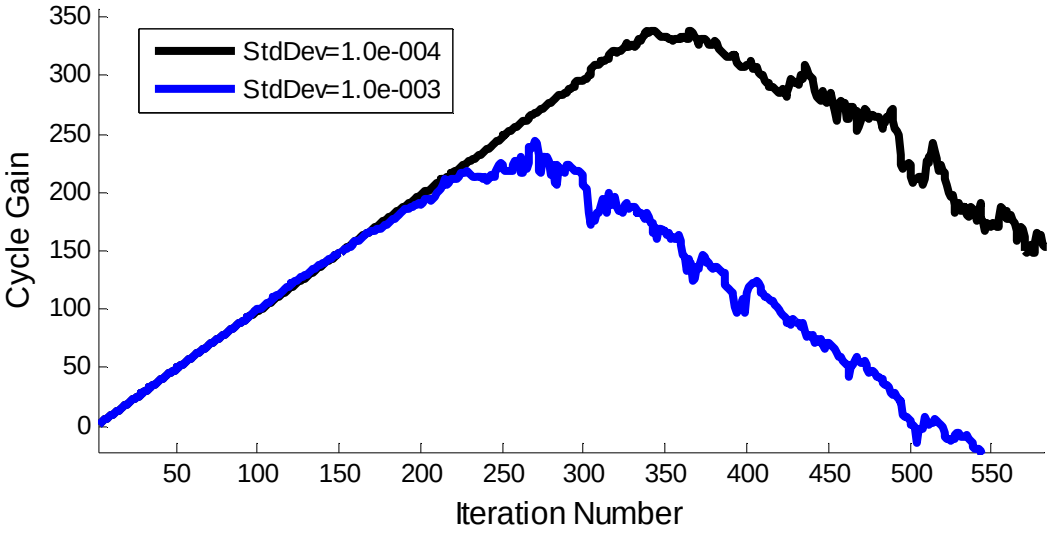

Figure 2. Plot of modal gain for the first mode versus iteration for a system with dominance ratio 0.99 and γ_n = 1.0 using α = 0.98 with two noise levels.

From the exercise above, one can see that turning off the extrapolation at some point in a simulation is desirable to avoid the elevated error levels after the fundamental mode eigenfunction estimate has converged. Another reason for turning off the acceleration is that extrapolation amplifies the higher order modes, which normally would be insignificant because of their fast decay rates. The use of acceleration increases the presence or these undesirable high frequency modes. For these reasons, this acceleration technique should always be turned off prior to computing tallies in active cycles. Several inactive cycles should be allowed after acceleration cutoff to allow the amplified modes to decay prior to the start of tallies. More buffer cycles will be needed for larger acceleration parameters. Detecting on-the-fly when to turn off the acceleration is currently under investigation, but this is a difficult problem because it involves detecting convergence of the fission source, which is an unresolved issue in MC.

5. APPLICATION TO MONTE CARLO NEUTRON TRANSPORT

Linear extrapolation was applied to Monte Carlo neutron transport using a grid to estimate the magnitude of the fission source density. The estimated magnitude of the fission source density in a grid box is computed by adding up the number of sites within the grid box and normalizing it by the number of total sites, such that the sum of all bins equals one. The fission source is extrapolated by first applying selection weights to each grid box according to the change in the estimated fission densities of each box observed from a single random transport cycle. The extrapolation parameter scales the grid box selection weights. Then, a stratified sampling routine selects the number of sites to use from each grid box based on the selection weights. Finally, the starting sites for the next iteration are sampled uniformly within each grid box from the fission sites in that box. These manipulations to the standard MC source iteration effectively push the fission source toward the fundamental mode distribution by exaggerating the changes observed from transport within a cycle. If the extrapolation computation ever results in a negative source within a grid box, then no source points are sampled from that box, which is a truncation.

6. RESULTS FROM TEST CASES

This paper will present results for a thick one-group one dimensional slab because the eigenvalues and eigenvectors are known with good precision using diffusion theory. The slab used has the following cross sections, and the scattering is isotropic.

$$\nu\Sigma_f = 0.5\,\text{cm}^{-1}$$
$$\Sigma_s = 0.5\,\text{cm}^{-1}$$
$$\Sigma_a = 0.5\,\text{cm}^{-1}$$
$$\Sigma_t = \Sigma_s + \Sigma_a = 1.0\,\text{cm}^{-1}$$

The slab thickness was selected to be 44.13 cm such that the dominance ratio is approximately 0.99. A nine region grid is used to evaluate the fission densities. By selecting such a coarse grid, the higher frequency modes are suppressed from influencing the acceleration. Accelerating on this grid is roughly equivalent to SRA with the cutoff mode set to 10 because only the first nine modes can be represented on the grid. Using Eq. (25) with this cutoff assumption, would suggest 8.0 as the optimal value for α; however, this was tested and found to be an unstable parameter. This instability arose because the grid is not an ideal filter. Higher frequency modes are allowed to poison the computation through the phenomenon known as aliasing. However, a more conservative extrapolation parameter of 4.0 was found to be stable by reducing α, iteratively. The always stable and therefore the most conservative estimate for the optimal α using Eq. (25) assumes that the eigenvalue of the mode just before the cutoff is 0. For this sample problem with a dominance ratio of 0.99, the conservative extrapolation parameter is 0.98.

To compare the Monte Carlo results with the theory presented above, the standard deviation of the mode coefficients was computed by calculating the mean and variance of each coefficient from 40 realizations at each iteration of the standard simulation. The standard deviation of the non-fundamental mode coefficients at each iteration was approximately 0.0024 and did not depend noticeably on the iteration or the mode. Calculations using $\alpha = 0.98$ and $\alpha = 4.0$ were performed starting with an initial guess containing only the fundamental mode and the first higher mode and using a Gaussian random variable with mean 0 and standard deviation of 0.0024. The magnitudes of the first mode coefficients, i.e. n =1, from Eqs. (16) and (21) averaged over 200 realizations are plotted with the average of 200 Monte Carlo (MC) simulations run with 16,000 neutrons per cycle in Fig. 3 and 4.

In Fig. 3 and 4, both the accelerated and standard MC simulations closely match the convergence paths predicted by the presented theory. The conservatively accelerated MC simulations realized an average gain of 87 cycles at cycle 110, which is approximately a 44% reduction in cycles, and the theory predicted an average gain of 91 cycles at cycle 108, which is a 46% reduction. This difference between the predicted gain and the realized gain is negligible because of the variance observed with gain calculations. In Fig. 3, the accelerated simulation clearly converges to a solution with higher error than the standard simulation because the first mode should converge to zero without noise. This error level is not particularly concerning in this case, but in Fig. 4 where acceleration was much more aggressive, the error in the accelerated simulation is nearly

double that of the standard. However, the aggressive acceleration lead to a maximum gain of 130 cycles at cycle 56, a savings of 70%, which was close to the 72% savings from a maximum gain of 136 cycles at cycle 53 predicted from the theoretical model.

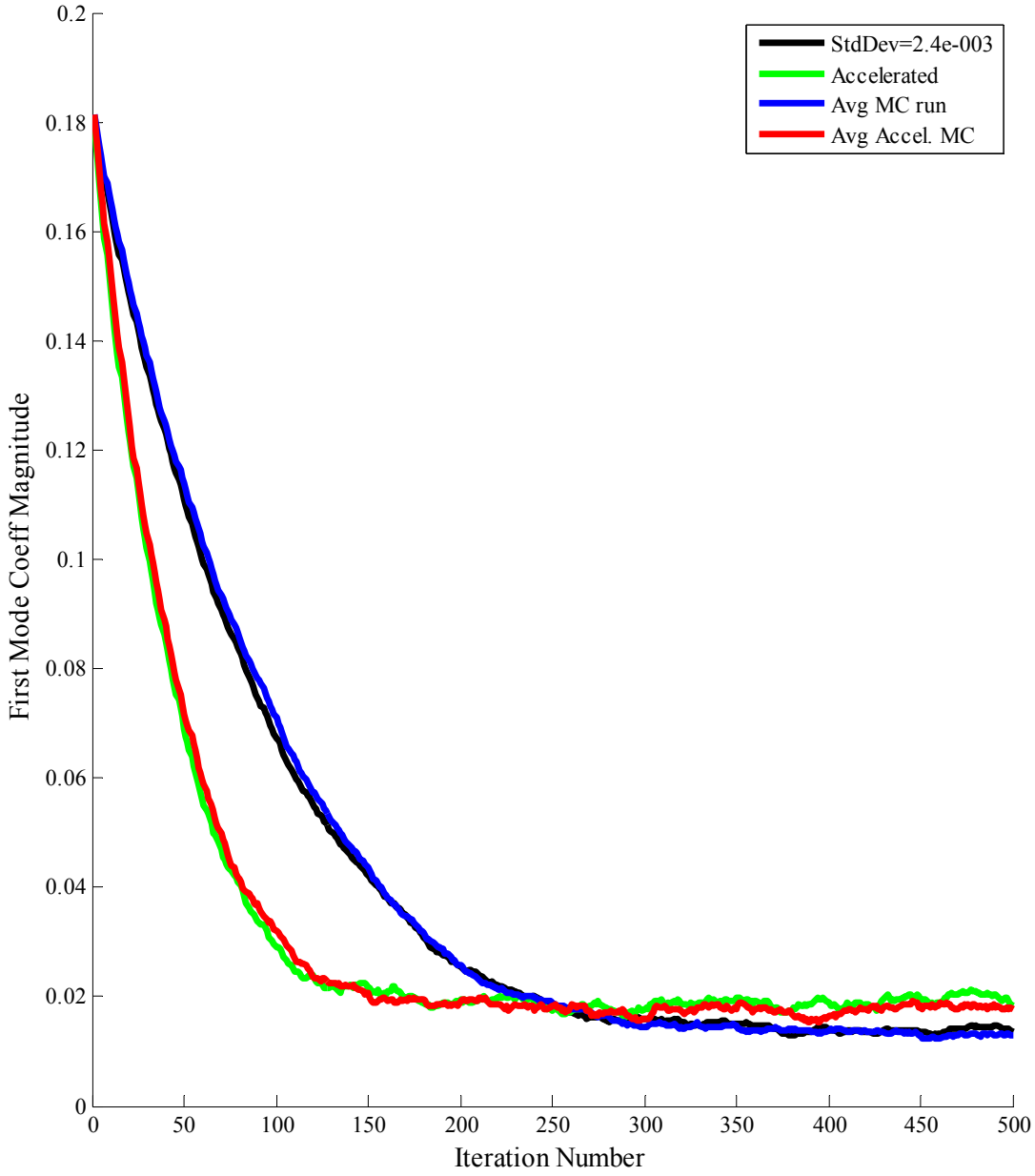

Figure 3. Plot of the magnitude of the first mode eigenfunction decomposition coefficient versus iteration for a system with dominance ratio 0.99 and γ_1 = 0.18 using a conservative extrapolation parameter, α = 0.98, for acceleration. The MC lines indicate that the results are from a 1-D Monte Carlo simulation and the other two lines are expected from theory.

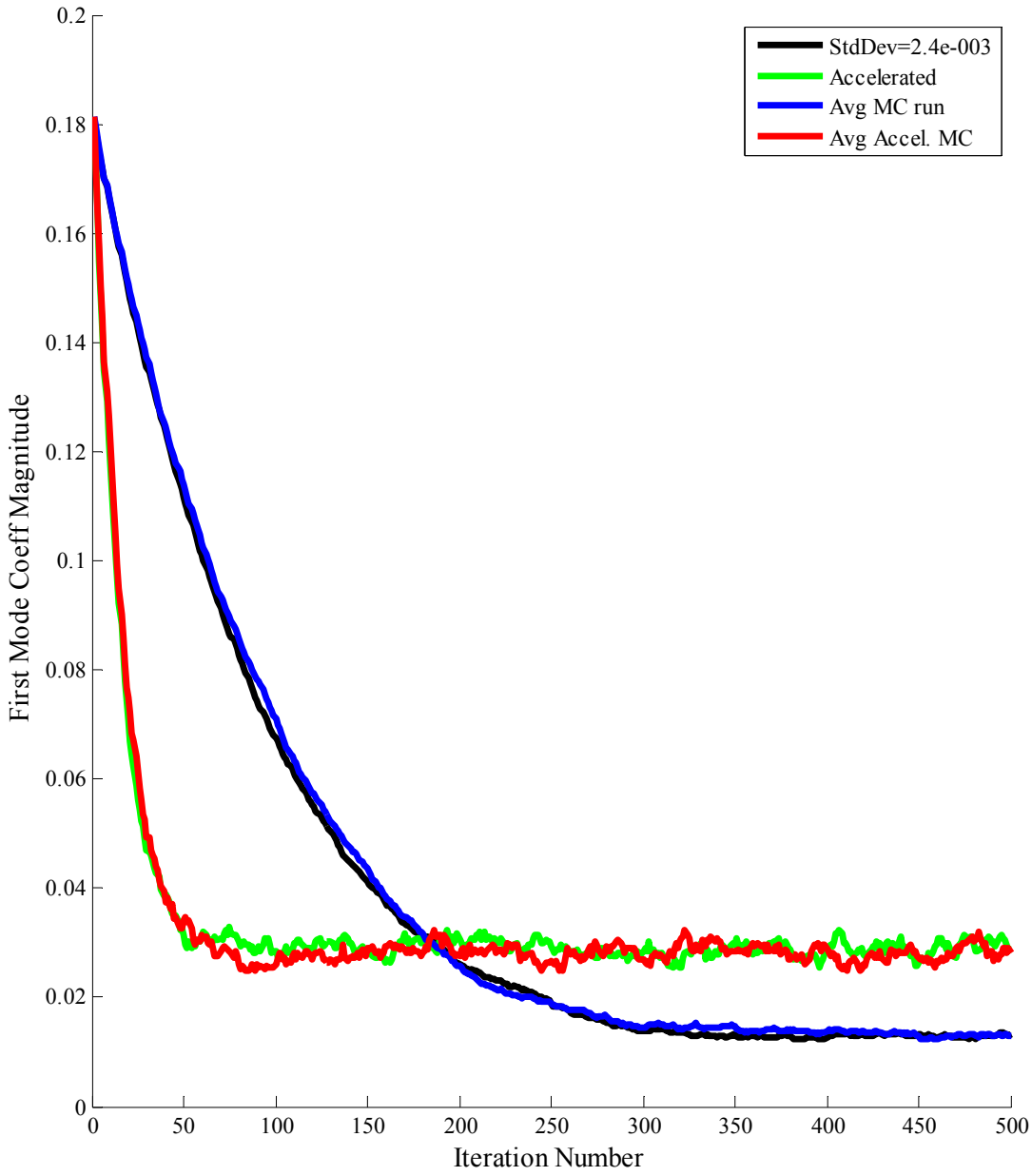

Figure 4. Plot of the magnitude of the first mode eigenfunction decomposition coefficient versus iteration for a system with dominance ratio 0.99 and γ_1 = 0.18 using α = 4.0 for acceleration. The MC lines indicate that the results are from a 1-D Monte Carlo simulation and the other two lines are expected from theory.

7. CONCLUSIONS

Results from the test problem presented in this paper indicate that the model presented for the power method with and without extrapolation is suitable for modeling stochastic analogs of these source iterations. SRA and linear extrapolation can successfully hasten convergence of the fundamental mode eigenfunction estimate with possible cycle savings up to 70%. The asymptotic analysis of the model and results obtained from Monte Carlo neutron transport simulations clearly indicate a need to determine the iteration where the extrapolation should be turned off because of the noise amplification that results from extrapolation.

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