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APPLICATION OF THE STOCHASTIC OSCILLATOR TO ASSESS SOURCE CONVERGENCE IN MONTE CARLO CRITICALITY CALCULATIONS

Paul K. Romano*
Knolls Atomic Power Laboratory
P.O. Box 1072, Schenectady, NY 12301

ABSTRACT

A novel method for assessing source convergence in Monte Carlo criticality calculations is presented here. The method is based on the stochastic oscillator, an indicator that is commonly used in the technical analysis of financial markets, and entails performing a posterior diagnostic test on the Shannon entropy of the source distribution. The stochastic oscillator takes advantage of the fact that when a scalar time series is increasing (or decreasing) monotonically, its value will be higher (or lower) than the previous values. Extensive testing on the OECD/NEA source convergence benchmark suite shows that the stochastic oscillator diagnostic performs very well. The relative merits of this method compared to previous approaches are discussed.

Key Words: Monte Carlo, Shannon entropy, source convergence, MC21, criticality

1. INTRODUCTION

In the power iteration method used to solve the *k*-eigenvalue transport equation, the fission source distribution converges at a rate slower than that of the eigenvalue. Unfortunately, it is too often the case that reactor analysts rely on convergence of the eigenvalue to determine how many batches to discard. Discarding too few batches can lead to gross errors in local tallies due to a non-stationary source and an erroneous eigenvalue. In the present work, a method for automatically assessing source convergence by performing a posterior diagnostic test on the Shannon entropy of the source distribution is developed.

2. THE STOCHASTIC OSCILLATOR DIAGNOSTIC

In this section, we will discuss how the Shannon entropy relates to the convergence of the source distribution and demonstrate how the stochastic oscillator can be applied to the Shannon entropy to develop a posterior diagnostic criterion for convergence.

2.1. Source Convergence and Shannon Entropy

* Affiliated with Massachusetts Institute of Technology, Department of Nuclear Science and Engineering, 77 Massachusetts Avenue, Cambridge, MA 02139
Email: romano7@mit.edu

It can be shown [1] that in the power iteration method for criticality problems, the higher-order terms in the source distribution die off as ρ^{n+1} whereas the higher-order terms in the eigenvalue die off as $\rho^n(1-\rho)$. Here ρ is the ratio of the first harmonic eigenvalue to the fundamental mode eigenvalue, *i.e.* the dominance ratio, and *n* is the number of iterations. For problems with a high dominance ratio, the eigenvalue may appear to be converged after a few iterations while the source distribution is still far from being converged. The error in the calculated eigenvalue due to higher harmonics will not be nearly as pronounced as the error in the source distribution at any iteration as a result of the extra damping from the $1-\rho$ term.

From the above considerations, the number of inactive batches in a Monte Carlo criticality simulation should be evaluated based on when the source distribution has reached stationarity, not the eigenvalue. However, assessing convergence of the source distribution is complicated by the fact that it is multi-dimensional. One way of overcoming this problem is to utilize a scalar metric called the Shannon entropy. Prior work has shown that the Shannon entropy converges to an arbitrary fixed value as the source distribution approaches stationarity [2]. In order to calculate the Shannon entropy, we superimpose a rectangular mesh over the spatial domain that contains all fissionable sources and tally the number of source sites that appear in each mesh bin. Then, the Shannon entropy can be calculated as:

$$H^{(n)} = -\sum_{i=1}^{p} \hat{S}_i^{(n)} \log_2 \hat{S}_i^{(n)} \qquad (1)$$

where $H^{(n)}$ is the Shannon entropy at the *n*-th batch, $\hat{S}_i^{(n)}$ is the percentage of source sites in the *i*-th bin at the *n*-th batch, and *p* is the total number of spatial bins. Assessing convergence of the source distribution becomes considerably less formidable when using Shannon entropy since one can look at a line-plot of the Shannon entropy versus batch in order to make a judgment on when the source distribution has converged.

2.2. Assessing Convergence via the Stochastic Oscillator

While visual inspection of a line-plot of the Shannon entropy is certainly a viable method of assessing source convergence, it places an unnecessary burden on the reactor analyst and necessitates making a subjective decision on how many batches to discard. As we will subsequently show, it is possible to automate this decision-making through the use of formulae.

A number of approaches for automatically assessing source convergence have been proposed. We review some of the more recent work as follows. Kitada and Takeda propose a convergence diagnostic based on the fission matrix [3]. Shim and Kim developed an on-the-fly criterion based on the inter-cycle correlation length [4]. Brown et al., having to deal with the inherent limitations of implementing routines in a production code with a large user base, investigated simpler posterior diagnostics using statistical tests on the Shannon entropy [5]. Ueki developed a step-refined on-the-fly convergence criterion based on the Wilcoxon signed rank sum [6]. The approach taken in the present work combines some of the salient features of Brown's suite of statistical tests and Ueki's Wilcoxon signed rank sum diagnostic. This allows for a simple implementation within a production Monte Carlo code while reliably producing estimates of the batch at which stationarity is reached.

The problem of detecting stationarity in the Shannon entropy is in many ways similar to the problem of determining trends in stock prices. In the technical analysis of financial markets, a number of indicators have been developed to ascertain whether the price of a stock is exhibiting a "bullish" trend where the price is increasing, a "bearish" trend where the price is decreasing, or whether it is "moving sideways" wherein the price is not trending appreciably in either direction. One such indicator is the stochastic oscillator [7]. The stochastic oscillator is based on the observation that when prices are increasing nearly monotonically, the current price will be high relative to the range of prices in the immediate past. Thus, when the price is not trending, we would expect that the current price will be confined within a finite range of prices.

The stochastic oscillator is a combination of two separate indicators. The first, referred to as %*K*, is defined as:

$$\%K = \frac{P - P_{\min}^{n}}{P_{\max}^{n} - P_{\min}^{n}} \tag{2}$$

where P is the current price, $P_{\min}^{n}$ is the minimum price over the last *n* observations, and $P_{\max}^{n}$ is the maximum price over the last *n* observations. When the price is trending upwards, %*K* will be close to unity since $P \cong P_{\max}^{n}$, and similarly, when the price is trending downwards, %*K* will be close to zero since $P \cong P_{\min}^{n}$. Rather than using the %*K* values as an indicator, a simple moving average of the last *m* values of %*K* is usually used for analyzing price movements and is called %*D*.

In a similar fashion, this idea can be applied to the Shannon entropy as a function of the batch number. Let us define

$$K^{(n)} = \frac{H^{(n)} - H_{\min}^{n,p}}{H_{\max}^{n,p} - H_{\min}^{n,p}} \tag{3}$$

where $H_{\min}^{n,p}$ and $H_{\max}^{n,p}$ are the minimum and maximum Shannon entropies over the last *p* batches, respectively. Once stationarity is reached, $K^{(n)}$ will fluctuate between zero and one such that $E\left[K^{(n)}\right] = 0.5$. Thus, the following criterion can be used to assess convergence of the source distribution:

$$\left|K^{(n)} - 0.5\right| < \varepsilon \quad \text{and} \quad \left|\frac{1}{m}\sum_{i=0}^{m-1} K^{(n+i)} - 0.5\right| < \varepsilon . \tag{4}$$

In words, this criterion requires that both $K^{(n)}$ and its average over the next *m* batches be within ε of 0.5.

An immediate drawback to this method can be seen in the fact that it requires three arbitrarily-chosen parameters, *p*, *m*, and ε. However, as will be shown from the results of extensive testing, a single parameter set performs very well in almost all problems.

To illustrate how the diagnostic works in practice, let us look at a typical Shannon entropy plot shown in Figure 1. We can explain the behavior of the Shannon entropy as follows. A point source was used for the initial source distribution giving us a very low initial entropy value since the source is concentrated all at one location. The entropy increases rapidly as the source spreads throughout the problem. The point at which the entropy hits its maximum represents the state in which the source is most evenly distributed throughout the problem geometry. From there on, the source will start to accumulate in the areas of highest fission density, causing the entropy to decrease until it reaches stationarity.

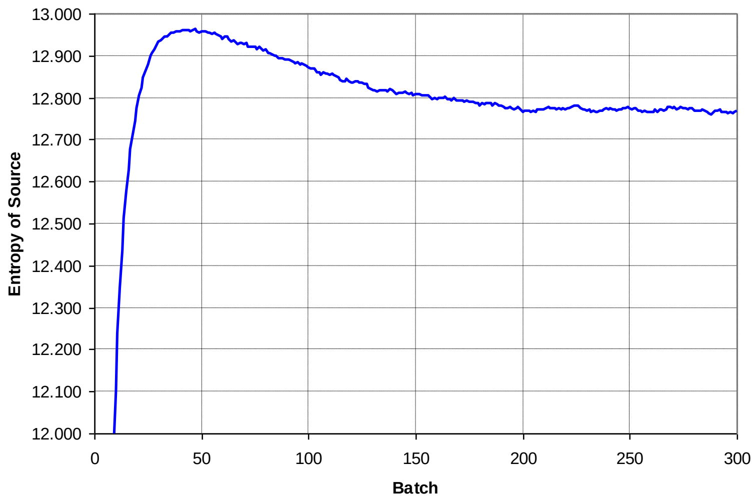

Figure 1. Typical Shannon Entropy plot for a point source.

In the first 40 batches where the entropy is trending upwards, $K^{(n)}$ is close to, if not, unity as we can see in Figure 2. Once the entropy hits its maximum and begins to make a downward trend, $K^{(n)}$ abruptly changes, going to zero in only a few batches. During this change, the first half of the criterion in Eq. (4) is met briefly, but clearly the average of $K^{(n)}$ over the next *m* batches will not be anywhere close to 0.5. From this point forward, the long downward trend in the entropy keeps the values of $K^{(n)}$ low until stationarity is finally reached around batch 200. It can clearly be seen in Figure 2 that once stationarity is reached, $K^{(n)}$ oscillates back and forth between zero and unity. Note that the average of $K^{(n)}$ stops at batch 250 since it is a forward average over 50 cycles.

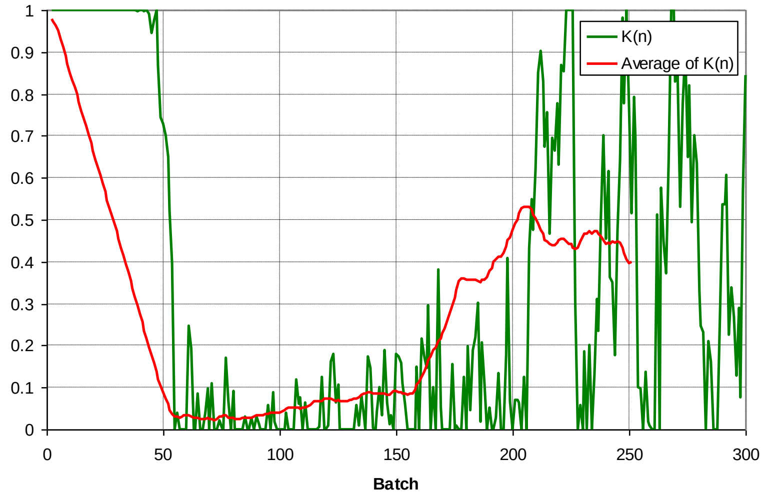

Figure 2. Stochastic oscillator $K^{(n)}$ and its moving average.

3. NUMERICAL RESULTS

To test the stochastic oscillator diagnostic, a routine was implemented in the MC21 Monte Carlo particle transport code [8] to calculate the Shannon entropy and apply the criterion from Eq. (4). The criterion was tested on the OECD/NEA source convergence benchmark problems [9] as these represent some of the most challenging source convergence problems. The poor source convergence in these problems is the result of the combination of high dominance ratios as well as undersampling of the fissionable regions. In the most extreme cases (Problem 1), convergence of the source distribution becomes very hard to diagnose due to a dominance ratio nearly unity and severe undersampling resulting from a highly decoupled geometry. For most problems, undersampling can be remedied by increasing the number of histories per batch. On the other hand, slow convergence due to a high dominance ratio will not be affected by the number of histories per batch and thus shows up even when solving problems using deterministic methods free of stochastic noise.

3.1. OECD/NEA Benchmark Problem 1

Problem 1 from the OECD/NEA benchmark suite is a checkerboard array of spent fuel in a concrete and water fuel storage vault. Each spent fuel assembly consists of a 15 x 15 lattice of Zr-clad fuel pins moderated by water and surrounded by a steel wall. The problem has vacuum boundary conditions on all outer sides. The geometry for this problem is shown in Figure 3.

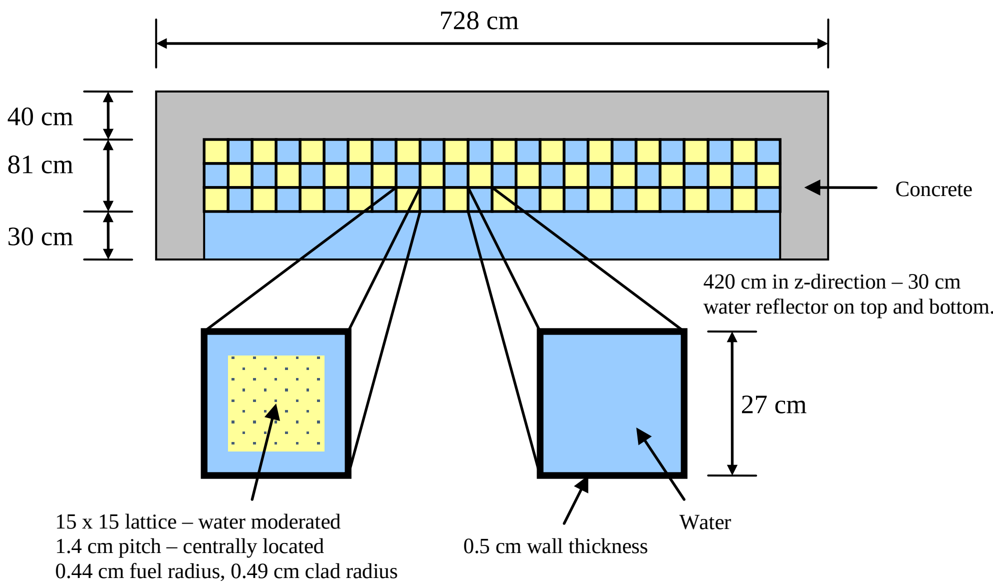

Figure 3. Geometry for OECD/NEA benchmark problem 1.

The specifications for this problem given by the Expert Group on Source Convergence will severely undersample the fissionable regions. At most, the Expert Group specifies running 5000 histories per batch. Given that there are over 8000 fuel pins, running 5000 histories per batch will not be nearly sufficient to sample every fuel pin at each batch. In order to isolate the poor convergence properties due to undersampling, the problem was run with a number of different histories per batch. All cases were started with a uniform source distribution over the array. Figure 4 shows an entropy plot for cases run with 5000, 20000, and 10000 histories per batch.

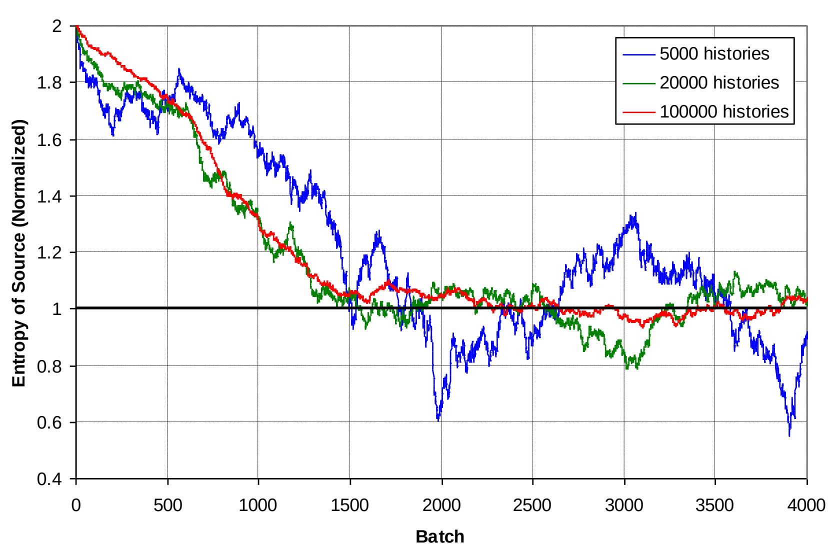

Figure 4. Entropy plot for OECD/NEA benchmark problem 1.

As can clearly be seen in Figure 4, running too few histories per batch leads to very big fluctuations in the source distribution due to stochastic noise. By increasing the number of histories per batch, these fluctuations can be dampened allowing for a better assessment of source convergence. Once entropy plots were obtained for a number of cases with varying histories per batch, each plot was visually inspected and a judgment made as to when the entropy converged. In addition, the stochastic oscillator diagnostic was applied using two different sets of parameters (p, m, ε) as defined above to compare with the assessment made via visual inspection. Table I shows the results of the visual inspection and application of the stochastic oscillator diagnostic.

Table I. Comparison of the number of batches for convergence in OECD/NEA benchmark problem 1 determined by visual inspection and by the stochastic oscillator diagnostic.

Histories per batch	Batch converged via inspection	p	m	ε	Batch converged via Eq. (4)
5000	Not converged	20	50	0.1	60
		500	500	0.1	Not converged
10000	2500	20	50	0.1	143
		500	500	0.1	2603
20000	1700	20	50	0.1	179
		500	500	0.1	2175
40000	1800	20	50	0.1	174
		500	500	0.1	1889
100000	1600	20	50	0.1	156
		500	500	0.1	3200

In all cases, the first parameter set (p = 20, m = 50, ε = 0.1) fails miserably due to the extremely high dominance ratio in this problem. The second parameter set performs reasonably well except in the case of 100000 histories per batch. Notice in Figure 4 that there is a slight decreasing trend in the entropy for this case from batch 1700 to 3100 that is likely due to the strong autocorrelation. As a result, the criterion for the stochastic oscillator diagnostic in Eq. (4) is not met until the trend reverses around batch 3200.

3.2. OECD/NEA Benchmark Problem 2

Problem 2 from the OECD/NEA benchmark suite is a pin-cell array with irradiated fuel. The fuel pin is divided into nine uniform axial regions as shown in Figure 5. We tested Case 2_3 [10] wherein the axial burnup profile is slightly asymmetric since this represented the worst case scenario as far as source convergence is concerned. Reflective boundary conditions are applied on all lateral sides and escape boundary conditions are applied on the top and bottom surfaces.

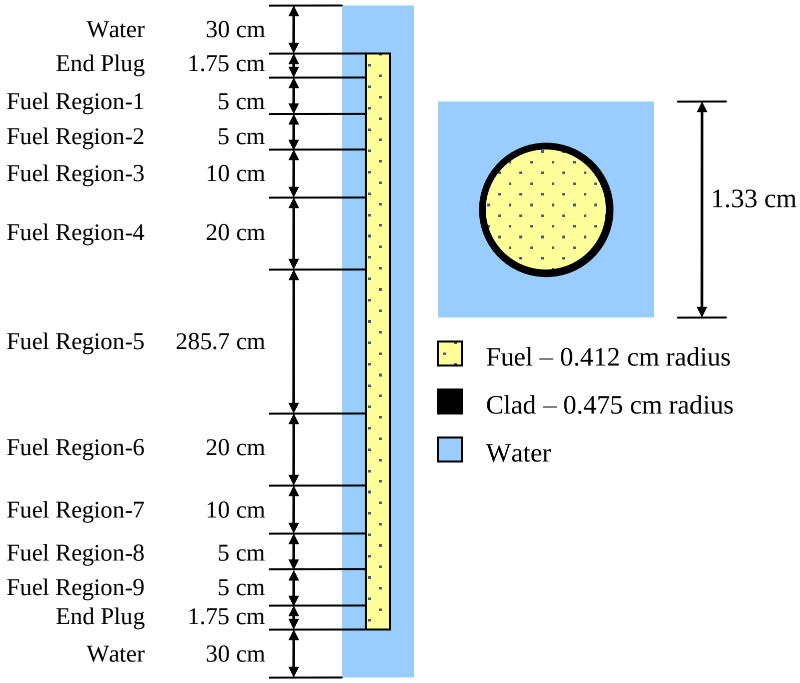

Figure 5. Geometry for OECD/NEA benchmark problem 2.

The specification for this problem calls for 100000 histories per batch. This is more than sufficient to sample all axial regions of the problem. While the dominance ratio of this problem is very high due to the long length of the fuel pin, the convergence to the true source distribution was found to be very smooth unlike in Problem 1 where the loose coupling of the problem led to strong autocorrelative trends in the Shannon entropy. Figure 6 shows the normalized Shannon entropy as a function of batch number.

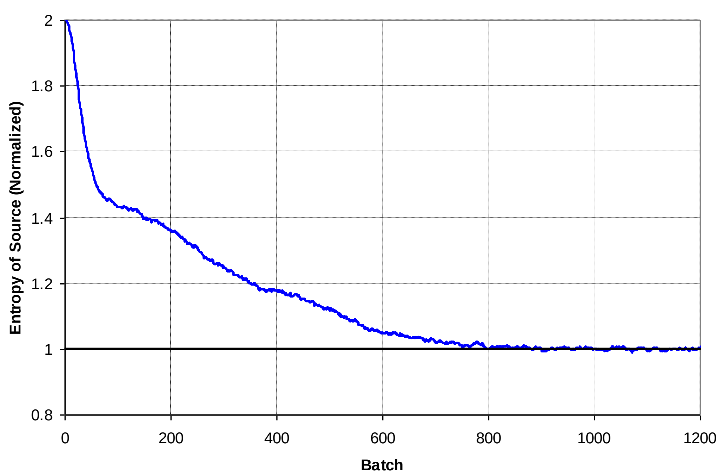

Figure 6. Entropy plot for OECD/NEA benchmark problem 2.

As can be seen from the above figure, the entropy clearly converges around batch 800. Applying the stochastic oscillator diagnostic criteria from Eq. (4) using the first parameter set from Problem 1 (p = 20, m = 50, ε = 0.1), we find that source convergence is attained at batch 722. The stochastic oscillator diagnostic performs well here thanks to the smooth decay of the higher harmonic modes and very limited stochastic noise once convergence is attained.

3.3. OECD/NEA Benchmark Problem 3

Problem 3 from the OECD/NEA benchmark suite is a one-dimensional problem with two slabs of uranyl nitrate solution separated by a thick slab of water. The width of one of the fissile slabs is held constant while the other two slabs are allowed to vary in width as shown in Figure 7. We tested Case 2 [11] in which the water slab is 30 cm and the second fissile slab is 18 cm, introducing an asymmetry into the system.

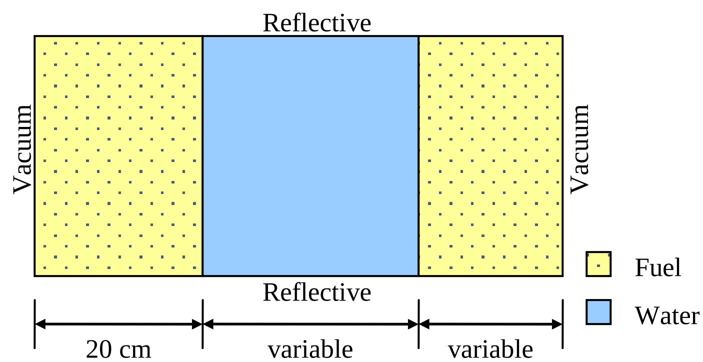

Figure 7. Geometry for OECD/NEA benchmark problem 3.

Running this problem with 5000 histories per batch is sufficient enough to mitigate convergence problems due to undersampling and allow us to make a proper assessment of stationarity. To get the slowest convergence possible, our initial source guess is a uniform source in the smaller slab. Figure 8 shows the normalized Shannon entropy for this problem as a function of the batch number.

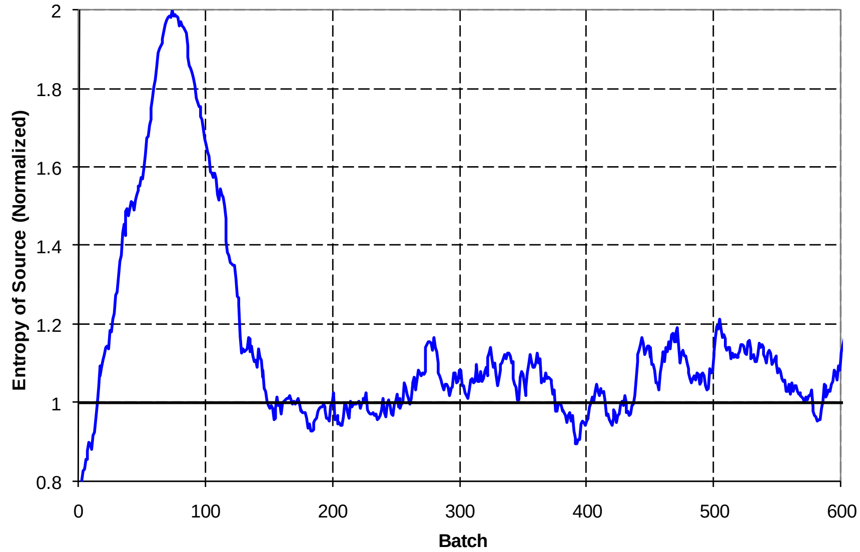

Figure 8: Entropy plot for OECD/NEA benchmark problem 3.

The initial overshoot seen in Figure 8 is typical of problems that are started with sources that do not sample the most important fissile regions. This is commonly encountered in situations where the user defines the starting source as a point source. Visually inspecting the entropy plot, we see that stationarity is reached around batch 170. Applying the stochastic oscillator diagnostic criteria from Eq. (4) again using the first parameter set from Problem 1 (p = 20, m = 50, ε = 0.1), we find that source convergence is attained at batch 163, showing excellent agreement with our visual inspection of the entropy plot.

3.4. OECD/NEA Benchmark Problem 4

The last problem from the OECD/NEA benchmark suite is a 5 x 5 x 1 array of interacting spheres made of uranium metal. The middle sphere in the array is slightly larger than all the others and hence has a disproportionate share of the power, similar to the situation seen in Problem 3. While Problem 3 has a fairly high dominance ratio (on the order of 0.95), this problem has a much lower dominance ratio and really only has convergence problems when stochastic undersampling is an issue. The geometry for Problem 4 is shown in Figure 9. It should be noted that the spheres of uranium metal are separated by air, not void.

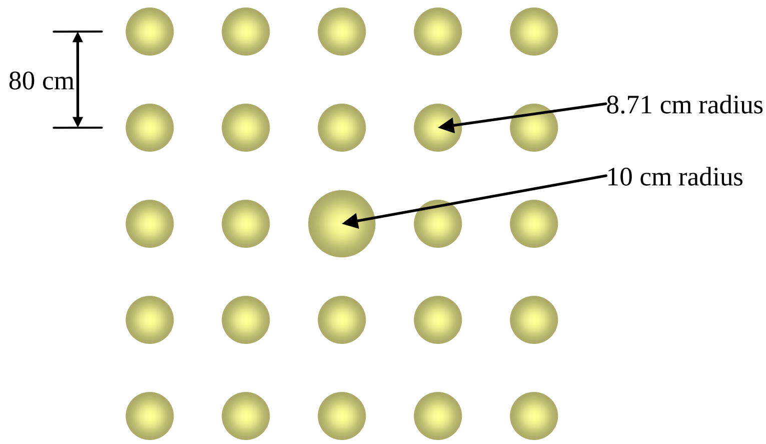

Figure 9: Geometry for OECD/NEA benchmark problem 4.

This problem was run with an initial uniform source distribution and 10000 histories per batch. Figure 10 shows the normalized Shannon entropy versus batch number obtained from this run.

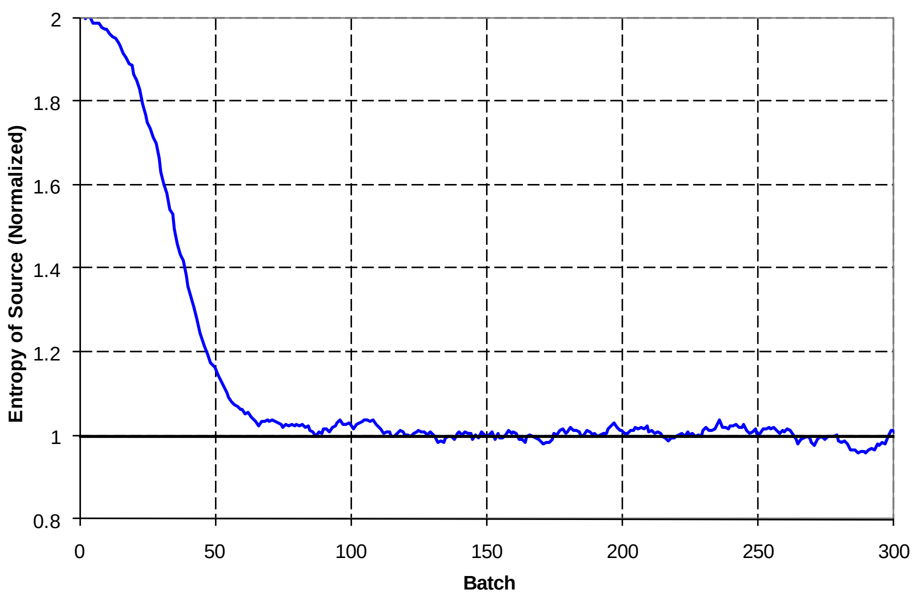

Figure 10: Entropy plot for OECD/NEA benchmark problem 4.

From the entropy plot, we see that the source distribution converges around batch 75 whereas applying the stochastic oscillator diagnostic with p = 20, m = 50, and ε = 0.1 shows convergence to be attained at batch 90. Our subjective assessment of convergence via inspection and that obtained from the stochastic oscillator diagnostic again show very good agreement.

4. CONCLUSIONS

The stochastic oscillator diagnostic developed in the current work represents a significant improvement over previous methods of automated assessment of source convergence in that little modification to existing Monte Carlo codes is required to calculate the needed parameters. In addition, the method provided a reliable indicator of convergence for the convergence benchmark problems evaluated except for the most challenging problem which was sensitive to undersampling and required a modified parameter set to achieve satisfactory performance. It should also be noted that the stochastic oscillator diagnostic was tested on a number of Naval Reactor (NR) core models and also showed very good performance in assessing source convergence.

Further investigations into optimizing the parameter set used for the stochastic oscillator diagnostic may prove to be fruitful. An obvious extension of the present work would be to look into ways of decreasing the number of parameters required for the stochastic oscillator diagnostic, either by introducing functional dependence of one parameter on another, e.g. $m = m(\varepsilon)$, or by correlating the performance of a parameter set to, say, the dominance ratio.

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