Title: CONVERGENCE TESTS FOR THE
FISSION SOURCE DISTRIBUTION
IN MCNP5

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Convergence Tests for the Fission Source Distribution in MCNP

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Abstract

Monte Carlo k-eigenvalue simulations rely on a converged fission source distribution for accurate tallies, and it can often be difficult to determine when the source distribution has converged to a stationary level. Currently, convergence is determined by running a given number of cycles and examining the trend of k_{eff}, the multiplication factor. A newly proposed method to determine convergence is to examine the trend of the entropy of the source distribution. This is considered a more sound approach because the entropy is not affected by eigenmode cancellation effects. Six different tests were created and applied to both k_{eff} and the entropy of the source distribution of five different problem types in MCNP. The goal was to enable MCNP to determine the cycle at which convergence is reached. This series of tests was successful in all but the most difficult cases, i.e. problems with a very high dominance ratio.

1. Introduction

Monte Carlo simulations estimate physical quantities by running many particle histories and averaging the resulting tallies, which are generated by given stochastic models. These histories are grouped into cycles, each of which has a fixed number of particle histories. Source iteration techniques are used to allow the source distribution to converge to and remain in an acceptable range of fluctuation around the true source distribution. Statistically, this convergence is known as reaching stationarity. Cycles are thus divided into two types: inactive, where the distribution is not yet converged, and active, where stationarity has been reached and tallies are taken. Only when the distribution has converged can valid tallies be taken, making it important to accurately determine when the simulation has converged to a stationary level.

The current method to determine convergence in the MCNP Transport Code is to perform a post-processing examination of the resulting k_{eff}. This quantity is integrated globally over the entire reactor. As will be shown Section 2, this is not always an accurate measure of the convergence of the source distribution. Due to eigenmode cancellation effects, k_{eff} can converge much faster than the source distribution. Thus, to determine convergence, the entropy of the source distribution must also be examined. This process is presented in Section 3.

Six different tests were examined in this work to gauge convergence. Each test was applied to five different reactor types, all of which converged in a unique manner. The tests and reactor types are explained in further detail in Section 4. Finally, the results of the tests are presented in Section 5 and discussed in Section 6.

2. Decay Effects of Eigenmodes

Due to the iterative nature of the k_{eff} computation, the dominance ratio, k_1/k_0 , greatly affects the convergence rate of k_{eff}. In Monte Carlo simulations, the cycle wise k_{eff} is calculated as

$$K_{eff}^{(n+1)} = K_{eff}^{(n)} \frac{\int M \cdot \Psi^{(n+1)} d\vec{r}}{\int M \cdot \Psi^{(n)} d\vec{r}} \tag{1}$$

where K_{eff} is the effective multiplication factor, M is the fission operator, and $\Psi^{(n)}$ is the angular flux after n cycles of the power iteration process. It can be shown[1] through manipulation of terms that this quantity can also be estimated as

$$K_{eff}^{(n+1)} \approx k_0 \left[1 + \left(\frac{a_1}{a_0} \right) \cdot \left(\frac{k_1}{k_0} \right)^n \cdot \left(\frac{k_1}{k_0} - 1 \right) \cdot G_1 + \cdots \right] \tag{2}$$

where

$$a_j = \int \Psi^{(0)} \cdot \vec{u}_j dV, \qquad k_0 > k_1 > k_2 > \cdots$$

and

$$G_m = \frac{\int M \cdot \vec{u}_m d\vec{r}}{\int M \cdot \vec{u}_0 d\vec{r}} .$$

The critical portions of Equation (2) are the terms

$$\left(\frac{k_1}{k_0} \right)^n \cdot \left(\frac{k_1}{k_0} - 1 \right).$$

The first term emphasizes how the cycle-wise convergence of k_{eff} is influenced by the dominance ratio. The second term is significant for reactors with high dominance ratios (e.g. $DR \geq 0.99$), as the k_{eff} calculation will converge very quickly, often much faster than the source distribution. This is due to the cancellation effects inherent in the whole core integrations, since positive and negative fluctuations will cancel over the domain. High dominance ratios are common in large reactors with small leakage, heavy-water reflected or moderated reactors, and loosely coupled systems.

3. Convergence to Stationarity

Two quantities can be used to test the convergence of the source distribution. The first is k_{eff}, and is currently the only quantity available to measure convergence in MCNP. The second quantity is a measure of the source distribution itself. Measure of this second quantity is preferred, since k_{eff} is integrated over the entire domain, potentially causing cancellation effects that make the problem appear to converge faster than it actually does.

To properly measure the convergence of the fission source distribution, it must first be characterized as a single number. This can be done through the Shannon's entropy. The fissionable regions of the reactor are divided into m spatial bins and a ratio S_j is taken of the number of source particles in a particular bin j to the total number of source particles. The entropy of that cycle is then estimated as

$$H(S) = -\sum_{j=1}^{m} S_j \log_2(S_j).$$

This provides a single number quantifying the source distribution that can be plotted verse cycle to examine convergence. If local quantities such as power distributions for assemblies such as fuel pins are investigated, the entropy of the source distribution must be examined because it is not affected by the cancellation effects associated with k_{eff} convergence.

4. Convergence Tests

Six different convergence tests were each applied to five different reactor types. The six tests were as follows:

1) Check if value has increased/decreased p times in a row

2) Check if average of previous q values has increased/decreased p times in a row

3) Check if slope of previous q values has changed sign

4) Check if slope of previous q values is within t-statistic

5) Check rate of change of average of previous q values

6) Normality check over previous q values

The first test is a simple one that can be used to determine whether the remaining tests should be run. Since at stationarity the distribution is normal, it is expected that if the value has increased or decreased p times in a row, then the problem is not yet be converged. For these problems $p = 5$.

The second test follows a similar design to the first test, but is applied to the average of the previous q values. Using an average instead of the actual values smoothes the data and allows for a more stable test instead of being misguided by noisy data due to too few particles per cycle. For all problems, q was varied among three values: $q = \{10,20,30\}$.

The third test checks the sign of the slope of the previous q values. When a change in sign occurs, it is expected that the problem has reached stationarity. At that point, the distribution also becomes normal, so the sign of the slope should fluctuate between positive and negative.

The fourth test is similar to the third test, but uses a t-statistic as the criteria for convergence[2]. The t-statistic is a way to determine if the slope of data is statistically zero. This is a standard statistical practice and is implemented as follows:

$$\text{Rejection region: } |t| > t_a$$

where t_a is the statistic from a table, based on $q - 2$ degrees of freedom. t is defined as

$$t = \frac{b}{s/\sqrt{SS_{xx}}}$$

where b is the slope of the data,

$$s = \sqrt{\frac{\sum(y_i - \bar{y})^2}{q - 2}}$$

and

$$SS_{xx} = \sum(x_i - \bar{x})^2 .$$

The fifth test checks the rate of change of the average of the previous q values from cycle to cycle. When stationarity is reached, the average should not vary significantly. The convergence criteria for this test is taken as

$$\text{Convergence region: } \frac{1}{n}\left(\sum_{i=1}^{n} y_i - \sum_{i=2}^{n+1} y_i\right) < 0.001 .$$

The sixth and final test is the Shapiro-Wilk normality test[3].   When the problem reaches convergence, the distributions of k_{eff} and the entropy become normal.   Thus, the convergence criterion is when the previous q values pass the Shapiro-Wilk normality test.   An algorithm for this is already implemented in the MCNP code and is used for this test.   The theory of the test is beyond the scope of this work, so it is not presented.
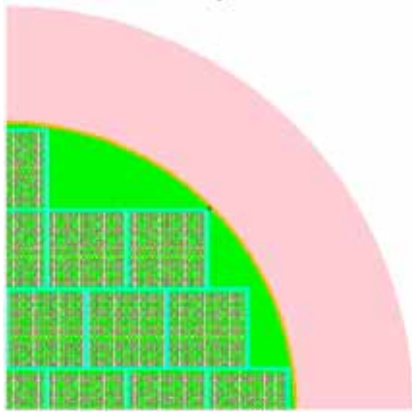

5. Results

On the following pages are the numerical results for each problem.   Each page begins with a brief description and illustration of the problem.   An in-depth discussion of each problem is not given as the exact make-up of each is not directly important.   Instead, these problems were chosen because of their resulting k_{eff} and entropy trends.   The plots of k_{eff} and entropy verse cycle are presented, as well as the cycle at which true convergence appears to be reached.   Next, the results of each six tests are shown for varying q.   The final predicted convergence point is taken as the maximum cycle of the series of tests.

Problem 1
Description
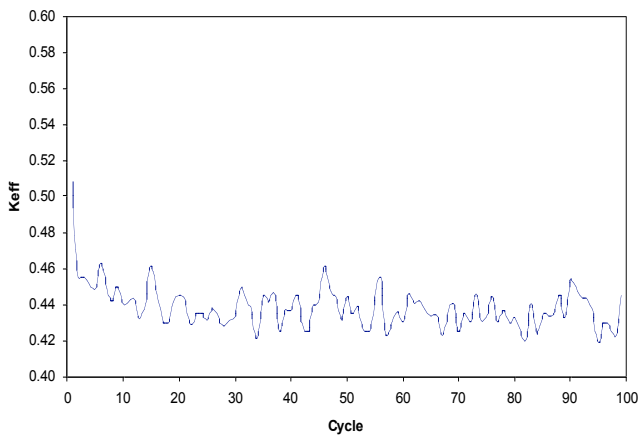Reactor Core – inp24
2000 Particles/Cycle

Convergence Plots

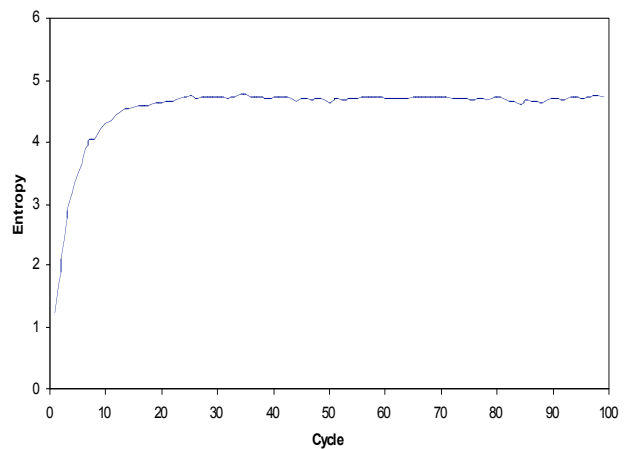Figure 1: k_{eff} Convergence
True k_{eff} Convergence: ~20

Figure 2: Entropy Convergence
True Entropy Convergence: ~20

Convergence Tests Results
Predicted k_{eff} Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	5	11	15	19	16	16		19
20	5	21	32	24	36	32		36
30	5	31	41	32	46	42		46

Predicted Entropy Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	17	10	32	37	32	39		39
20	17	31	42	43	43	44		44
30	17	46	48	50	49	51		51

Problem 2

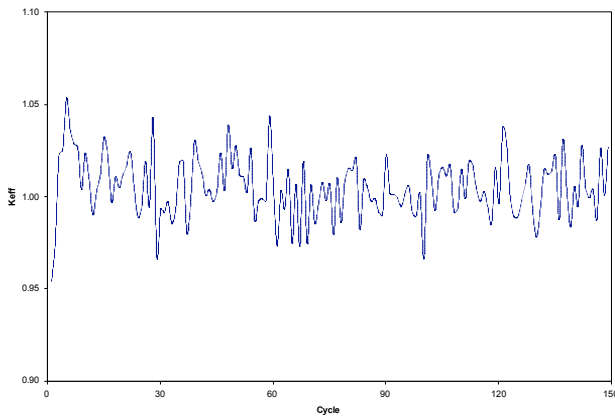## Description
Reactor Core – PNL33i
5000 Particles/Cycle
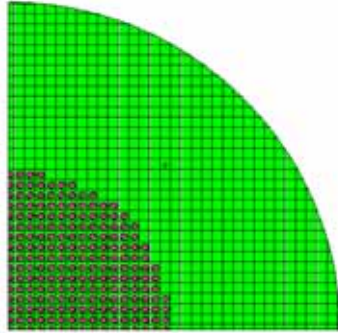
Convergence Plots

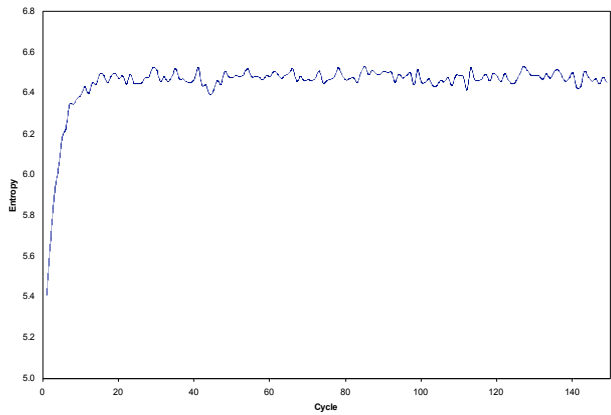Figure 3: k_{eff} Convergence
True k_{eff} Convergence: ~20

Figure 4: Entropy Convergence
True Entropy Convergence: ~20

Convergence Tests Results

Predicted k_{eff} Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	6	10	11	19	12	15		19
20	6	20	20	23	21	25		25
30	6	30	30	32	46	35		46

Predicted Entropy Convergence

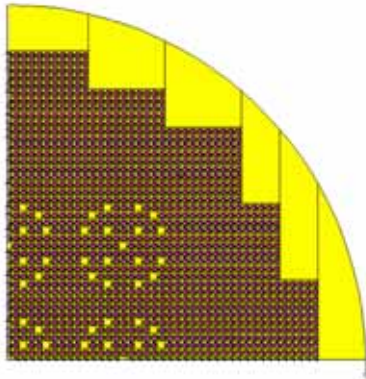| Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	8	10	22	24	24	26		26
20	8	29	33	33	34	37		37
30	8	38	42	43	43	44		44

Problem 3

Description

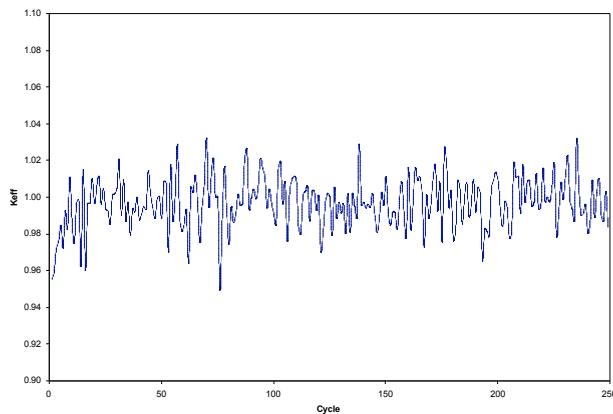Reactor Core – bawxi2
5000 Particles/Cycle

Convergence Plots

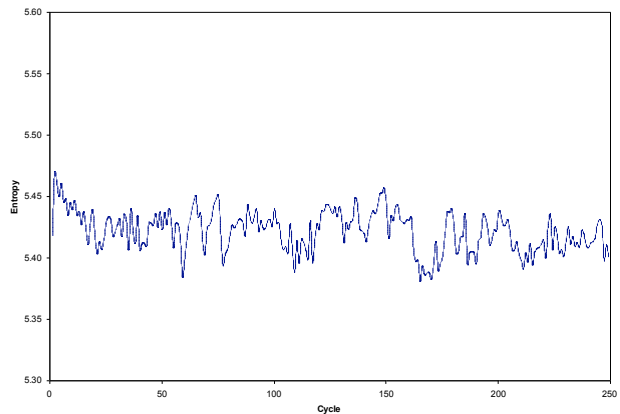Figure 5: k_{eff} Convergence
True k_{eff} Convergence: ~20

Figure 6: Entropy Convergence
True Entropy Convergence: ~20

Convergence Tests Results

Predicted k_{eff} Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	6	10	14	17	14	15		17
20	6	20	27	25	36	28		36
30	6	30	37	34	44	40		44

Predicted Entropy Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	5	10	10	18	26	15		26
20	5	20	31	21	33	35		35
30	5	30	44	31	46	35		46

Problem 4

Description
Array of Spheres – test4s
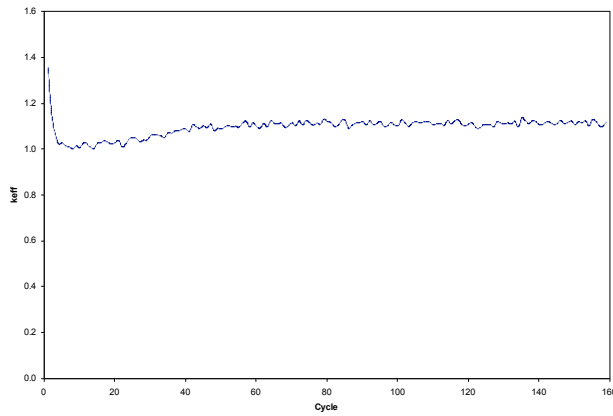5000 Particles/Cycle
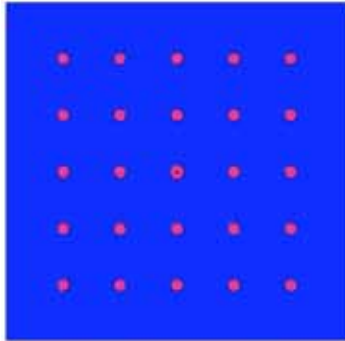
Convergence Plots

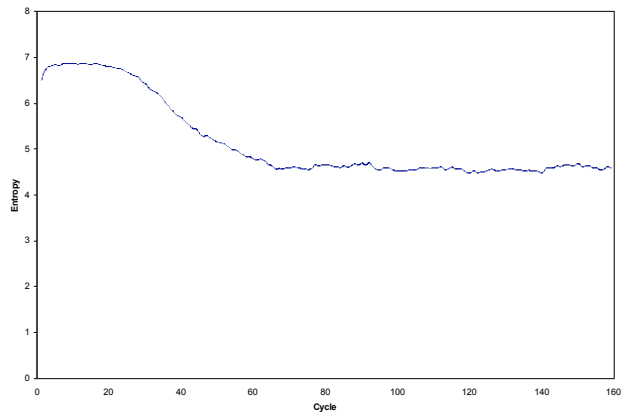Figure 7: k_{eff} Convergence
True k_{eff} Convergence: ~50

Figure 8: Entropy Convergence
True Entropy Convergence: ~70

Convergence Tests Results

Predicted k_{eff} Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	5	13	13	15	15	17		17
20	5	23	22	58	23	25		58
30	5	32	31	33	31	35		35

Predicted Entropy Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	6	12	15	15	16	18		18
20	6	37	21	85	22	25		85
30	6	58	90	97	91	97		97

Problem 5

Description
Fuel Storage Vault – bench1
2000 Particles/Cycle
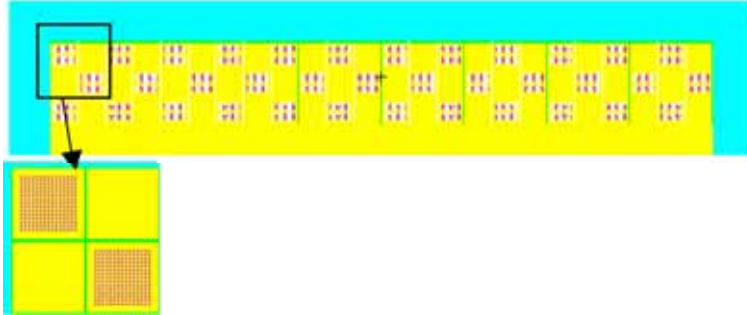
Convergence Plots

Figure 9: k_{eff} Convergence
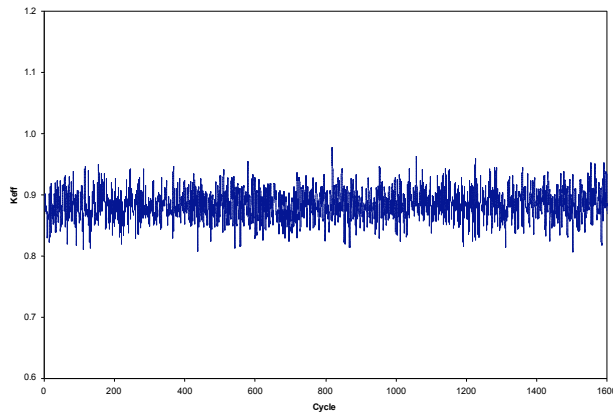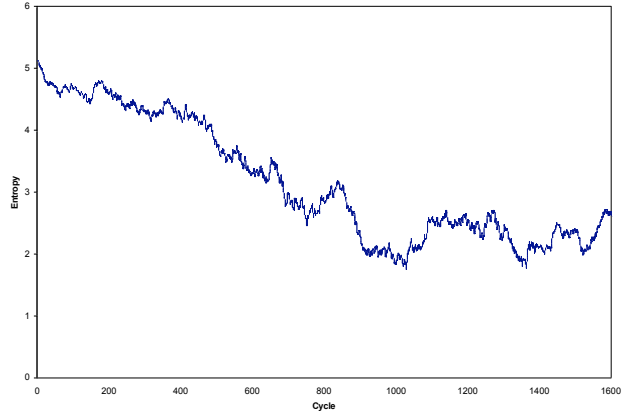True k_{eff} Convergence: ~10

Figure 10: Entropy Convergence
True Entropy Convergence: ~900

Convergence Tests Results

Predicted k_{eff} Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	5	10	13	14	13	15		15
20	5	20	20	21	30	25		30
30	5	30	30	33	31	35		35

Predicted Entropy Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	7	10	35	35	36	36		36
20	7	20	71	51	72	74		74
30	7	48	76	73	77	78		78

6. Discussion

The first test consistently under predicted the convergence point, and it can be reasonably assured that if the first test fails, the problem is not converged. Once it passes, however, further tests should be run to determine if the problem is truly converged.

The second test predicted much higher values of convergence than the first test, even though it was similar. This is because it took averages of the previous q values. It was not consistent in correctly predicting convergence, especially for $q = 10$, and should not be used as a stand-alone test.

The third and forth tests were very similar to each other, though they sometimes gave considerably different results. Neither test predicted a consistently higher convergence point. Test four, however, often proved the most rigorous of the six tests when $q = 10$.

The fifth and sixth test seemed to predict the highest convergence points out of all the tests. This is important because the combination of these tests almost always ensured that the problem was converged. While the convergence criteria for the fifth test (i.e. that the change in average was less than 0.001) was arbitrarily chosen, it did seem to work considerably well. It was clear in the sixth test that the more data points used, the better the test performed.

It should be noted that while certain problems did have large fluctuations in their k_{eff} and entropy plots (especially in problem 2 and 3), the convergence tests were still able to accurately predict when the problem reached a stationary level. The series of tests only failed for problem 5 where the data did not follow an exponential or logarithmic trend.

7. Conclusion

An automated and rigorous method to determine convergence of the source distribution to the fundamental mode in MCNP would be very beneficial to ensuring accurate tallies. Data can often have such large fluctuations due to the number of particles per cycle that it is difficult to properly determine the point of true convergence. Predicting this point of convergence can be effectively done with a series of tests as was shown in this work. These tests must be applied to both the entropy of the source distribution and k_{eff}, especially if local quantities such as power distributions in fuel bundles are examined. In most cases, the series of tests applied in this work predicted sufficient points of convergence. Only in the most difficult problem (problem 5) did the tests fail.

There are several areas that this work could be extended to. While these tests worked in most cases, other tests should be created and applied to the problems that failed. Also, a new routine to determine the dominance ratio should be implemented into MCNP so that the user can have an indication of whether his problem is a slowly converging type. Finally, it would be beneficial to allow the user to test the fluctuations of the data (and, hence, the number of particles per cycle) to ensure that they are sufficiently smooth.

References

[1] T. Ueki and F.B. Brown, "Informatics Approach to Stationarity Diagnostics of the Monte Carlo Fission Source Distribution," Trans. Am. Nuc, **89**, 458 (2003).

[2] S. Kokoska and C. Nevison, *Statistical Tables and Formulae*. New York, NY: Springer-Verlag,1991

[3] S. S. Shapiro and M. B. Wilk, "An Analysis of Variance Test for Normality (Complete Samples)," Biometrika, **52**, 591 (1965).