International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2011)
Rio de Janeiro, RJ, Brazil, May 8-12, 2011, on CD-ROM, Latin American Section (LAS) / American Nuclear Society (ANS)
ISBN 978-85-63688-00-2

CONVERGENCE DIAGNOSTICS FOR EIGENVALUE PROBLEMS WITH LINEAR REGRESSION MODEL

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ABSTRACT

Although the Monte Carlo method has been extensively used for criticality/eigenvalue problems, a reliable, robust, and efficient convergence diagnostics method is still desired. Most methods are based on integral parameters (multiplication factor, entropy) and either condense the local distribution information into a single value (e.g., entropy) or even disregard it. We propose to employ the detailed cycle-by-cycle local flux evolution obtained by using mesh tally mechanism to assess the source and flux convergence. By applying a linear regression model to each individual mesh in a mesh tally for convergence diagnostics, a global convergence criterion can be obtained. We exemplify this method on two problems and obtain promising diagnostics results.

Key Words: Monte Carlo, fission source convergence diagnostics, flux distribution based diagnostics, linear regression model.

1. INTRODUCTION

This paper examines the use of Monte Carlo method in eigenvalue or criticality problems. The initial guess of the source distribution in eigenvalue problems is frequently significantly different from the converged one, so a reliable convergence diagnostics is desired to guarantee that collecting data takes place only after the convergence of the source or flux distribution is achieved. Even when k_{eff} is the primary interest in the simulation of eigenvalue problems, just focusing on the convergence of k_{eff} may be misleading. The cause of potential false positive diagnostics is the faster convergence rate of k_{eff} than that of the source distribution. Therefore, basing the convergence diagnostics on the source distribution is much more reliable. As an example, the Shannon entropy method [1] converts the mesh-based source distribution to a single value in order to represent the status of the system and perform convergence check. This method is implemented into MCNP5[2] as a convergence diagnostics indictor, but due to the discarding of the local source information, the entropy indicator reports false positive diagnostics at times for large loosely-coupled problems[3] [4]. As a potential remedy, we propose to analyze the trends of the cycle-based flux distribution, which corresponds to the source distribution, using mesh tally in order to determine the convergence.

2. LINEAR REGRESSION MODEL

In the simulation of eigenvalue problems, the mesh tally may be used to records fluxes in all specified meshes together with relative errors based on the contributions of each particle.

Generally, only a single total mesh tally result is reported, such as in MCNP5, to represent the average volume fluxes for all active generations. As a result, no cycle-based flux data, which record the estimated volume fluxes after each generation, are available. We propose to establish the cycle-based flux first, and observe the changing trends in estimated fluxes in each mesh to determine how many generations are needed as inactive generations. This observation procedure could be enhanced by describing the cycle-based flux behavior with the time series theory, in which fluxes in the current generation contain not only random noises, but also dependence from the fluxes in the previous generation. This model is accurate but complex; thus, in this paper we apply a simpler model—linear regression model [5]—to approximate the behavior of the mesh tally evolution.

A linear model between independent predictors X_i and responders Y_i is expressed as

$$Y_i = \beta_0 + \beta_1 \times X_i + \varepsilon_i \,, \tag{1}$$

where β_0 and β_1 are coefficients of the linear regression model; and ε_i is an independent random error term generally following a normal distribution N(0,σ^2). Therefore, three unknown parameters, β_0, β_1, and σ^2, need to be estimated by available observations. For n sets of observations (x_1,y_1) to (x_n,y_n), representing random variables X_i,andY_i, the least square estimator of the coefficient β_1 is

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}, \text{ where } \bar{x} = \frac{\sum_{i=1}^{n} x_i}{n} \text{ and } \bar{y} = \frac{\sum_{i=1}^{n} y_i}{n}. \tag{2}$$

In addition, the least square estimator of the coefficient β_0 is

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \times \bar{x} \tag{3}$$

The estimate of the standard deviation of $\hat{\beta}_1$ is

$$\sigma(\hat{\beta}_1) = \frac{\hat{\sigma}}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}}\,, \tag{4}$$

where $\hat{\sigma}$ is the estimated standard deviation of the random error term given by

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 \times x_i)}{n-2}\,. \tag{5}$$

We treat the cycle-based fluxes as the responders to the assigned predictors, a sequence of integrals from 1 to *n*. Under the condition of convergence, the responders should oscillate along an expected value, which means the estimated slope coefficient $\hat{\beta}_1$ is close to zero. Otherwise, the slope coefficient has a relative large absolute value, which indicates that the changing of the flux is still ongoing. The length, *n*, of the sequence of predictors and responses should be chosen large enough to fully represent the changing trend and reduce the affects from the random noise.

3. DIAGNOSTICS METHODS

In a regression process, we generally discard the mesh tally results from the first n_o generations, since some abnormal behavior of the mesh tally may exist during the initialization. In this study we used $n_o = 10$. Then, we pick the mesh fluxes from the next *n* cycles as the regression set and perform linear regression. After that, we discard the first flux in the regression set and add the next mesh flux into the regression set. The re-constructed new regression set with the same size *n* is used to perform the linear regression again. We propose to conduct the hypothesis test for the slope coefficient $\hat{\beta}_1$. Note that for optimum efficiency it may be sufficient to perform the hypothesis test only after each *m* cycles (where *m* is some fraction of *n*) rather than after each cycle.

The hypothesis test

$$H_0: \beta_1=0 \text{ vs. } H_a: \beta_1 \neq 0$$

for the coefficient $\hat{\beta}_1$ is to identify whether the coefficient is zero, which concludes that the responders have no linear dependence on the predictors, or not. For each regression, the estimated $\hat{\beta}_1$ follows a t-distribution with *n-2* degrees of freedom, so we choose the t-value as

$$t = \frac{\hat{\beta}_1}{\sigma(\hat{\beta}_1)} . \tag{6}$$

We compare the t-value and the standard t-distribution with the significance level α If the t-value is greater than the 1-α/2 quantile of the t-distribution, $t_{1-\alpha/2,n-2}$, we reject the null hypothesis and take the opposite one that $\hat{\beta}_1$ does not equal 0. Otherwise, we accept the null hypothesis; therefore conclude that the flux has converged in the specific mesh. We perform the hypothesis test in all the meshes for the consecutive regression procedure and summarize the acceptance of the null hypothesis at the first time for each mesh, respectively. With the discarded n_0 initial generations, we obtain a table containing the index of the generations satisfying null hypothesis in each mesh. The maximum number in this table is the global convergence diagnostics result.

In this diagnostics procedure, we need to specify two parameters: the size of the regression mode, *n*; and the significant level α. The size *n* should be chosen to be big enough to override the impact of the random oscillations and reduce the variance of the regression model, but a too large *n*, which demands more generations, is not acceptable either because in the transition to the convergence portion, the flat oscillation may overwrite the changing part. The significance level α defines the probability of false negative. It is frequently set to 0.10 and we use similar values in this paper for comparison. More analysis about the influence of the significance level is in later parts of this paper.

In addition to the t-distribution diagnostics, an absolute value threshold is also applicable to the regression model. This approach determines the maximum number of the regression with the absolute value of coefficient $\hat{\beta}_1$ smaller than a particular artificial threshold. However, choosing the threshold value is subjective and depends on the simulated system and user experience. Therefore, we will not detail or exemplify that method in this paper, but we would like to clarify the capability of this alternative approach.

4. ONE-DIMENSIONAL TEST PROBLEM

We first demonstrate the capability of the linear regression diagnostics with a one-dimensional one-group problem. The system contains two types of fission materials: high reactivity material (HRM) and low reactivity material (LRM), with cross-sections listed in Table I. The system size is 9 MFP(mean free path). Three regions exist in the system as shown in Figure 1: -4.5cm to -2.0cm with HRM, -2.0cm to 2.0cm with LRM, and 2.0cm to 4.5cm with HRM. We employ vacuum boundary conditions to both external boundaries at -4.5cm and 4.5cm. A single point source is located at -4.0cm, but it does not take long for the neutron distribution to reach the right HRM region because of the small MFP of the system. However, the LRM in the middle still causes the weakly coupled disconnection between the two HRM region; thus, the fission source distribution needs many generations to be converged. Although this point source does not cause any observable problem in this test simulation, more cautions, which will be explained later, are needed to initialize the source distribution. Actually, we can compute the dominance ratio, which turns out to be 0.9811, with the modified power iteration method [6] [7]. Although the dominance ratio is not over 0.99 the source convergence is still slow due to weak coupling. We simulate the problem with 40,000 particles per generation for 400 generations, and divide the system into 100 equal-size meshes to obtain the mesh tally. The same mesh tally is used for the computation of the entropy. Figure 2 shows the entropy evolution, which seems to indicate that the convergence is reached after ~150 generations.

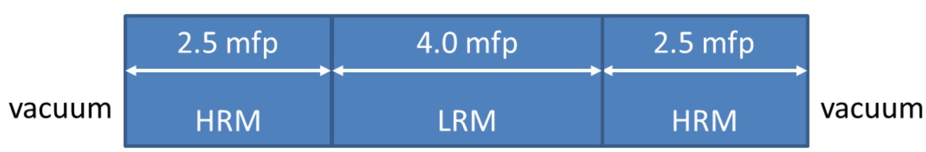


Figure 1. Test problem schematic

Table I. Material data for the one-dimensional problem

	HRM	LRM
Σ_t	1.0 cm^{-1}	1.0 cm^{-1}
Σ_c	0.1 cm^{-1}	0.45 cm^{-1}

Σ_s	0.8 cm^{-1}	0.5 cm^{-1}
$\nu\Sigma_f$	0.3 cm^{-1}	0.15 cm^{-1}
Σ_f	0.1 cm^{-1}	0.05 cm^{-1}
ν	3.0	3.0

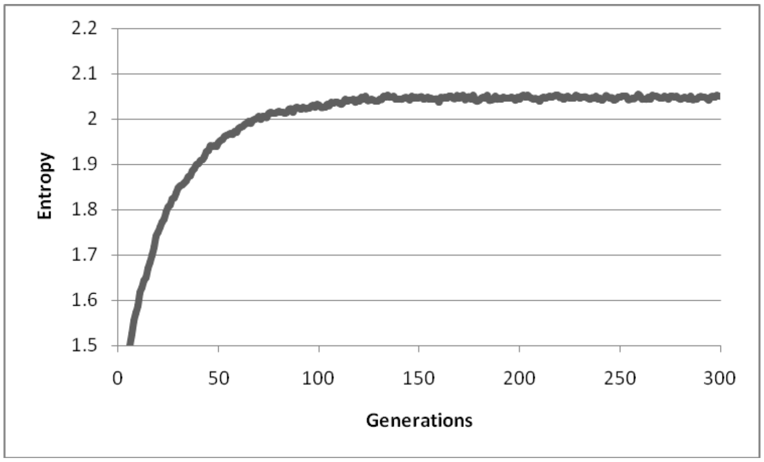


Figure 2. Entropy evolution for the one-dimensional problem with a single point source

We discard the first 10 generations and perform our linear regression diagnostics upon the mesh tally with the significance level α=0.10. We illustrate the impact of the regression size *n* by summarizing the diagnostics result for different sizes *n*, varying from 3 to 101 with step size 2, and plotting them in Figure 3. The y axis represents the final convergence diagnostics results including the initially discarded 10 generations.

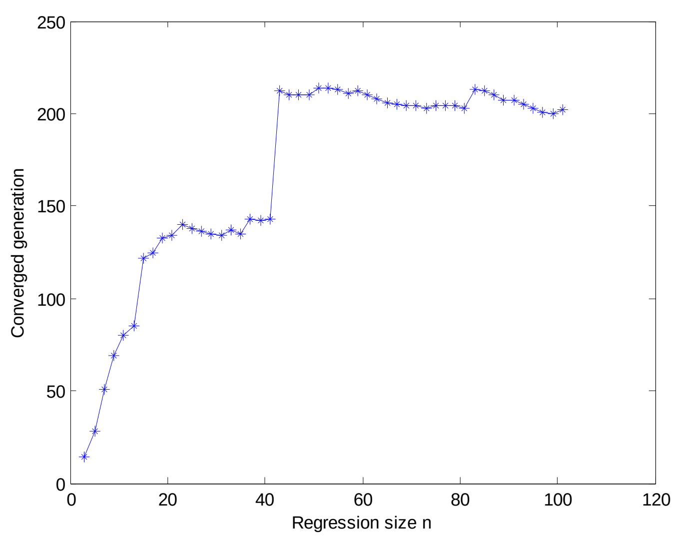


Figure 3. Diagnostics results with significance level 0.10 versus different regression size n for the one dimensianl problem with a single point source

This figure clearly shows that a relatively small number of cycle *n*, in this case smaller than 50, cannot capture the slow changing trend of the fission source redistribution. When *n* is sufficiently large, the diagnostics results are relatively stable and round 200, which validates the consistency of the linear regression diagnostics with different (but sufficient) size *n*. Compared to the entropy indicator, this result is stricter at this significance level. We change the significance level α to be 0.20 and depict a similar diagnostics curve in Figure 4. This time, the average diagnostics result is slightly stricter than the 0.10 case.

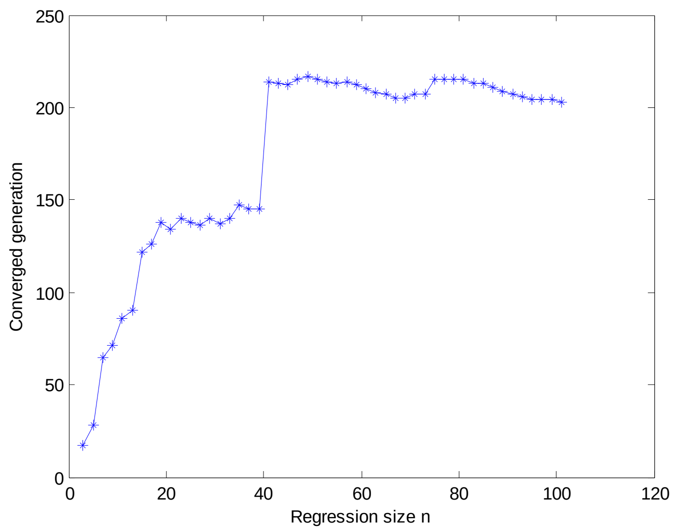


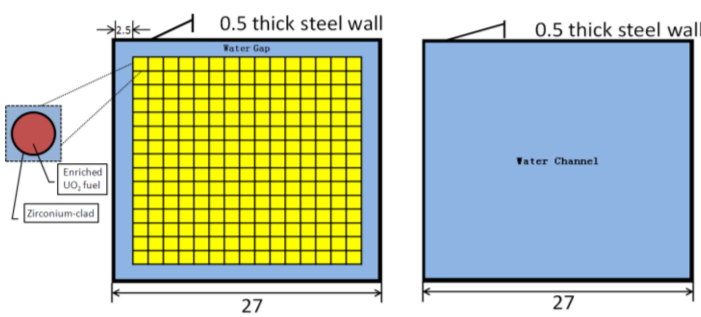
Figure 4. Diagnostics results with significance level 0.20 versus different regression size n for the one dimensional problem with a single point source

For this simple test problem, the linear regression diagnostics method yields results relatively consistent with the entropy indicator (~200 vs. ~150 cycles, respectively), for the 0.20, 0.10 significance levels and regression size is sufficiently large to stabilize results. Unlike the entropy indicator, which is a posterior one especially in MCNP5, this method can provide diagnostics during the simulation requiring as overhead just one mesh tally. Once the diagnostics reports that the system has converged, we could begin "active cycles" with all requested tallies.

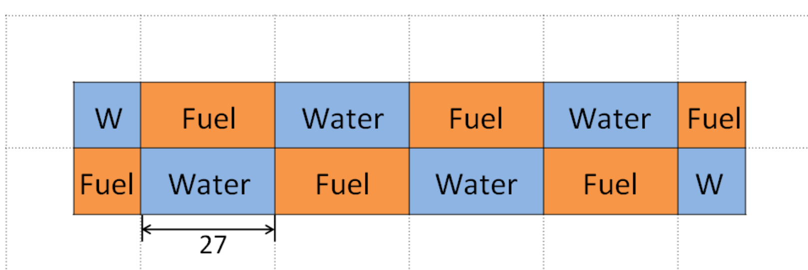
Before moving to the next example, we would like to clarify several issues to understand this method better. Since the method relies on the flux mesh tally, a zero-flux mesh generally does not indicate convergence but inadequate sampling and may thus endanger the diagnostics if checked only for trend. Therefore, every mesh should report some flux estimate after the initially discarded n_0 generations. Although in this problem we choose to use a single point source in the left HRM region, neutrons have travelled to all regions of the system and produced non-zero tallies after 10 generations. However, in a general case, the presence of enough particles is highly desired for the diagnostics. Another important feature of the method that needs to be pointed out is the choice of the significance level. The hypothesis test is based on the null hypothesis that β_1=0; in other words, to perform the hypothesis test, we assume to accept the null hypothesis unless we obtain strong enough evidence to reject the null hypothesis. One effect of this feature is that reducing the significance level is actually restricting the diagnostics; this is the reason the 0.20 level diagnostics gives a stricter result in the comparison. However, since the tail part of the t-distribution is relatively small, changing of the significance level in the tail parts would not affect the diagnostics results much. The other effect of the hypothesis test is that the diagnostics method is conservative and tends to make under-estimate of the convergence diagnostics. As a result, we suggest maintaining general number of inactive generations even after the diagnostics and before the tallying simulation.

5. SIMPLIFIED BENCHMARK PROBLEM

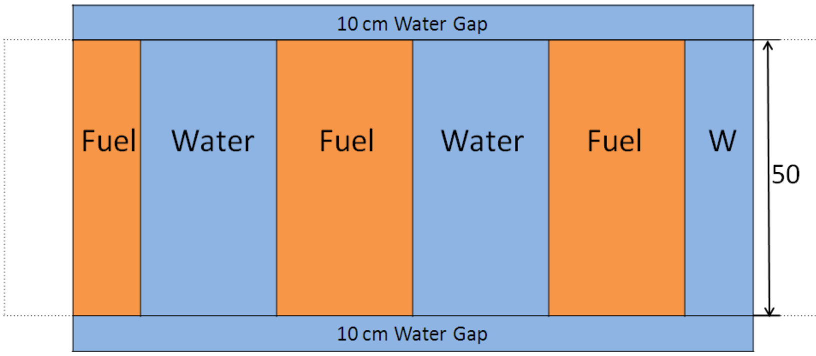
We used this method to analyze a real-life-like problem—a simplified version of the OECD/NEA storage fuel pool problem [8]. We maintain the fuel assembly structure and the materials, which contains U235 enriched up to ~5%, used in the benchmark description as shown in Figure 5(a). Compared to the original benchmark specifications, we simplify the array composition as shown in Figure 5(b) with reflective boundary conditions in x and y directions. The corner elements are one quarter of the full size element, and the other elements are half size. We also shorten the vertical size of the fuel assembly to 50cm in height, and cover the system with 10cm water gap at the top and bottom of the system with vacuum boundary conditions in the z direction. Therefore, this system maintains the loosely-coupled property of the original system but with a reduced size, which results in a reduction of the computational resources needed.



(a) Fuel assembly and water gap



(b) Horizontal cross section view of the system



(c) Vertical front view of the system

Figure 5. Geometry of the simplified problem

We simulate this problem in MCNP5 with 50,000 particles per generation. The initial source distribution is uniform along y and z directions, but 99% of neutrons focus on the first column of the array, i.e., 0 to 13.5cm along the x direction. Therefore, we expect a re-distribution of the neutron source all over the system after convergence. We divide the system into ten partitions along the x direction, three partitions along the y direction, and five partitions along the z direction without the water top and bottom; in other word, 150 meshes are used for the mesh tally. One simulation was used to generate a data set of the cycle-based mesh fluxes for 300 generations.

We first use the entropy indicator. Figure 6 shows the entropy evolution using a slightly different mesh structure from the one used for the mesh tally: only two even partitions exist along y direction; the partitions along the other directions remain the same. The entropy plot suggests that the source distribution has converged after ~150 generations.

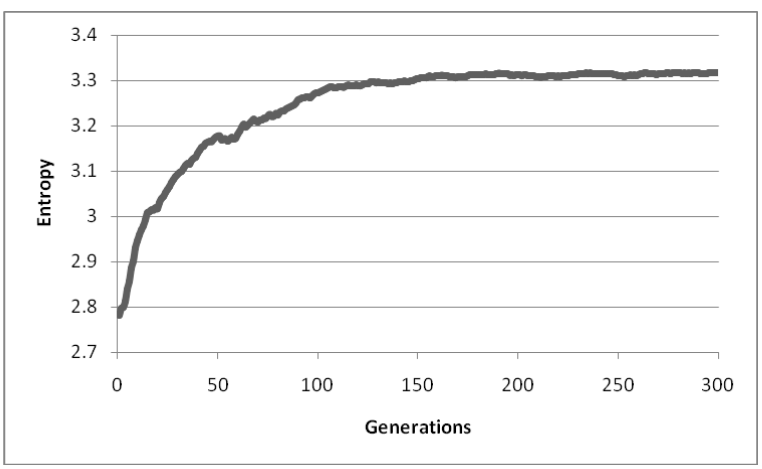


Figure 6. Entropy evolution for the simplified benchmark problem

We then apply the linear regression diagnostics to this problem by analyzing the 300 cycle-based mesh fluxes. We choose the significance level to 0.10 first and plot the diagnostics results versus the regression size *n* in Figure 7. A reasonable large regression size *n* is greater than 40 for this case; and the diagnostics results are relatively stable around 160, which is consistent with the entropy indicator. We then change the significant level to 0.20, and similar diagnostics results are shown in Figure 8. The diagnostics results are around 160, which is similar to the previous case. One unexpected trend is present in both of the figures when the regression size is too large. This abnormal behavior occurs because the chosen size is too large compared with the 300 generations simulation. As a result, the diagnostics criterion will report the maximum available generation for the limited data set. Therefore, we would like to repeat our statement that a too large regression size does not always give a meaningful result This behavior can be avoided by limiting the length of regression size relative to the total number of generations or increasing the number of generations to allow the longer regression size.

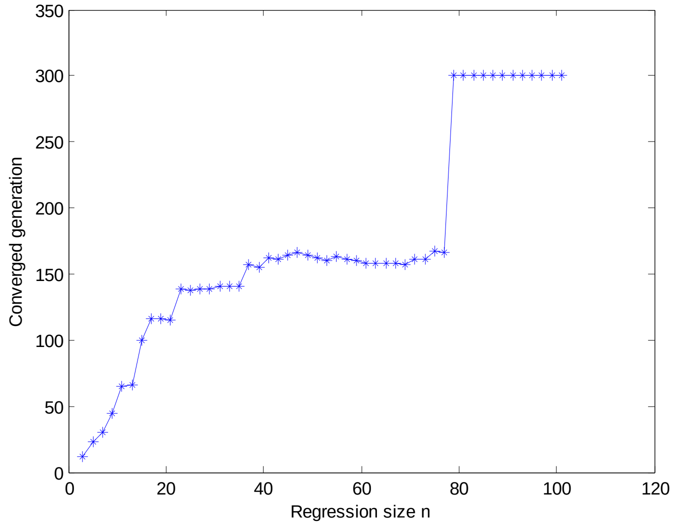


Figure 7. Diagnostics results with significance level 0.10 versus different regression size *n* for the simplified benchmark problem

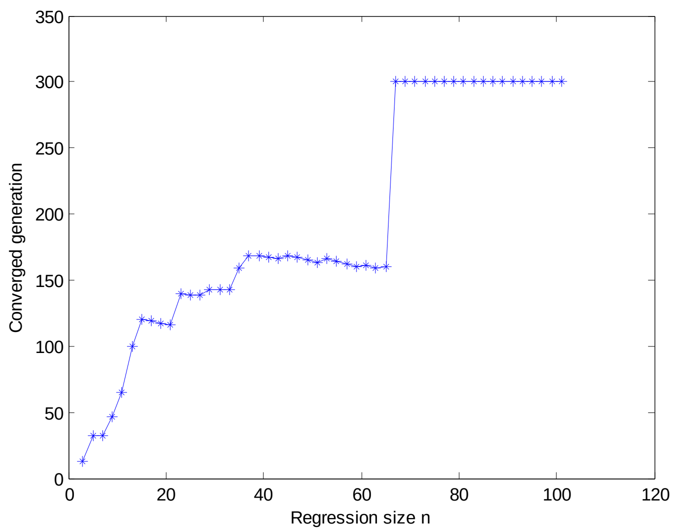


Figure 8. Diagnostics results with significance level 0.20 versus different regression size *n* fo r the simplified benchmark problem

In order to validate our diagnostics results, we pick a mesh near the left boundary, which has high flux initially because of the initial source distribution. Then along with the re-distribution of the fission source, the flux in the mesh changes and finally reaches convergence as shown in Figure 9. The initial jump is due to the inaccurate initial guess of k_{eff}, which is also the reason that we discard the first ten generations. After that, the flux behaves normally and converges after ~150 generations, which validates the entropy indicator and our linear regression diagnostics results. Actually, from Figure 9, we may find that the flux changes with an exponential behavior rather than a linear behavior. To examine the impact, we transform the flux to the logarithmic scale and perform the linear regression diagnostics again. The transformation turns out to have little impact on the diagnostics results, so we do not perform the transformation in general. This behavior is actually comprehensible: for a large flux change, both will detect the non-convergence; and for a small flux changes (in the converged stage) the linear relation is a reasonable approximation to exponential, and less expensive.

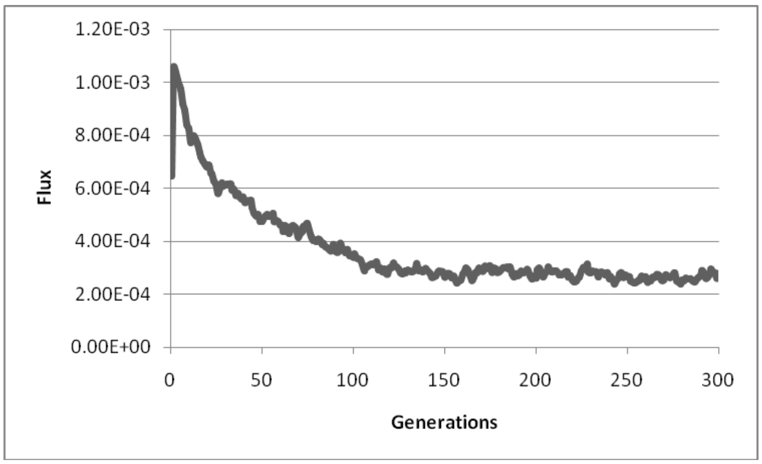


Figure 8. Flux evolution in a particular mesh for the simplified benchmark problem

6. CONCLUSIONS AND FUTURE WORK

In this paper, we propose a linear regression diagnostics method, which is based on the cycle-based mesh tally. It utilizes the local information of the source or flux re-distribution, which significantly enhances its reliability. We apply this method to a simple one-dimensional problem and a real-life simplified benchmark problem. In both cases, the diagnostics method provides accurate diagnostics results, consistent with the entropy indicator. Moreover, due to its use of local information, we expect that this method will work for more challenging cases where the entropy indicator could fail, such as the problems analyzed in Ref. 3 and 4. In our future work, we intend to apply this method to more complex problems to verify its validity, and if confirmed, fully implement in a production-type Monte Carlo code.

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