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The Optimal Source Bias Method based on RMC code

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ABSTRACT

When criticality calculation is performed with Reactor Monte Carlo (RMC) code for reactor analysis, the fission source iterative method is selected. There are two strategies to sample the fission neutrons in each fissile region: the conventional Proportional Stratified Sampling Method that focuses on the real physical process, and the author-developed Optimal Stratified Sampling Method that focuses on the optimal mathematics treatment. The Optimal Stratified Sampling Method have the effect of global variance reduction and could be easily implemented with the use of optimal source bias coefficients. However, the calculation of optimal source bias coefficients needs the values of variances in advance, which is almost impossible. To meet the requirement, a Batch Approximate Method is then put forward. The Batch Approximate Method based on the Batch algorithm and Shannon Entropy Diagnosis, eliminates the correlation among cycles during the criticality calculation. Combining the Optimal Stratified Sampling Method and the Batch Approximate Method, the Optimal Source Bias Method is established and developed in RMC code. The Optimal Source Bias Method was tested with a standard Pressurized Water Reactor assembly. The effect of global variance reduction was found, as well as the flattening of variance distribution. So, the new method is valuable for the high fidelity computation of the RMC code.

1. Introduction

The Monte Carlo method has received wide attention in recent years, especially in the field of reactor physical calculation, and a lot of Monte Carlo codes were developed those year, such as the RMC code (Wang et al., 2015). The Reactor Monte Carlo code (RMC) is a Monte Carlo code for reactor core analysis, it is developed by Department of Engineering Physics at Tsinghua University, Beijing, China. It can finish both criticality calculation and fix source calculation. The RMC code now has a lot of advanced functions, such as on-the-fly nuclear cross sections processing (Liu et al., 2016), random geometry capability treatment (Liu et al., 2015), and it just finished the calculation of BEAVRS benchmark (Liu et al., 2017).

The criticality problem (Li et al., 2010) is characterized by calculating k_{eff}, which solves the eigenvalue of the neutron transport equation. In reactor physics, k_{eff} is regarded as the ratio of the children neutrons number to the father neutrons number between the adjacent neutron cycles (X-5 Monte Carlo Team, 2003). So, in order to calculate k_{eff}, the fission source iterative method (Nease et al., 2008) is used. That means the fission neutrons produced in the current cycle is the initial source of the next cycle. So, the number of source neutrons sampled in each fissile region is in direct proportion to the fission neutrons produced in the last cycle. This makes sense physically, but not mathematically. Therefore, there are some tough questions:

How many fission neutrons should be sampled for a certain fissile region to minimize the global variance?

How should the source neutrons be spatial distributed per cycle to achieve mathematical optimization?

Facing those problems, the conventional method is based on the real physical process. That means the number of source neutrons sampled in a certain fissile region is exact the total number of fission neutrons produced in that fissile region, and the spatial distribution of source neutrons is the same as the flux distribution. After mathematic analysis, we could find that the conventional method has not reached the optimum, and still has room for improvement.

In order to deal with the questions, the authors came up with a new method to achieve the optimal spatial distribution of source neutrons, the method named Optimal Source Bias Method (OSBM). The new method based on the Optimal Stratified Sampling Method (Blomquist and Monte, 1997), it has the effect of global variance

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reduction and can be easily implemented with the use of Optimal Source Bias Coefficients.

However, the calculation of Optimal Source Bias Coefficients needs the values of variances in advance, which is almost impossible. To meet the requirement, a Batch Approximate Method is then put forward. The Batch Approximate Method make a combination of Batch Algorithm (Gelbard and Prael, 1990) and Shannon Entropy Diagnosis (Ueki and Brown, 2005), eliminates the correlation among cycles during the criticality calculation.

The Optimal Source Bias Method for Monte Carlo criticality calculation is established after mathematical derivation. Then, it is developed in RMC code, tested with a standard Pressurized Water Reactor assembly. The calculation results show that the new method have the effect of global variance reduction. As well as that the distribution of variances are spatially flattened out. In fact, this method is not only meaningful for the variance reduction (Shi et al., 2017, Shi et al., 2018), but also useful for the research on the underestimate of the variance (MacMillan, 1973).

In this paper, the train of thought of the Optimal Source Bias Method is given in Section 2, where the necessary mathematical derivation and equations are outlined, especially the two basic methods: Optimal Stratified Sampling Method and Batch Approximate Method. Section 3 presents the calculation flow of the Optimal Source Bias Method, and some advices for implementing the method in the Monte Carlo code is also given. Section 4 provides the numerical results and comparisons. In the end, there is a conclusion about the work.

2. Theory

Stratified Sampling Method (SSM) has received extensive attention in mathematical statistics (David et al., 2008). When the population is composed of several parts with obvious differences, in order to make the sample more objectively show the overall situation, the population is often divided into distinct parts according to different features. Then sample according to the proportion of each part in the population, this sampling method is called Stratified Sampling Method, and the stratified parts are called "stratification". Stratified Sampling Method is to change the population probability distribution into stratified probability distribution. So, the Stratified Sampling Method can be used as a kind of variance reduction technique.

At present, the fission source iterative method is used in the Reactor Monte Carlo (RMC) code when doing criticality calculation. That means, the fission neutrons produced in each fissile region by the current cycle are used as the initial source neutrons of the next cycle. So, when we focus on the spatial distribution probability of the fission neutrons in each fissile region, the sampling process can be regarded as Stratified Sampling process, and fissile regions act as the "stratification".

During the conventional fission source iterative method, the numbers of source neutrons sampled in each region are decided by Proportional Stratified Sampling Method (PSSM) – the conventional method, show as the Eq. (1)

$$n_i = N \cdot p_i \tag{1}$$

where, N is the total number of source neutrons in each cycle; p_i is the producing probability of fission neutrons in the ith fissile region for PSSM and n_i is the number of source neutrons sampled in the ith fissile region for PSSM. However, after mathematic analysis, the Proportional Stratified Sampling Method is not optimal and still have room for improvement, such as the Optimal Stratified Sampling Method (OSSM), show as Eq. (2)

$$\tilde{n}_i = N \cdot \tilde{p}_i \tag{2}$$

where, $\tilde{p}_i$ is the producing probability of fission neutrons in the ith fissile region for OSSM and $\tilde{n}_i$ is the number of source neutrons sampled in the ith fissile region for OSSM.

In fact, the PSSM that focuses on the real physical process and OSSM that focuses on the optimal mathematics treatment are both Stratified Sampling Method, but their sampling strategies are totally different which will lead to different calculated variances.

The Optimal Stratified Sampling Method can be deduced from Lagrangian Multiplier Method (Xu et al., 2005) or Schwarz Inequality (Xu et al., 2005), and it can achieve global variance reduction. As we can see from the mathematical derivation in the following section, the exact OSSM show as Eq. (3)

$$\tilde{n}_i = N \cdot \tilde{p}_i = N \cdot p_i \frac{\sigma_i}{\sum_{j=1}^{m} p_j \sigma_j} = N \cdot p_i \cdot c_i \tag{3}$$

where, σ_i is the variance in the ith fissile region, i is the serial number of a specific fissile region; c_i is the Optimal Source Bias Coefficient.

In order to achieve the Optimal Stratified Sampling Method, we need to know the Optimal Source Bias Coefficients first. However, the calculation of the Optimal Source Bias Coefficients needs the variances in advance. Without the value of the variances, it is impossible to achieve the Optimal Stratified Sampling Method directly. So, the Optimal Stratified Sampling Method is like a Zero-variance theory, you can't really do it, you can only approximate it.

A Batch Approximate Method is then put forward for this situation. The approach is to assume that the results of each cycle is accurate enough, and each cycle during criticality calculation are independent of each other. Then the variances in the current cycle could be approximated by the variances in the last cycle. So, there are two jobs to be done for implementing the Optimal Stratified Sampling Method. One is to set a large sample size for each cycle; another one is to eliminate the correlation among cycles.

However, the fission source iterative method leads to the correlation among cycles, not only makes the assumption of each cycle are independent of each other fails, but also results in the underestimate of variance. Meanwhile, the underestimate of variance will affects the evaluation of global variance reduction. So, some methods for reducing the underestimate of variance are also used during the Optimal Stratified Sampling Method. For the perspective of versatility and reliability, the batch algorithm is selected, and a simple and effective method based on Shannon entropy diagnosis for determining the batch length M is introduced. We call it Batch Approximate Method.

So, the Optimal Source Bias Method includes two parts: the Optimal Stratified Sampling Method for global variance reduction; the Batch Approximate Method for supporting the implementation of the Optimal Stratified Sampling Method.

2.1. Optimal Stratified Sampling Method

The Monte Carlo calculation use expectations to estimate the real values, and use variances to restrict the errors. Let f(x) be the probability density function in region D, consider the following mathematical expectation calculation$R$:

$$R = \int_D g(x) f(x) dx = E[g] \tag{4}$$

Region D is decomposed into the sum of m two disjoint subregions $D = \bigcup_{i=1}^{m} D_i$, $D_j \bigcap D_k = 0$ $(j \neq k)$, let

$$f_i(x) = \begin{cases} f(x)/p_i, & x \in D_i \\ 0, & x \notin D_i \end{cases} \tag{5}$$