International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

INSTRUCTIVE CONCEPTS ABOUT THE MONTE CARLO FISSION SOURCE DISTRIBUTION

Brian R. Nease
Commissariat á l'Énergie Atomique (CEA)
Saclay, France
bnease@gmail.com

Taro Ueki
Department of Chemical and Nuclear Engineering
University of New Mexico
Albuquerque, NM
tueki@unm.edu

Thomas M. Sutton
Knolls Atomic Power Laboratory
Schenectady, NY
sutton@kapl.gov

Forrest B. Brown
Los Alamos National Laboratory
Los Alamos, NM
fbrown@lanl.gov

ABSTRACT

Treatment of the fluctuation and noise of the fission source distribution in Monte Carlo nuclear criticality calculations is essential to understanding and correctly modeling the process of source iterations. The theory related to source normalization and conditioning is presented in a format that could be used in a graduate level Monte Carlo course. These discussions will hopefully promote innovative ideas to solve problems related to the fission source distribution.

Key Words: Monte Carlo, fission source, eigenvalue, noise, normalization

1. INTRODUCTION

Nuclear criticality calculations account for a significant portion of Nuclear Engineering (NE) Monte Carlo (MC) simulations. However, rigorous treatments of the fission source iteration process is rarely covered in graduate level NE MC textbooks [1,2], despite the importance of its implications. This process introduces bias and correlations into the estimates of the effective neutron multiplication factor and the fission source distribution. Especially for academic purposes it is critical to derive models of these quantities to understand how they depend on the user-specified conditions such as the number of neutrons per cycle, etc.

In this paper, we present a thorough discussion of the theory related to the fission source distribution in stationarity, including the fluctuation and noise terms. It has been compiled from several sources [3-5] originating from Lieberoth's work [6] and includes a new proof. This material is suitable for a graduate level MC course. An understanding of Proability Theory, Real Analysis, and the basic MC principles are necessary to fully appreciate the material.

There are three main topics related to the source iteration procedure that are discussed: normalization of the fission source distribution, asymptotic linearity of the noise propagation process, and the inherent bias of fundamental mode eigenvalue and eigenmode. Since the topics are related to the fission source distribution, it is convienient to present them all together within the same context. The normalization of the source distribution will be discussed first, arguing the order of magnitude in terms of total starter-neutron weight. This will be important for the next section where the asymptotic linearity of the noise propagation will be derived, which leads to several implications about cycle correlations and how they relate to the eigenvalues of the problem. Finally, the bias inherent to the source iterations in MC criticality calculations will be derived.

2. MONTE CARLO (MC) TRANSPORT THEORY

Production level MC codes such as MCNP and Tripoli solve criticality (k-eigenvalue) problems via the source iteration method. At the start of a run, a batch of neutrons is sampled according to some initial distribution and tracked until termination or leakage. Using the distribution of spatial locations where fission events occurred, the next batch of neutrons is then sampled and tracked. This process is repeated until the distribution converges, such that it fluctuates around the true fundamental mode distribution. At this point, accurate tallies can be made.

The first step in formalizing the source iteration process is to treat the normalization of the fission source term $S(\vec{r})$. Determining the order of magnitude in terms of total stater-neutron weight is important since it affects the propagation of noise and fluctuation through cycles and the magnitude of the bias from the true fundamental mode eigenvalue and eigenfunction, k_0 and $S_0(\vec{r})$.

2.1 Fission Source Normalization

The neutrons in the initial cycle of a MC calculation are sampled according to some user-specified distribution, and through source iteration the distribution is updated each cycle so that it eventually matches the true source distribution within statistical fluctuations. Any tallies taken before the distribution has converged to the stationarity fluctuation range around the fundamental mode will be biased, and so those initial tallies are ignored. Once the distribution is converged, the distribution is said to be stationary and accurate tallies can begin. For our purposes, we only consider the distribution in its stationary state. The topic of convergence of the fission source distribution is not rigorously covered here.

Throughout this paper we assume that the total weight of starter-neutrons in each cycle is constant. After simulating all of the neutrons in a particular cycle, an unnormalized realization of the fission source distribution can be expressed as the collection of fission sites and their corresponding statistical weights (i.e. the distribution of fission-born neutrons produced in cycle *m*):

$$\hat{S}^{(m)}\left(\vec{r}\right)=\sum_{i=1}^{C^{(m)}} w_i^{(m)}\delta\left(\vec{r}-\vec{r}_i\right). \tag{1}$$

The hat above $\hat{S}^{(m)}\left(\vec{r}\right)$ is used to indicate a stochastic unnormalized realization of the fission source distribution, $C^{(m)}$ is the number of collision site(s) with non-zero fission cross sections in cycle *m*, $w_i^{(m)}$ is the statistical weight assigned to the corresponding collision site $\vec{r}_i$, i.e. $w_{b,i}\nu\Sigma_f/\Sigma_t$ using the weight immediately before the collision at $\vec{r}_i$ and conventional cross section notation, and δ is a Dirac delta function such that $\int\delta\left(\vec{r}-\vec{r}_i\right)\left(f\right)dV=f\left(\vec{r}_i\right)$ and $\delta\left(\vec{r}-\vec{r}_i\right)=0$ when $\vec{r}\neq\vec{r}_i$. The particle weights are normalized such that

$$\sum_{i=1}^{C^{(m)}} w_i^{(m)}=\int_V \hat{S}^{(m)}\left(\vec{r}\right)dV\,. \tag{2}$$

where V is the domain of spatial coordinates It should be observed from Eq. (2) that the integrated source distribution is dependent on the number of fission sites, and hence the number of neutrons used each cycle:

$$\int_V \hat{S}^{(m)}\left(\vec{r}\right)dV\simeq O\left(N\right), \tag{3}$$

where N is the total weight of starter-neutrons in each cycle, equal to the number of stater-neutrons in the initial cycle. For our analysis, we wish to represent the expected MC fission source distribution $S\left(\vec{r}\right)$ as a normalized quantity, independent of the number of neutrons used in each MC cycle. This will be useful when discussing the linearity of the process and quantifying the bias.

Each normalized realization of the stationary fission source distribution $\hat{S}^{(m)}\left(\vec{r}\right)/N$, $m=1,2,\ldots$ matches the expected MC source distribution $S\left(\vec{r}\right)$ within statistical fluctuations. Thus, we can formulate that a particular realization of the source distribution at cycle *m* can be written as a combination of a deterministic part $S\left(\vec{r}\right)$ and a fluctuating part $\hat{e}^{(m)}\left(\vec{r}\right)$

$$\hat{S}^{(m)}\left(\vec{r}\right)=NS\left(\vec{r}\right)+\sqrt{N}\hat{e}^{(m)}\left(\vec{r}\right). \tag{4}$$

with scaling terms N and $\sqrt{N}$. From Eq. (4), the expected value of the source distribution can be defined as

$$S\left(\vec{r}\right)\equiv\frac{1}{N}E\left[\hat{S}^{(m)}\left(\vec{r}\right)\right]. \tag{5}$$

Here the notation $E[\bullet]$ is to be understood as the ensemble average of realizations of $\hat{S}^{(m)}\left(\vec{r}\right)$ over an infinite number of runs from the same initial source distribution. Since $\int_V \hat{S}^{(m)}\left(\vec{r}\right)dV\simeq O\left(N\right)$ by Eq. (3), it is clear that $\int_V S\left(\vec{r}\right)dV\simeq O\left(1\right)$ by Eq. (5), i.e., it is independent of the total weight of starter neutrons per cycle. Eqs. (4) and (5) imply that

$$E\left[\hat{e}^{(m)}\left(\vec{r}\right)\right]=0\,. \tag{6}$$

Eq. (5) and the definition of variance yields

$$\mathrm{var}\left[\int_V \widehat{S}^{(m)}(\vec{r})\,dV\right] \equiv E\left[\left\{\int_V \widehat{S}^{(m)}(\vec{r})\,dV - N\int_V S(\vec{r})dV\right\}^2\right]. \quad (7)$$

We apply Eq. (4) to the right hand side of Eq (7) to obtain

$$\mathrm{var}\left[\int_V \widehat{S}^{(m)}(\vec{r})\,dV\right] = NE\left[\left\{\int_V \widehat{e}^{(m)}(\vec{r})\,dV\right\}^2\right]. \quad (8)$$

Taking into account particle population dynamics as in previous work [3-6], it is assumed that

$$\mathrm{var}\left[\int_V \widehat{S}^{(m)}(\vec{r})\,dV\right] \simeq O(N). \quad (9)$$

Eqs (9) and (8) yield

$$\int_V \widehat{e}^{(m)}(\vec{r})dV \simeq O(1). \quad (10)$$

In this way, we have consistently formalized scaling arguments in terms of the total weight of starter neutrons per cycle using only the population dynamics assumption that $\mathrm{var}\left[\int_V \widehat{S}^{(m)}(\vec{r})dV\right] \simeq O(N)$.

Now, the fundamental mode eigenvalue after cycle *m* is estimated as

$$\widehat{k}^{(m)} = \frac{1}{N}\int_V \widehat{S}^{(m)}(\vec{r})dV \quad (11)$$

and the expected eigenvalue is

$$k \equiv E\left[\widehat{k}^{(m)}\right] = \int_V S(\vec{r})dV\,. \quad (12)$$

2.2 Asymptotic Linearity of the Fission Source and Fluctuation

We now derive the propogation of the cycle-wise fission source and fluctuation. The neutron source locations for cycle $m+1$ are selected based on the distribution (i.e. the fission sites and collection of weights) from cycle *m*. Recalling Eqs. (1) - (2), the probability that a particular fission site $\vec{r}_j$ is chosen as a starter-neutron source location in the cycle $m+1$ is determined from the weight distribution of the previous cycle *m* as

$$p^{(m+1)}\left(\vec{r} = \vec{r}_j\right) = \frac{w_j^{(m)}}{\sum_{i=1}^{C^{(m)}} w_i^{(m)}}. \quad (13)$$

Since *N* is the total weight of starter neutrons, it is expected that $N\ p^{(m+1)}\left(\vec{r} = \vec{r}_j\right)$ will start at that particular fission site $\vec{r}_j$.

Using the kernel $\mathbf{H}\left(\vec{r}_j \rightarrow \vec{r}\right)$, defined as the expected next-generation fission-born-neutron weight at $\vec{r}$ given the unit fission-born-neutron weight at $\vec{r}_j$, the expected distribution of weights for all neutrons that will start at $\vec{r}$ after simulating all neutron histories in cycle $m+1$ assuming that the unit weight at $\vec{r}_j$ is the only weight produced in cycle *m* is

$$E\left[\widehat{S}^{(m+1)}\left(\vec{r}\right) \mid \widehat{S}^{(m)}\left(\vec{r}\right)=\delta\left(\vec{r}-\vec{r}_j\right)\right]=N\ \mathbf{H}\left(\vec{r}_j \to \vec{r}\right). \tag{14}$$

If Eq. (14) is multiplied by $p^{(m+1)}\left(\vec{r}=\vec{r}_j\right)$ from Eq. (13) and is summed over all possible fission sites $\left(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_{C^{(m)}}\right)$, then the expected weight distribution given the distribution of weights $\widehat{S}^{(m)}\left(\vec{r}\right)$ in Eq. (1) is

$$E\left[\widehat{S}^{(m+1)}\left(\vec{r}\right) \mid \widehat{S}^{(m)}\left(\vec{r}\right)=\sum_{i=1}^{C^{(m)}} w_i^{(m)}\delta\left(\vec{r}-\vec{r}_i\right)\right] \tag{15}$$

$$=\sum_{j=1}^{C^{(m)}} E\left[\widehat{S}^{(m+1)}\left(\vec{r}\right) \mid \widehat{S}^{(m)}\left(\vec{r}\right)=\delta\left(\vec{r}-\vec{r}_j\right)\right] p^{(m+1)}\left(\vec{r}=\vec{r}_j\right) \tag{16}$$

$$=N\frac{\sum_{j=1}^{C^{(m)}} w_j^{(m)}\mathbf{H}\left(\vec{r}_j \to \vec{r}\right)}{\sum_{j=1}^{C^{(m)}} w_j^{(m)}}. \tag{17}$$

The numerator of Eq. (17) can be manipulated as

$$\sum_{j=1}^{C^{(m)}} w_j^{(m)}\mathbf{H}\left(\vec{r}_j - \vec{r}\right)=\sum_{j=1}^{C^{(m)}} w_j^{(m)}\mathbf{H}\left(\vec{r}_j \to \vec{r}\right)\int_V \delta\left(\vec{r}'-\vec{r}_j\right)dV' \tag{18}$$

$$=\int_V \sum_{j=1}^{C^{(m)}} w_j^{(m)}\delta\left(\vec{r}'-\vec{r}_j\right)\mathbf{H}\left(\vec{r}_j \to \vec{r}\right)dV' \tag{19}$$

$$=\int_V \sum_{j=1}^{C^{(m)}} w_j^{(m)}\delta\left(\vec{r}'-\vec{r}_j\right)\mathbf{H}\left(\vec{r}' \to \vec{r}\right)dV'. \tag{20}$$

Eq. (20) is obtained from the relation $\delta\left(x-y\right)f\left(x\right)=\delta\left(x-y\right)f\left(y\right)$. Applying Eq. (1) to Eq. (20) yields

$$\sum_{j=1}^{C^{(m)}} w_j^{(m)}\mathbf{H}\left(\vec{r}_j - \vec{r}\right)=\int_V \widehat{S}^{(m)}\left(\vec{r}'\right)\mathbf{H}\left(\vec{r}' \to \vec{r}\right)dV' \tag{21}$$

Using Eq. (2) and Eq. (21), the expected source distribution described by Eq. (17) is rewritten as

$$E\left[\widehat{S}^{(m+1)}\left(\vec{r}\right) \mid \widehat{S}^{(m)}\left(\vec{r}\right)\right]=N\frac{\int \widehat{S}^{(m)}\left(\vec{r}'\right)\mathbf{H}\left(\vec{r}' \to \vec{r}\right)dV'}{\int \widehat{S}^{(m)}\left(\vec{r}'\right)dV'}. \tag{22}$$

This is a conditional distribution that represents the expected source distribution at the end of cycle $m+1$ given the source distribution $\widehat{S}^{(m)}\left(\vec{r}\right)$ at the end of cycle *m*.

The stochastic equation describing $\widehat{S}^{(m+1)}$ can then be written as

$$\widehat{S}^{(m+1)}\left(\vec{r}\right)=N\frac{\int \widehat{S}^{(m)}\left(\vec{r}'\right)\mathbf{H}\left(\vec{r}' \to \vec{r}\right)dV'}{\int \widehat{S}^{(m)}\left(\vec{r}'\right)dV'}+\sqrt{N}\widehat{\varepsilon}^{(m+1)}\left(\vec{r}\right). \tag{23}$$

The fluctuating term $\hat{\varepsilon}^{(m+1)}(\vec{r})$ is a random noise component resulting from population (total weight) normalization of starting neutrons and subsequent tracking. As before, the N and $\sqrt{N}$ are scaling terms. Eq. (23) is perhaps more recognizable after applying (11), which yields

$$\hat{S}^{(m+1)}(\vec{r}) = \frac{1}{\hat{k}^{(m)}} \int \hat{S}^{(m)}(\vec{r}\,')\mathbf{H}(\vec{r}\,' \to \vec{r})\,dV' + \sqrt{N}\hat{\varepsilon}^{(m+1)}(\vec{r}) . \tag{24}$$

Eqs. (22) and (23) imply that $\hat{\varepsilon}^{(m)}(\vec{r})$ satisfies

$$E\left[\hat{\varepsilon}^{(m+1)}(\vec{r}) \mid \hat{S}^{(m)}(\vec{r})\right] = 0 . \tag{25}$$

This result further implies that

$$E\left[\hat{\varepsilon}^{(m+1)}(\vec{r})\right] = E\left[E\left[\hat{\varepsilon}^{(m+1)}(\vec{r}) \mid \hat{S}^{(m)}(\vec{r})\right]\right] = 0 . \tag{26}$$

No assumptions about the distribution of $\hat{\varepsilon}^{(m)}(\vec{r})$ are made. In other words, any iteration scheme of fixed total starter-neutron weight per cycle can be treated by Eq. (24) except the superhistory method [4]. It is important to note that following directly from Eqs. (4) and (25),

$$E\left[\hat{\varepsilon}^{(m+1)}(\vec{r}) \mid \hat{e}^{(m)}(\vec{r})\right] = 0 . \tag{27}$$

Eq. (24) describes a realization of the source iteration from cycle m to m+1, while the fission source eigenvalue equation [3-5] is

$$S_0(\vec{r}) = \frac{1}{k_0} \int_V \mathbf{H}(\vec{r}\,' \to \vec{r}) S_0(\vec{r}\,')\,dV' , \tag{28}$$

where k_0 and $S_0(\vec{r})$ are the true fundamental mode eigenvalue and eigenfunction, as refered to before.

We next derive an expression describing the fission source fluctuation $\hat{e}^{(m)}(\vec{r})$ similar in form to Eq. (24). Substituting Eq. (4) into Eq. (23) and dividing through by N results in

$$S(\vec{r}) + \frac{1}{\sqrt{N}}\hat{e}^{(m+1)}(\vec{r}) = \frac{\int_V \left[NS(\vec{r}\,') + \sqrt{N}\hat{e}^{(m)}(\vec{r}\,')\right] H(\vec{r}\,' \to \vec{r})\,dV'}{\int_V \left[NS(\vec{r}\,') + \sqrt{N}\hat{e}^{(m)}(\vec{r}\,')\right] dV'} + \frac{1}{\sqrt{N}}\hat{\varepsilon}^{(m+1)}(\vec{r}) \tag{29}$$

To reduce Eq. (29) further, the first term on the right hand side (RHS) of the equation must be manipulated. First, N^{-1} is applied throughout. Next, the numerator is expanded and Eq. (12) is applied to the denominator resulting in

$$\frac{\int_V H(\vec{r}\,' \to \vec{r}) S(\vec{r}\,')\,dV' + \frac{1}{\sqrt{N}} \int_V H(\vec{r}\,' \to \vec{r})\hat{e}^{(m)}(\vec{r}\,')\,dV'}{k\left(1 + \frac{1}{k\sqrt{N}} \int_V \hat{e}^{(m)}(\vec{r}\,')\,dV'\right)} \tag{30}$$

At this point, the denominator is in the form $(1+x)^{-1}$ with $x<1$, which can also be written in series form as $1 - x + x^2 - x^3 + \cdots$. Rewriting the denominator this way yields

$$\left[\frac{1}{k}\int_V H(\vec{r}'\to\vec{r})S(\vec{r}')dV' + \frac{1}{k\sqrt{N}}\int_V H(\vec{r}'\to\vec{r})\hat{e}^{(m)}(\vec{r}')dV'\right] \times\left(1-\frac{1}{k\sqrt{N}}\int_V \hat{e}^{(m)}(\vec{r}')dV' + \frac{1}{k^2 N}\left(\int_V \hat{e}^{(m)}(\vec{r}')dV'\right)\left(\int_V \hat{e}^{(m)}(\vec{r}'')dV''\right)-\cdots\right) \quad (31)$$

All terms are multiplied out and the terms of order N^{-a}, $a \geq 1$, are combined into a leading order term $O\left(N^{-1}\right)$, yielding

$$\frac{1}{k}\int_V H(\vec{r}'\to\vec{r})S(\vec{r}')dV' + \frac{1}{k\sqrt{N}}\int_V H(\vec{r}'\to\vec{r})\hat{e}^{(m)}(\vec{r}')dV' - \frac{1}{k^2\sqrt{N}}\int_V H(\vec{r}''\to\vec{r})S(\vec{r}'')dV''\int_V \hat{e}^{(m)}(\vec{r}')dV' + O\left(N^{-1}\right) \quad (32)$$

A kernel term is defined

$$\mathbf{A}(\vec{r}'\to\vec{r}) = \frac{1}{k}\left[H(\vec{r}'\to\vec{r}) - \frac{1}{k}\int_V H(\vec{r}''\to\vec{r})S(\vec{r}'')dV''\right] \quad (33)$$

allowing Eq. (32) to be simplified to

$$\frac{1}{k}\int_V H(\vec{r}'\to\vec{r})S(\vec{r}')dV' + \frac{1}{\sqrt{N}}\int_V \mathbf{A}(\vec{r}'\to\vec{r})\hat{e}^{(m)}(\vec{r}')dV' + O\left(N^{-1}\right) \quad (34)$$

Now that the first term on the RHS of Eq. (29) has been manipulated into this form, it can be substituted back into Eq. (29) to obtain

$$S(\vec{r}) + \frac{1}{\sqrt{N}}\hat{e}^{(m+1)}(\vec{r}) = \frac{1}{k}\int_V H(\vec{r}'\to\vec{r})S(\vec{r}')dV' + \frac{1}{\sqrt{N}}\int_V \mathbf{A}(\vec{r}'\to\vec{r})\hat{e}^{(m)}(\vec{r}')dV' + \frac{1}{\sqrt{N}}\hat{\varepsilon}^{(m+1)}(\vec{r}) + O\left(N^{-1}\right) \quad (35)$$

Taking the expectation and using Eqs (6) and (26), we obtain

$$S(\vec{r}) = \frac{1}{k}\int_V H(\vec{r}'\to\vec{r})S(\vec{r}')dV' + O\left(N^{-1}\right). \quad (36)$$

Subtracting Eq. (36) from Eq. (35) and multiplying through by $\sqrt{N}$ yields

$$\hat{e}^{(m+1)}(\vec{r}) = \int_V \mathbf{A}(\vec{r}'\to\vec{r})\hat{e}^{(m)}(\vec{r}')dV' + \hat{\varepsilon}^{(m+1)}(\vec{r}) + O\left(N^{-1/2}\right) \quad (37)$$

Eq. (37) describes how the fluctuation of the fission source distribution changes cycle-to-cycle. However, we must still show that Eq (37) is the fundamental form of error propagation. To do this, we introduce the operator $\mathbf{A}_0(\vec{r}'\to\vec{r})$:

$$\mathbf{A}_0(\vec{r}'\to\vec{r}) = \frac{1}{k_0}\left[H(\vec{r}'\to\vec{r}) - S_0(\vec{r})\right]. \quad (38)$$

As will be shown in the next section, there exists bias in the MC solutions such that

$$S(\vec{r}) - S_0(\vec{r}) = O\left(N^{-1}\right) \quad (39)$$

$$k - k_0 = O\left(N^{-1}\right). \quad (40)$$

From Eqs. (28), (39) and (40), it is clear that

$$\mathbf{A}\left(\vec{r}'\to\vec{r}\right)=\mathbf{A}_0\left(\vec{r}'\to\vec{r}\right)+O\left(N^{-1}\right). \tag{41}$$

Applying $\mathbf{A}_0\left(\vec{r}'\to\vec{r}\right)$ to Eq. (37) and using operator notation such that

$$\mathbf{A}_0\hat{e}^{(m)}=\int\mathbf{A}_0\left(\vec{r}'\to\vec{r}\right)\hat{e}^{(m)}\left(\vec{r}'\right)dV', \tag{42}$$

yields the working form

$$\hat{e}^{(m+1)}=\mathbf{A}_0\hat{e}^{(m)}+\hat{\varepsilon}^{(m+1)}+O\left(N^{-1/2}\right). \tag{43}$$

$\mathbf{A}_0$ is termed the Noise Propagation operator and its eigenvalues are k_j/k_0, $j=1,2,\ldots$, where k_j is the *j*-th eigenvalue of $\mathbf{H}\left(\vec{r}'\to\vec{r}\right)$, $|k_0|>|k_1|\geq|k_2|\geq|k_3|\geq\cdots$, in Eq (28) [7]. Note that the "*j*" in k_j/k_0 starts at 1 and therefore the magnitudes of the eigenvalues of $\mathbf{A}_0$ are smaller than unity.

Eq. (43) is an important equation in many regards since it describes how noise and fluctuation propagate throughout the cycles. The eigenvalues of $\mathbf{A}_0$ are related to the strength of the correlations between MC cycles, though an in-depth analysis of this is not given in this paper; we will suffice to say that the larger the eigenvalues, the stronger the correlations. Also, Eq. (43) illustrates the asymptotic linearity of the process (or Markov nature). The process can be represented in terms of discrete time events as

$$\cdots\to\hat{e}^{(i)}\xrightarrow{\;\hat{\varepsilon}^{(i+1)}\downarrow\;}\hat{e}^{(i+1)}\xrightarrow{\;\hat{\varepsilon}^{(i+2)}\downarrow\;}\hat{e}^{(i+2)}\xrightarrow{\;\hat{\varepsilon}^{(i+3)}\downarrow\;}\hat{e}^{(i+3)}\to\cdots$$

Each particular state of the source fluctuation $\hat{e}^{(i+1)}$ is completely determined by the previous state $\hat{e}^{(i)}$ and the generated noise $\hat{\varepsilon}^{(i+1)}$.

2.3 Bias of Fission Source Distribution and Fundamental Eigenvalue

In this final section, the biases of k and $S\left(\vec{r}\right)$ from k_0 and $S_0\left(\vec{r}\right)$ are derived. Here, corresponding to Eq (12), $S_0\left(\vec{r}\right)$ is normalized to be

$$k_0=\int_V S_0\left(\vec{r}\right)dV \tag{44}$$

These biases are caused by the ratio of the two stochastic estimators in Eq. (24). However, as will be shown, the bias is inversely proportional to the total weight of starter neutrons per cycle. Therefore, the bias can be made much smaller than the statistical fluctuations and a correct result can be obtained.

Recall Eqs (36) and (28). Subtract Eq (28) from Eq (36) to

$$S\left(\vec{r}\right)-S_0\left(\vec{r}\right)-\int_V H\left(\vec{r}'\to\vec{r}\right)\left[\frac{S\left(\vec{r}'\right)}{k}-\frac{S_0\left(\vec{r}'\right)}{k_0}\right]dV'=O\left(N^{-1}\right). \tag{45}$$

A bias of order $O\left(N^{-a}\right)$ is allowed to exist between the exact solution and the MC solution such that

$$S\left(\vec{r}\right)-S_0\left(\vec{r}\right)=O\left(N^{-a}\right), \tag{46}$$

which implies that

$$k - k_0 = O\left(N^{-a}\right), \tag{47}$$

by Eqs. (12) and (44). Using Eqs. (46) and (47), Eq. (45) can be rewritten

$$O\left(N^{-a}\right) = O\left(N^{-1}\right). \tag{48}$$

It is clear that the order of bias must be equivalent, i.e. $a = 1$, otherwise the RHS and LHS of Eq. (48) will differ by orders of magnitude as $N \to \infty$. Thus, a bias exists when evaluating the fission source distribution and its associated eigenvalue by MC iterative source methods

$$S(\vec{r}) - S_0(\vec{r}) = O\left(N^{-1}\right) \tag{49}$$

$$k - k_0 = O\left(N^{-1}\right). \tag{50}$$

Thus, using sufficient numbers of neutrons per cycle, MC calculations are able to obtain accurate results such that the bias is much smaller than the standard error of the calcualation. These biases were also derived by Dubi and Elperin based on the faithful Markov chain analysis of continuous-space source-iteration Monte Carlo procedures, which initially led to an upper bound of $O(N^{-1/2})$ [8] and the subsequent tightning to $O(N^{-1})$ [9].

In practice, the bias in the k estimate is considered negligible when reasonable numbers of neutrons per cycle are used (most modern calculations use thousands or tens of thousands of neutrons per cycle). However, with MC calculations being used more frequently for power calculations (where the distribution must be known in small regions), it is important to make sure that each region of importance is properly sampled with sufficient numbers of neutrons. (See [10] for numerical examples of the bias in k_{eff} and fission rate distributions for realistic problems.)

3. CONCLUSIONS

A solid theoretical treatment of the MC fission source normalization and conditioning is critical for those doing research in MC criticality calculation methodologies. These proofs and derivations will help to broaden understanding of the MC process and will provide different representations of quantities, which could potentially be used to tackle other important problems such as confidence interval estimation of the fission source distribution, etc. Due to the complexity of the material, we feel it would best be presented for PhD level students studying Monte Carlo methods.

REFERENCES

[1] S.A. Dupree & S.K.Fraley, *A Monte Carlo Primer, A Practical Approach to Radiation Transport*, Kluwer Academic/Plenum Publishers, New York, NY 2002.

[2] I. Lax & L. Koblinger, *Monte Carlo Particle Transport Methods: Neutron and Photon*, CRC Press, Boca Raton, FL 1991.

[3] E.M. Gelbard & R.E. Prael, “Monte Carlo Work at Argonne National Laboratory,” ANL-75-2, Argonne National Laboratory, (1974).

[4] R.J. Brissenden & A.R. Garlick, "Biases in the Estimation of keff and its Error by Monte Carlo Methods," Annals of Nuclear Energy, **13**, pp. 63-83 (1986).

[5] T.M. Sutton & F.B. Brown, "Analysis of the Monte Carlo Eigenvalue Bias," (unpublished), (1991).

[6] J. Lieberoth, "A Monte Carlo Technique to Solve the Static Eigenvalue Problem of the Boltzmann Transport Equation", *Nukleonik*, **11**, 213 (1968).

[7] T. Ueki, F.B. Brown, D.K. Parsons, and J.S. Warsa, "Time Series Analysis of Monte Carlo Fission Sources: I. Dominance Ratio Computation," Nuclear Science and Engineering, 148, 374-390, (2004).

[8] T. Elperin & A. Dubi, "On the Markov Chain Analysis of Source Iteration Monte Carlo Procedures for Criticality Problems: I," *Nuclear Science and Engineering*, **91**, pp. 59-76 (1985).

[9] A. Dubi & T. Elperin, "On the Markov Chain Analysis of Source Iteration Monte Carlo Procedures for Criticality Problems: II," *Nuclear Science and Engineering*, **91**, pp. 77-83 (1985).

[10] F.B. Brown, "A Review of Monte Carlo Criticality Calculations – Convergence, Bias, Statistics," in CD-ROM proceedings of International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics (M&C 2009) Saratoga Springs, NY (2009).