Accelerated Monte Carlo Eigenvalue Calculations

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This paper reviews methods that have been suggested for improving the source convergence in Monte Carlo eigenvalue calculations; the super-history powering method, the Wieland method, the stratified-source sampling, the fission matrix method, and the semi-fixed-source fission matrix method are considered. The super-history powering method[1] was designed to reduce the source bias. The Wielandt method was adapted from deterministic eigenvalue calculations to address the systems with a dominance ratio close to unity.[2] The stratified-source sampling[3] can improve the source convergence in loosely-coupled multi-component systems. The source convergence can also be accelerated through the zero-variance scheme that was recently adapted[4] for MC eigenvalue calculations. The fission matrix method[5] can accelerate the fission source, and provide the higher mode source eigenfunctions and eigenvalues. Recently, the semi-fixed-source fission matrix method[6] was suggested to improve the stability of the fission matrix method. Moreover, this method allows for an efficient parallelization of Monte Carlo eigenvalue calculations on an arbitrary number of processors. The zero-variance scheme and the semi-fixed-source fission matrix method are being developed within the NURESIM Integrated Project[7].

I. INTRODUCTION

The computational demands of Monte Carlo (MC) eigenvalue calculations restrict their large scale utilization; an efficient parallelization or source convergence acceleration is therefore of general interest. In contrast to deterministic acceleration techniques that address systems with a dominance ratio close to unity, the MC acceleration techniques have to take more aspects into account. This is due to statistical source sampling that causes the bias of the k_{eff} estimator and stationary source distribution,[1] and can make dominant components "invisible" in loosely-coupled multi-component systems.[8] Theory of the MC fission source is introduced in Sec. II in more detail.

A number of acceleration techniques have been suggested for MC eigenvalue calculations, see Sec. III. For instance, the super-history powering method[1] can reduce the inter-generational correlation of unimportant neutrons, which reduces the source bias, and accelerates the calculation, see Sec. III A. An MC adaptation[2] of the Wielandt method addresses systems with a dominance ratio close to unity, see Sec. III B. The stratified source-sampling technique[3] might be suitable for loosely-coupled multi-component systems, see Sec. III C. The source convergence can also be accelerated through the zero-variance scheme, see Sec. III D.[4] It has been observed that the fission matrix (FM) method[5] can accelerate the convergence of the MC fission source, see Sec. III E. This method can also provide higher mode eigenvalues and source eigenfunctions; however, some instability issues limit wider application of the method.[9]

However, none of the acceleration method mentioned above can itself reduce the computing time as much as an efficient parallelization. At present, multi-core processors and multi-processor computers are commonly used. Moreover, it is expected that the number of cores in a single processor will grow with time. Only parallel calculations can take advantage of such computers.

The problem of the efficient parallelization can be resolved using an approximate semi-fixed source in the FM method, which also stabilizes the FM method,[6] see Sec. III F.

II. CONVERGENCE OF THE MC FISSION SOURCE

The stationary distribution of fission neutrons $s(\mathbf{r})$ is given by the eigenvalue equation

$$ks(\mathbf{r}) = Fs(\mathbf{r}), \tag{1}$$

where the operator F applied on $s(\mathbf{r})$ gives the next generation fission source, and k is the eigenvalue. F is defined as

$$Fs(\mathbf{r}) \equiv \int_V f(\mathbf{r}' \to \mathbf{r}) s(\mathbf{r}') \, \mathrm{d}^3 r', \tag{2}$$

where the fission kernel $f(\mathbf{r}' \to \mathbf{r})$ is an expected number of first generation fission neutrons produced per unit volume at $\mathbf{r}$ resulting from a fission neutron born at $\mathbf{r}'$. The angle dependency is not considered, as the fission neutrons are emitted isotropically. The energy dependency is, for simplicity, commonly skipped since the inter-generational correlation of the source energy spectra is negligible. This does not compromise the results as all equations may embody the energy coordinate.

Let the eigenfunctions $s_j(\mathbf{r})$ and eigenvalues k_j of F be ordered, $k_0 > |k_1| > |k_2| > \dots$. Then, the fundamental mode $s_0(\mathbf{r})$ represents the physical stationary source, and

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the corresponding k_0 is equal to k_{eff} of the system. $s_0(\mathbf{r})$ is commonly computed by the power iteration

$$s_0^{(n)}(\mathbf{r}) = F s_0^{(n-1)}(\mathbf{r}), \qquad n = 0, 1, \ldots, \tag{3}$$

where $s_0^{(0)}(\mathbf{r})$ is an initial nontrivial guess. (Usually, $s_0^{(n)}(\mathbf{r})$ is also normalized in each step.)

In MC eigenvalue calculations, the source of the net weight m is iterated by the stochastic adaptation of the power iteration,

$$s_{\text{mc}}^{(n)}(\mathbf{r}) \xleftarrow{m} F_{\text{mc}} s_{\text{mc}}^{(n-1)}(\mathbf{r}), \qquad n = 1, 2, \ldots, \tag{4}$$

where $F_{\text{mc}} s_{\text{mc}}^{(n-1)}(\mathbf{r})$ is randomly sampled from $F s_{\text{mc}}^{(n-1)}(\mathbf{r})$. In the case of non-analogue MC calculations, $F_{\text{mc}} s_{\text{mc}}^{(n-1)}(\mathbf{r})$ can be represented by the so-called fission store that is a large set $\mathcal{S}^{(n)}$,

$$\mathcal{S}^{(n)} = \{\{\mathbf{r}_i^{(n)}, w_i^{(n)}\} | i = 1, 2, \ldots, q^{(n)}\}, \tag{5}$$

of $q^{(n)}$ fission neutrons, $q^{(n)} \gg m$, of various weights $w_i^{(n)}$ and positions $\mathbf{r}_i^{(n)}$. $\mathcal{S}^{(n)}$ is formed during the neutron transport simulation; each collision where fission is possible is considered as a new fission site with the weight

$$w_i = w_n \bar{\nu} \frac{\sigma_{\text{f}}}{\sigma_{\text{t}}}, \tag{6}$$

where w_n is the weight of the neutron before the collision, $\bar{\nu}$ is an averaged number of fission neutrons, and $\frac{\sigma_{\text{f}}}{\sigma_{\text{t}}}$ is the probability of fission.

$\mathcal{S}^{(n)}$ contains considerably more fission sites than required; thus, $s_{\text{mc}}^{(n)}(\mathbf{r})$ must be randomly sampled from $\mathcal{S}^{(n)}$. This can be accomplished by Algorithm II.1. In order to reduce the memory requirements for the fission store, another method, described by Algorithm II.2, is commonly used.[10] The advantage of Algorithm II.2 is that the fission store is not needed, and $s_{\text{mc}}^{(n)}(\mathbf{r})$ is sampled directly during the neutron transport simulation. The disadvantage is that the number of fission neutrons in the sampled MC source may considerably fluctuate around m, which requires additional weight normalization. Moreover, a k_{eff} estimation is needed for the first cycle.

Algorithm II.1 Sampling the MC fission source from $\mathcal{S}^{(n)}$.

1: Generate $\mathcal{S}^{(n)}$ during the nth cycle.
2: **for** $j = 0$ to m **do**
3: Generate a random number $\xi \in \langle 0, 1)$.
4: Find l, $\sum_{i=1}^{l-1} w_i < \xi \sum_i w_i \leq \sum_{i=1}^{l} w_i$
5: Put a fission neutron with coordinates of the lth fission site from $\mathcal{S}^{(n)}$ and unity importance into the new fission source.
6: **end for**

The convergence rate of the power iteration is derived in Sec. II A. The stationary MC fission source is always biased, which is explained in Sec. II B. Sec. II C explains the importance of a good choice of the initial MC fission source. Sec. II D describes diagnostics techniques for the MC source convergence.

Algorithm II.2 Direct sampling of the MC fission source.

1: **for** all fission sites $i = 1, 2, \ldots$ generated during the nth cycle **do**
2: Compute $q_i = w_n \bar{\nu} \frac{\sigma_{\text{f}}}{\sigma_{\text{t}}} \frac{1}{k_{\text{eff}}}$.
3: Find an integer number p_i so that $p_i \leq q_i < p_i + 1$
4: Generate a random number $\xi \in \langle 0, 1)$
5: **if** $\xi \leq q_i - p_i$ **then**
6: If $p_i > 0$ then add a fission site of the weight $p_i > 0$ into the new fission source.
7: **else**
8: Add a fission site of the weight $p_i + 1$ into the new fission source.
9: **end if**
10: **end for**

A. Convergence Rate of Power Iteration

The convergence rate of the power iteration is given by the dominance ratio of F, i.e. $s^{(n)}(\mathbf{r})$ converges to $s_0(\mathbf{r})$ as $O((k_1/k_0)^n)$.[11] This can be easily derived. Any real function in the domain of F can be expressed as a weighted sum of the eigenfunctions $s_i(\mathbf{r})$ of F; therefore

$$\exists \gamma_i, \ i = 0, 1, \ldots, \ s^{(0)}(\mathbf{r}) = \sum_i \gamma_i s_i(\mathbf{r}). \tag{7}$$

Equations (3) end (7) yield

$$\begin{aligned} s^{(n)}(\mathbf{r}) &= F^n \sum_i \gamma_i s_i(\mathbf{r}) \\ &= \sum_i \gamma_i F^n s_i(\mathbf{r}) \\ &= \sum_i \gamma_i k_i^n s_i(\mathbf{r}). \end{aligned} \tag{8}$$

If (8) is multiplied by k_0^n then

$$\frac{s^{(n)}}{k_0^n}(\mathbf{r}) = \gamma_0 s_0(\mathbf{r}) + \left(\frac{k_1}{k_0}\right)^n \gamma_1 s_1(\mathbf{r}) + \left(\frac{k_2}{k_0}\right)^n \gamma_2 s_2(\mathbf{r}) + \ldots \tag{9}$$

Since $|k_1/k_0| > |k_2/k_0| > \ldots$ $s^{(n)}(\mathbf{r})$ converges to $s_0(\mathbf{r})$ as $O\left((k_1/k_0)^n\right)$. The convergence rate of the power iteration is therefore given by the dominance ratio (the ratio of the second largest to the largest eigenvalue).

Therefore, the fission source converges slowly in systems with a dominance ratio close to unity (typically loosely coupled multi-component systems and large symmetric systems).

B. Bias of the Stationary MC Fission Source

Random sampling introduces errors into the MC source in each cycle. Although these errors decay, net error propagation over cycles causes the expected source $E(s_{\rm mc}^{(n)}(\mathbf{r}))$ to converge not to $s_0(\mathbf{r})$ but to a biased stationary distribution $s_{0,m}(\mathbf{r})$. The difference between $s_0(\mathbf{r})$ and $s_{0,m}(\mathbf{r})$ is of the order $O(1/m)$.[1] The source bias can cause under-sampling of the dominant components, and overestimation of the neutron leakage, resulting in an underestimation of $k_{\rm eff}$.

$E(s_{\rm mc}^{(n)}(\mathbf{r}))$ converges to $s_{0,m}(\mathbf{r})$ at the rate of $O\left((k_1/k_0)^n\right)$;[12] thus, a large number of inactive cycles is required in systems with a dominance ratio close to unity. Naturally, $s_{\rm mc}^{(n)}(\mathbf{r})$ contains noise of the order $O(1/\sqrt{m})$, and therefore can never be equal to $s_{0,m}(\mathbf{r})$, which complicates the source convergence diagnostics.[13]

The bias of the stationary MC fission source can be explained physically. If fission neutrons are located in relatively poorly multiplying places in cycle $n-1$ then

$$\int_V F s_{\rm mc}^{(n-1)}(\mathbf{r})\,\mathrm{d}^3 r < m k_{\rm eff}, \tag{10}$$

and the importance of fission neutrons in cycle n must be increased by more than a factor of $k_{\rm eff}$. The neutron batch is thus artificially kept in unimportant places. As a result, the relatively highly and poorly multiplying places have a decreased and increased intensity of the stationary MC fission source $s_{0,m}(\mathbf{r})$, respectively, compared to $s_0(\mathbf{r})$. This can happen when m is insufficiently small.

The biased stationary MC fission source causes a bias in the $k_{\rm eff}$ estimator, resulting in underestimation of the value of $k_{\rm eff}$. This is caused partially by an increased neutron leakage from the system due to the increased intensity of the MC fission source in peripheral places, and partially by the reduced intensity of the MC fission source in highly multiplying places.

C. Initial MC Fission Source

An important issue in MC eigenvalue calculations is the so-called "$k_{\rm eff}$ of the world problem".[8] This problem is caused by an unsuitable choice of the initial source $s_{\rm mc}^{(0)}(\mathbf{r})$, and can be observed in a loosely-coupled array of fissile components. If fission neutrons are not present in dominant components in the initial cycle then the dominant components may stay "invisible" during many cycles. During these cycles, the source convergence is not governed by the dominance ratio of the whole system, but by the dominance ratio of the system consisting of those components where the fission source is present. The MC fission source diverges to an incorrect distribution, and $k_{\rm eff}$ is underestimated while the fission source is not present in the dominant components. Therefore, the fission source $s_{\rm MC}^{(0)}$ should be sufficiently sampled in the dominant components.

D. MC Source Convergence Diagnostics

In systems with a dominance ratio close to unity, the convergence of the $k_{\rm eff}$ estimate is much faster than the convergence of the fission source. Therefore, a converged $k_{\rm eff}$ estimate does not guarantee a converged fission source; the fission source may completely change within several cycles in a loosely-coupled multi-component system. Thus, the source convergence should be diagnosed directly by observing the fission source over the cycles.

The fission source convergence can be diagnosed[13–18] by the Shannon entropy of the normalized binned source distribution $\boldsymbol{s}_b^{(n)}$ from the nth cycle,

$$(\boldsymbol{s}_b^{(n)})_i = \int_{V_i} \hat{s}^{(n)}(\boldsymbol{r})\mathrm{d}^3 r, \tag{11}$$

where b is the total number of spatial regions, and i is the bin number. The Shannon entropy h is defined as

$$h(\boldsymbol{s}_b^{(n)}) = -\sum_{i=1}^{b} (\boldsymbol{s}_b^{(n)})_i \log_2 (\boldsymbol{s}_b^{(n)})_i. \tag{12}$$

$h(\boldsymbol{s}_b^{(n)})$ attains the maximum $\log_2 b$ when $\boldsymbol{s}_b^{(n)}$ is uniform, and it attains the minimum value at zero when the whole source is located in a particular source bin. The source distribution can be diagnosed in terms of randomness by computing $h(\boldsymbol{s}_b^{(n)})$ at each cycle. The relative entropy is not sensitive to binning mesh refinement in the limit of sufficiently fine meshes.

The posterior relative entropy $d(\boldsymbol{s}_b^{(n)}\|\boldsymbol{t}_b)$ was also suggested between the binned fission source $\boldsymbol{s}_b^{(n)}$ in the nth cycle and the average MC source over the second half of the active cycles $\boldsymbol{t}_b$,

$$d(\boldsymbol{s}_b^{(n)}\|\boldsymbol{t}_b) = \sum_{i=1}^{b} (\boldsymbol{s}_b^{(n)})_i \log_2 \left(\frac{(\boldsymbol{s}_b^{(n)})_i}{(\boldsymbol{t}_b)_i} \right). \tag{13}$$

$d(\boldsymbol{s}_b^{(n)}\|\boldsymbol{t}_b)$ is the statistical distance between $\boldsymbol{s}_b^{(n)}$ and $\boldsymbol{t}_b$; it is nonnegative, and becomes zero only when $\boldsymbol{s}_b^{(n)} = \boldsymbol{t}_b$. $d(\boldsymbol{s}_b^{(n)}\|\boldsymbol{t}_b)$ should cross the average of $d(\boldsymbol{s}_b^{(n)}\|\boldsymbol{t}_b)$ over the second half of the active cycles before the first active cycle. Indeed, posterior relative entropy can only be found at the end of the calculation to determine whether the source was converged before the first active cycle.

III. ACCELERATION OF THE MC FISSION SOURCE CONVERGENCE

The efficiency of a calculation may be expressed by the figure-of-merit (FOM),

$$FOM = \frac{1}{\sigma^2 t}, \tag{14}$$

where t is the total computational time, and σ is the relative standard deviation of a calculated quantity.

Improving the FOM of MC eigenvalue calculations in systems with a dominance ratio close to unity is commonly done by dividing inactive cycles into several stages; the batch size is periodically increased in each subsequent stage so that the source bias does not exceed the error caused by the slow convergence rate.[10] A number of other methods have been proposed to accelerate the source convergence. This section introduces those that are well described and published in the open literature.

A. Super-History Powering

The super-history powering method[1] reduces the source bias by altering the source normalization scheme. Each cycle consists of l neutron generations (instead of one only). The neutron population $s_{\mathrm{mc}}^{(n,g+1)}(\mathbf{r})$ in cycle n and generation $g+1$ is sampled from $Fs_{\mathrm{mc}}^{(n,g)}(\mathbf{r})$, but is not normalized to m, but to

$$\frac{1}{k_{\mathrm{eff}}}\int_V Fs_{\mathrm{mc}}^{(n,g)}(\mathbf{r})\,\mathrm{d}^3r, \tag{15}$$

where k_{eff} is the eigenvalue estimate. The fission source $s^{(n,1)}(\mathbf{r})$ in the first generation in cycle n is sampled by m fission neutrons from the fission store produced in the last generation l in the previous cycle,

$$s_{\mathrm{mc}}^{(n,1)}(\mathbf{r}) \xleftarrow{m} \frac{Fs_{\mathrm{mc}}^{(n-1,l)}(\mathbf{r})}{k_{\mathrm{eff}}}, \tag{16}$$

where l-values up to 10 are easy to cope with.[1]

The population may grow or decay depending on whether the fission neutrons are located in more or less multiplying places. The fission source in relatively highly multiplying places is prioritized, which reduces the source bias.

B. Wielandt's Method

The Wielandt method is one of many acceleration techniques for deterministic eigenvalue calculations that have been applied to reactor analysis. In deterministic calculations, the method usually guarantees a rapid and stable convergence in systems with a dominance ratio close to unity.

The MC adaptation[2] of the Wielandt method suggests an enhancement of the intensity of neutron interaction between more distant places. A fission neutron with a parent particle weight w is emitted within the current cycle from each collision with probability

$$\frac{\Sigma_{\mathrm{f}}}{\Sigma_{\mathrm{t}}}\frac{\nu}{k_{\mathrm{e}}}, \tag{17}$$

where the chosen k_{e} must be larger than k_{eff}. New fission neutrons are tracked by the same random walk process as other particles; they may produce progenies that are also tracked within the current cycle until their deaths by escape, Russian roulette and so on. If $k_{\mathrm{e}} < k_{\mathrm{eff}}$ then the fission chain will not terminate within the current cycle.

The apparent k-eigenvalue k_{w} of the system is computed by a standard k_{eff} estimator. The correct k_{eff} of the system is then given as

$$k_{\mathrm{eff}} = \left(\frac{1}{k_{\mathrm{w}}} + \frac{1}{k_{\mathrm{e}}}\right)^{-1}. \tag{18}$$

Fission neutrons for the subsequent cycle are produced in each collision with probability

$$w\frac{\Sigma_{\mathrm{f}}}{\Sigma_{\mathrm{t}}}\frac{\nu}{k_{\mathrm{w}}} = w\frac{\Sigma_{\mathrm{f}}}{\Sigma_{\mathrm{t}}}\nu\left(\frac{1}{k_{\mathrm{eff}}} - \frac{1}{k_{\mathrm{e}}}\right). \tag{19}$$

If k_{e} is reasonably selected, i.e. $k_{\mathrm{e}} > k_{\mathrm{eff}}$, then the expected number of fission neutrons per collision is smaller than in standard MC calculations. However, all neutrons tracked within the current cycle (including the new fission neutrons) may produce new fission neutrons for the subsequent cycle; thus, the number of first generation fission neutrons is preserved in each cycle. This causes the fission neutrons to be more spread out within a cycle than in standard MC calculations.

This method is similar to the super-history powering where the new fission neutrons are also tracked within the current cycle. In contrast to the super-history powering method, the neutron population always decays completely within a cycle. Moreover, fission neutrons for the subsequent cycle are sampled using all neutron histories in the cycle, not only using the very last generation.

This adaptation of the Wielandt method decreases the number of cycles needed for convergence. However, a numerical test calculation shows[2] that the reduction of the total number of cycles does not compensate for the increased computer time per cycle. The method increases the total computing time to obtain a converged fission source, and worsens the FOM of the k_{eff} estimate.

C. Stratified Source Sampling

The problem of losing an important component in weakly-coupled multi-component systems was addressed in the stratified source-sampling technique.[3] The system must be divided into a spatial mesh with b regions. Before sampling a new source $s_{mc}^{(n)}(\mathbf{r})$, the expected normalized source net weight $\langle w\rangle_i^{(n)}$ in region i is computed as

$$\langle w\rangle_i^{(n)} = \frac{m\int_{V_i} Fs_{\mathrm{mc}}^{(n-1)}(\mathbf{r})\,\mathrm{d}^3r}{\int_V Fs_{\mathrm{mc}}^{(n-1)}(\mathbf{r})\,\mathrm{d}^3r}, \tag{20}$$

and a low weight cutoff threshold, w_{cutt}, is specified. The net-number of fission neutrons in respective mesh regions is computed by Algorithm III.1 in each cycle. The locations of fission neutrons are sampled from the fission store with a probability proportional to the site weights.

Algorithm III.1 Stratified source sampling in cycle n.

1: **for** each region $i = 1, 2, \ldots$ **do**
2: Compute $\langle w \rangle_i^{(n)}$ by Eq. (20).
3: **if** $\langle w \rangle_i^{(n)} < w_{\text{cutt}}$ **then**
4: With probability $p = \langle w \rangle_i^{(n)}$ neutron starts from cell i carrying a unit weight; with probability $1 - p$ no source is sampled in region i.
5: **else**
6: Find $\tilde{m}$ as the nearest integer to $\langle w \rangle_i^{(n)}$.
7: **if** $\tilde{m} = 0$ **then**
8: A neutron starts from region i with a weight $\langle w \rangle_i^{(n)}$.
9: **else**
10: $\tilde{m}$ neutrons start from region i, each with a weight $\langle w \rangle_i^{(n)} / \tilde{m}$.
11: **end if**
12: **end if**
13: **end for**

D. Zero-Variance Scheme

The zero-variance scheme is known to be well-fitted for shielding calculations where a response R from small detectors is needed in large multiplying systems;

$$R = \int \eta_\chi(\mathbf{P}) \chi(\mathbf{P}) \, \mathrm{d}\mathbf{P} = \int \eta_\psi(\mathbf{P}) \psi(\mathbf{P}) \, \mathrm{d}\mathbf{P}, \tag{21}$$

where $\chi(\mathbf{P}) \equiv \chi(\mathbf{r}, \Omega, E)$ and $\psi(\mathbf{P})$ are the emission and collision density, respectively; and $\eta_\chi(\mathbf{P})$ and $\eta_\psi(\mathbf{P})$ are the detector response functions with respect to $\chi(\mathbf{P})$ and $\psi(\mathbf{P})$, respectively. $\chi(\mathbf{P})$ and $\psi(\mathbf{P})$ are given by steady-state transport equations,

$$\chi(\mathbf{P}) = s(\mathbf{P}) + \int K(\mathbf{P}' \to \mathbf{P}) \chi(\mathbf{P}') \, \mathrm{d}\mathbf{P}', \tag{22}$$

and

$$\psi(\mathbf{P}) = s(\mathbf{P}) + \int L(\mathbf{P}' \to \mathbf{P}) \psi(\mathbf{P}') \, \mathrm{d}\mathbf{P}', \tag{23}$$

where the transport kernels K and L are given as

$$K(\mathbf{P}' \to \mathbf{P}) \equiv T(\mathbf{r}' \to \mathbf{r}, \Omega', E') C(\mathbf{r}, \Omega' \to \Omega, E' \to E), \tag{24}$$

and

$$L(\mathbf{P}' \to \mathbf{P}) \equiv C(\mathbf{r}, \Omega' \to \Omega, E' \to E) T(\mathbf{r}' \to \mathbf{r}, \Omega', E'), \tag{25}$$

respectively. The transition kernel

$$T(\mathbf{r}' \to \mathbf{r}, \Omega', E') \, \mathrm{d}V \tag{26}$$

is the probability that a particle starting a flight path at $\mathbf{r}'$ will have its next collision in $\mathrm{d}V$ at $\mathbf{r}$. The collision kernel

$$C(\mathbf{r}, \Omega' \to \Omega, E' \to E) \, \mathrm{d}\Omega \, \mathrm{d}E \tag{27}$$

is the probability that a particle will exit a collision at $\mathbf{r}'$ with direction Ω in $\mathrm{d}\Omega$ and energy E in $\mathrm{d}E$.

During the neutron transport simulation, the transport kernel $L(\mathbf{P}' \to \mathbf{P})$ is biased using the adjoint form of $\psi(\mathbf{P})$ as

$$\bar{L}(\mathbf{P}' \to \mathbf{P}) \equiv L(\mathbf{P}' \to \mathbf{P}) \frac{\psi^*(\mathbf{P})}{\psi^*(\mathbf{P}')}, \tag{28}$$

which must be compensated by a suitable change of the particle weight w, so that wL is conserved. The adjoint form $\psi^*(\mathbf{P})$ is the solution of the adjoint equation

$$\psi^*(\mathbf{P}) = \eta_\psi + \int L(\mathbf{P} \to \mathbf{P}') \psi^*(\mathbf{P}') \, \mathrm{d}\mathbf{P}'. \tag{29}$$

Similarly, the adjoint form of $\chi(\mathbf{P})$ can be obtained, and used for biasing the transport kernel $K(\mathbf{P}' \to \mathbf{P})$.

Recently, a zero-variance scheme was derived for eigenvalue calculations.[4] The k_{eff} eigenvalue is obtained from a detector response

$$R = \int \frac{\nu \Sigma_f(\mathbf{P})}{\Sigma_t(\mathbf{P})} \psi(\mathbf{P}) \, \mathrm{d}\mathbf{P}. \tag{30}$$

Thus, the detector response function $\eta_\psi = \nu \Sigma_f(\mathbf{P}) / \Sigma_t(\mathbf{P})$. This is possible since

$$k_{\text{eff}} = \frac{\int F s_{\text{mc}}^{(n)}(\mathbf{P}) \, \mathrm{d}\mathbf{P}}{\int s_{\text{mc}}^{(n)}(\mathbf{P}) \, \mathrm{d}\mathbf{P}} = \frac{\int \frac{\nu \Sigma_f(\mathbf{P})}{\Sigma_t(\mathbf{P})} \psi(\mathbf{P}) \, \mathrm{d}\mathbf{P}}{\int s_{\text{mc}}^{(n)}(\mathbf{P}) \, \mathrm{d}\mathbf{P}}, \tag{31}$$

where $\int s(n)(\mathbf{P}) \, \mathrm{d}\mathbf{P}$ is the known neutron batch size.

It has been shown that the FOM in computing k_{eff} may be increased by about 70% when only the collision kernel is biased.[19] Biasing the transition kernel is time consuming, resulting in a reduction the FOM of the calculation. Acceleration of the fission source convergence may be expected when the collision kernel is biased in successive cycles.

E. Fission Matrix Method

When the system is spatially discretized, the operator F in Eq. (1) can be approximated by the fission matrix $\mathbb{F}$.[5,20] The (i, j)th element of $\mathbb{F}$ represents the probability that a fission neutron born in region j causes the subsequent birth of a fission neutron in region i,

$$(\mathbb{F})_{i,j} = \frac{\int_{V_i} \mathrm{d}^3 r \int_{V_j} \mathrm{d}^3 r' f(\mathbf{r}' \to \mathbf{r}) s_0(\mathbf{r}')}{\int_{V_j} s_0(\mathbf{r}') \, \mathrm{d}^3 r'}. \tag{32}$$

Kaplan[5] proposed biasing the MC fission source through variance reduction techniques using the fundamental eigenvector of $\mathbb{F}$.

Carter and McCormick[21] suggested forming the "cycle fission matrix" in each cycle as

$$(\mathbb{F}^{(n)})_{i,j} = \frac{\int_{V_i} \mathrm{d}^3 r \int_{V_j} \mathrm{d}^3 r' f(\mathbf{r}' \to \mathbf{r}) s_{\text{mc}}^{(n-1)}(\mathbf{r}')}{\int_{V_j} s_{\text{mc}}^{(n-1)}(\mathbf{r}') \, \mathrm{d}^3 r'}, \tag{33}$$

and modifying the weights $w_i^{(n)}$ of fission neutrons in region j in the fission store as

$$w_i^{(n)} \leftarrow \frac{\left(\mathbf{s}_{\mathrm{fm}}^{(n)}\right)_j}{\left(\mathbf{s}_{\mathrm{fm}}^{(n-1)}\right)_j} w_i^{(n)}, \quad \forall j, \tag{34}$$

where $\mathbf{s}_{\mathrm{fm}}^{(n)}$ is the fundamental eigenvector of $\mathbb{F}^{(n)}$.

Kadotani, et al.[22] proposed correcting the weights $w_i^{(n)}$ of the fission neutrons in region j as

$$w_i^{(n)} \leftarrow \frac{\left(\mathbf{s}_{\mathrm{fm}}^{(n)}\right)_j}{\left(\mathbf{s}_{\mathrm{mc}}^{(n)}\right)_j} w_i^{(n)}, \quad \forall j, \tag{35}$$

where

$$\left(\mathbf{s}_{\mathrm{mc}}^{(n)}\right)_j = \int_{V_j} s_{\mathrm{mc}}^{(n)}(\mathbf{r})\,\mathrm{d}^3 r. \tag{36}$$

(Vectors $\mathbf{s}_{\mathrm{mc}}^{(n)}$ and $\mathbf{s}_{\mathrm{fm}}^{(n)}$ should be normalized to the same number.) This correction was intended for all cycles, both inactive and active.

Kitada and Takeda[23] tested Eq. (35) on a large core model, and recommended using the method only during inactive cycles due to the unexpected behavior of the fundamental eigenvector $\mathbf{s}_{\mathrm{fm}}^{(n)}$. In fact, all attempts at using the fission matrix computed by MC have met with limited success due to the problematic convergence of $\mathbf{s}_{\mathrm{fm}}^{(n)}$,[9] although the convergence may be improved by using the "cumulative fission matrix"

$$\left(\mathbb{F}^{(n)}\right)_{i,j} = \frac{\sum_{l=0}^{n-1} \int_{V_i} \mathrm{d}^3 r \int_{V_j} \mathrm{d}^3 r' f(\mathbf{r}' \to \mathbf{r}) s_{\mathrm{mc}}^{(l)}(\mathbf{r}')}{\sum_{l=0}^{n-1} \int_{V_j} s_{\mathrm{mc}}^{(l)}(\mathbf{r}')\,\mathrm{d}^3 r'}. \tag{37}$$

However, using the cumulative fission matrix is also problematic. The cumulative fission matrix formed in the first cycle might be very noisy, depending on m and the initial MC fission source. If the matrix contains highly overestimated entries then $\mathbf{s}_{\mathrm{fm}}^{(n)}$ typically has very few nonzero elements. After source normalization, e.g. by Eq. (35), the source can be located in a relatively small volume; thus, only a very small part of the cumulative fission matrix can be improved in the subsequent cycle. This may result in a very slow source convergence since the fundamental eigenvector can change its shape considerably in each cycle. In an extreme case, the source could be positioned in regions that do not relate to the corrupted elements of the fission matrix, which can result in the divergence of $\mathbf{s}_{\mathrm{fm}}^{(n)}$.

The convergence of FM methods have been diagnosed when the relative difference between corresponding elements of $\mathbf{s}_{\mathrm{fm}}^{(n)}$ and $\mathbf{s}_{\mathrm{fm}}^{(n-1)}$ have dropped below a certain small number ε,[23]

$$\varepsilon > \left| \frac{\left(\mathbf{s}_{\mathrm{fm}}^{(n)}\right)_j - \left(\mathbf{s}_{\mathrm{fm}}^{(n-1)}\right)_j}{\left(\mathbf{s}_{\mathrm{fm}}^{(n-1)}\right)_j} \right|, \quad \forall j. \tag{38}$$

F. Semi-Fixed-Source FM Method

Numerical test calculations indicate[6] that the instability of the FM method is caused by sampling the elements of the fission matrix using various numbers of fission neutrons. This causes an imbalanced precision of elements of the fission matrix, resulting in a large error of its fundamental eigenvector. The new "semi-fixed-source FM method"[6] samples all regions with an equal number of fission neutrons in all cycles, which insures that all elements of the fission matrix converge at the same rate. The weights $w_i^{(n)}$ of all fission neutrons in region j in the fission store are modified as

$$w_i^{(n)} \leftarrow \frac{m}{d} \frac{w_i^{(n)}}{\left(\mathbf{s}_{\mathrm{mc}}^{(n)}\right)_j}, \quad \forall j, \tag{39}$$

where $\left(\mathbf{s}_{\mathrm{mc}}^{(n)}\right)_j$ is defined by Eq. (36). If the number of fission neutron is fixed in all mesh regions then the regions should have varied volumes V_i so that the source can converge to $s_0(\mathbf{r})$. However, since $s_0(\mathbf{r})$ is not known the ideal mesh can not be designed. An approximate mesh will cause a bias of the fission matrix. However, it was shown, using the mean value theorems, that if the mesh regions in the approximate mesh are sufficiently small then the bias of the fission matrix is minimized.

It was suggested that the convergence of the semi-fixed-source method can be diagnosed when the relative distance between $\mathbf{s}_{\mathrm{fm}}^{(n_i)}$ and $\mathbf{s}_{\mathrm{fm}}^{(n_{i-1})}$ drops below ε,

$$\varepsilon > \frac{\left\| \mathbf{s}_{\mathrm{fm}}^{(n_i)} - \mathbf{s}_{\mathrm{fm}}^{(n_{i-1})} \right\|}{\left\| \mathbf{s}_{\mathrm{fm}}^{(n_{i-1})} \right\|}, \tag{40}$$

rather than using criterion (38). Since the relative change of the fundamental eigenvector between two subsequent cycles also depends on the neutron batch size m, and a small batch might not be sufficient to considerably improve the cumulative fission matrix and its eigenvectors, the number of cycles $(n_1, n_2, \ldots)$ where $\mathbf{s}_{\mathrm{fm}}^{(n)}$ is computed can, for instance, grow geometrically.

The method can provide k_{eff}, the fission source, neutron flux, gamma heat deposition, power, detector response etc., at any place, when the convergence is diagnosed, and no further simulation is needed.[6] Contrary to the existing methods in MC eigenvalue calculations the semi-fixed-source FM method can also be efficiently parallelized.

IV. CONCLUSIONS

The main methods of accelerating the MC eigenvalue calculations (improving the FOM) were briefly described.

Super-History Powering

The super-history powering method is suitable for reducing the MC source bias. Therefore, a smaller neutron batch size than in a standard MC calculation may be specified to reach the required source bias. This allows a faster source iteration, i.e. source convergence acceleration. A possible drawback of the method is that the last generation in a cycle may contain a considerably smaller number of neutrons than required for the subsequent cycle; therefore, relatively few fission neutrons with a large weight may be generated, which may have a negative effect. The method is implemented in the MONK code.

Wielandt's Method

The MC adaptation of the Wielandt method addresses systems with a dominance ratio close to unity; however, as numerical test calculations indicate, the method does not improve the FOM of MC eigenvalue calculations. This could be explained by the fact that the method samples the fission source for the subsequent cycle using all generations from the current cycle; the initial generations are, however, less converged than the last generations. The method may decrease the bias of the MC source, similarly to the super-history powering method.

Stratified Source Sampling

The stratified source sampling method demonstrated an improved convergence of the fission source in a multi-component system. The impact on the source bias as well as the ability to increase the FOM in systems with a dominance ratio close to unity was not tested.

Zero-Variance Scheme

The zero-variance scheme was recently derived for eigenvalue calculations, and numerically tested. The FOM of the zero-variance scheme in eigenvalue calculations is smaller than in shielding calculations since the criticality response function may be more or less uniform in a well designed reactor. Therefore, the adjoint form of $\psi(\mathbf{P})$ does not have large spatial gradients inside the core. However, numerical tests indicate a considerably increased FOM when computing the k_{eff}, and possible acceleration of the fission source convergence. The method is being implemented into the TRIPOLI-4 code[24] within the NURESIM Integrated Project[7].

Fission Matrix Method

The fission matrix method has many times showed its potential to accelerate the fission source, especially when a large neutron batch size was specified for both the FM method and the standard MC calculation. However, the efficiency of a standard MC calculation is sensitive to the neutron batch size. If the batch size is reduced while still providing an acceptable source bias then the MC calculation has a better FOM while the fission matrix method may become instable.

Semi-Fixed-Source FM Method

The instability issue of the FM method was recently addressed in the semi-fixed-source FM method. The method samples all elements of the fission matrix using an equal number of neutrons in all cycles, which insures a stable convergence, and improves the efficiency compared to the existing FM methods. Numerical tests indicate that the performance of the semi-fixed-source FM method is comparable to standard MC eigenvalue calculations with an optimized neutron batch size. In practice, however, a considerable acceleration can be reached for two reasons. First, the efficiency of standard MC eigenvalue calculations is sensitive to the neutron batch size while the semi-fixed-source method is not. Second, standard MC eigenvalue calculations do not utilize data obtained from inactive cycles. The semi-fixed-source FM method, however, can provide a k_{eff} estimation as well as spatial distributions of neutron flux and power at the moment when the convergence is diagnosed; all data from the full simulation is utilized. Moreover, the method can provide higher mode k-eigenvalues and source eigenfunctions and the dominance ratio. The semi-fixed-source FM method can be parallelized efficiently in contrast to standard MC eigenvalue calculations, which is its greatest advantage. This allows for the full utilization of multi-core processors and multi-processor computers. The method will be implemented into the TRIPOLI-4 code[24] within the NURESIM Integrated Project[7].

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