Annals of Nuclear Energy 36 (2009) 7–14

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Convergence of the second eigenfunction in Monte Carlo power iteration

Toshihiro Yamamoto *

Nuclear Technology and Education Center, Japan Atomic Energy Agency, 2-4 Shirakata Shirane, Tokai-mura, Naka-gun, Ibaraki-ken 319-1195, Japan

ARTICLE INFO

Article history:
Received 28 August 2008
Received in revised form 7 November 2008
Accepted 10 November 2008
Available online 23 December 2008

ABSTRACT

The conditions of convergence in a modified Monte Carlo power iteration method to generate the eigenfunction with the second largest criticality eigenvalue, which was originally proposed by Booth, have been defined with a different approach. In this work, the first and second eigenvectors composed of two volume-integrated fission source intensities defined in two-partitioned regions are used for deriving the convergence conditions. The conditions of convergence as shown by Booth are found to be true in the limit of a small amplitude of the first eigenfunction. Following the method that uses two estimates of the second eigenvalue defined in two-partitioned regions, a new method for removing the fundamental mode eigenfunction from the fission source distributions has been developed. Because of the explicit removal of the first eigenfunction, the validity of this method is convincing as a technique for obtaining the second eigenfunction. Although this method needs the first eigenfunction and eigenvalue, and the subtraction of the first eigenfunction from the fission source distribution, it has the advantage that the adjoint mode calculation which is in general difficult for continuous energy Monte Carlo codes is not required.

1. Introduction

A method for obtaining the higher-order eigenfunctions in Monte Carlo criticality calculations, which may be useful for nuclear reactor analyses and nuclear criticality safety evaluations, will enhance the versatility of the Monte Carlo method in the field of nuclear applications.

An elaborate technique to obtain the higher-order eigenfunctions in Monte Carlo criticality calculations were proposed in the references (Booth, 2003, 2006; Booth and Gubernatis, 2008; Gubernatis and Booth, 2008). For example, to obtain the second eigenfunction, the method partitions the whole space into two regions. In the course of the power iteration, the component of the eigenfunction in each region is adjusted such that the estimate of the eigenvalue in each region is forced to be equal to each other (Booth, 2003). The superiority of the method is its simplicity. The lower-order eigenfunctions are not needed to estimate the higher-order eigenfunctions, which is an outstanding feature of the method. In addition, it is worth noting that particles of negative weights were introduced firstly in Monte Carlo criticality calculations. However, only a plausibility argument was given to the proof that this method surely converges to the higher-order eigenfunctions. Booth (2006) adopted another technique for higher-order eigenvalues and eigenfunctions, which is different from Booth (2003). Other subsequent recent papers (Booth and Gubernatis, 2008; Gubernatis and Booth, 2008) are extensions or applications to the method in Booth (2006). However, the technique in Booth (2003) is still fascinating because of its simplicity, and further investigation on the technique is worth while. Thus, this paper attempts to develop a new understanding as to the conditions required for convergence of the method in Booth (2003).

2. Review of power iteration for the largest eigenvalue

In the power iteration method for a fundamental mode eigenvalue calculation, the initial fission source distribution, which may be far from the fundamental mode, is given at the beginning of the calculation. The convergence of the fission source distribution toward the fundamental mode was already proved in many literatures (Urbatsch, 1996; Naito and Yang, 2004). The ratio of a higher-order eigenfunction's magnitude to the fundamental mode's one attenuates at each power iteration, then the fission source distribution converges to the fundamental mode. Let the fission source distribution and the ith mode eigenfunction be $P(\boldsymbol{r})$ and $\varphi_i(\boldsymbol{r})$, $i = 1, 2, \ldots$, respectively. The fission source distribution is given by

$$P(\boldsymbol{r}) = \int \Sigma_f(\boldsymbol{r}, E)\phi(\boldsymbol{r}, E)\,\mathrm{d}E, \tag{1}$$

where

$\Sigma_f(\boldsymbol{r}, E)$ = macroscopic fission cross-section of neutron energy E at position $\boldsymbol{r}$,

$\phi(\boldsymbol{r}, E)$ = neutron flux of neutron energy E at position $\boldsymbol{r}$.

The ith eigenvalue k_i associated with the ith eigenfunction $\varphi_i(\boldsymbol{r})$ is ordered $k_1 > k_2 \geqslant k_3 \geqslant, \ldots, > 0$ where the eigenvalues are

* Tel.: +81 29 284 3845; fax: +81 29 282 6040.
E-mail address: elsavonbrabant@yahoo.co.jp.

0306-4549/$ - see front matter © 2008 Elsevier Ltd. All rights reserved.
doi:10.1016/j.anucene.2008.11.004

assumed to be real and positive. Here, k_1 is the fundamental mode eigenvalue and called neutron effective multiplication factor k_{eff}. An operator $\boldsymbol{A}$, which is relevant to a single power iteration, is introduced, then

$$\boldsymbol{A}\varphi_i(\boldsymbol{r}) = k_i\varphi_i(\boldsymbol{r}). \tag{2}$$

Because of completeness, an arbitrary fission source distribution $P(\boldsymbol{r})$ can be expanded as a linear combination of the eigenfunctions

$$P(\boldsymbol{r}) = \sum_{i=1}^{\infty} a_i\varphi_i(\boldsymbol{r}), \tag{3}$$

where a_i is an amplitude of the ith eigenfunction. $P(\boldsymbol{r})$ is normalized at each iteration throughout the Monte Carlo calculation. For example,

$$N = \int |P(\boldsymbol{r})|\mathrm{d}\boldsymbol{r}, \tag{4}$$

where N is the number of particles per iteration. Applying the operator $\boldsymbol{A}$ to $P(\boldsymbol{r})$ stands for obtaining the fission source distribution on the next iteration

$$\boldsymbol{A}P(\boldsymbol{r}) = \sum_{i=1}^{\infty} a_i k_i\varphi_i(\boldsymbol{r}). \tag{5}$$

Since $k_1 > k_2 \geqslant k_3 \geqslant, \ldots, > 0$, applying the operator $\boldsymbol{A}$ many times has the limit as

$$\lim_{n\to\infty} \frac{1}{k_1^n}\boldsymbol{A}^n P(\boldsymbol{r}) = a_1\varphi_1(\boldsymbol{r}), \tag{6}$$

where only the eigenfunction with the largest eigenvalue survives. That is why the power iteration cannot lead to the higher-order eigenfunctions without introducing some extra techniques for obtaining the higher-order eigenfunctions.

3. Review of methods for obtaining the higher-order eigenfunctions

3.1. Hotelling's method for Monte Carlo calculations

Hotelling's method is known as a technique for obtaining the higher-order eigenfunctions (Hashimoto and Nishina, 1991). The method removes the fundamental mode eigenfunction from $P(\boldsymbol{r})$ by making use of the adjoint eigenfunctions and the orthogonality between the forward and adjoint eigenfunction. The orthogonality is

$$\int\int \phi_m^*(\boldsymbol{r},E)\chi(E)\phi_n(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}\,\mathrm{d}E = 0 \quad \text{for } m\neq n, \tag{7}$$

where

$\phi_m^*(\boldsymbol{r},E)$ = mth order adjoint flux,

$\chi(E)$ = fission spectrum of energy E.

With this orthogonality, the amplitude of the first eigenfunction a_1 in Eq. (3) is given as

$$a_1 = \int\int \phi_1^*(\boldsymbol{r},E)\chi(E)P(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}\,\mathrm{d}E \Big/ \int\int \phi_1^*(\boldsymbol{r},E)\chi(E)\phi_1(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}\,\mathrm{d}E \tag{8}$$

The component of the first eigenfunction in Eq. (3) can be easily removed from $P(\boldsymbol{r})$ as

$$P(\boldsymbol{r}) - a_1\varphi_1(\boldsymbol{r}). \tag{9}$$

Since the first eigenfunction is removed by applying Eq. (3) each iteration, the fission source distribution converges toward the second eigenfunction that has the second-largest eigenvalue. This method, however, has two difficulties for Monte Carlo calculations. First, a capability of the criticality calculation in adjoint mode has been installed in no contemporary continuous energy Monte Carlo code. Hotelling's method could not be applied to continuous energy Monte Carlo calculations before development of the adjoint mode calculation in continuous energy. Secondly, since eigenfunctions are represented by point particles in Monte Carlo calculations, the integrations in Eq. (8) and the pointwise subtraction in Eq. (9) are in general difficult to conduct unless a technique similar to the point detector as proposed by Booth (2003) or a discretization of space and energy is introduced. Consequently, in view of the present status of the Monte Carlo method, the use of Hotelling's method seems not to be suitable for obtaining the higher-order eigenfunctions in Monte Calro criticality calculations.

3.2. Method using two estimates of the second eigenfunctions

A method proposed by Booth (2003) can obtain the second eigenfunction via a modified power iteration without knowing the first eigenfunction. This method partitions the space into two regions R_{I} and R_{II}. Two $k_2's$ in the nth iteration are defined as

$$k_2^{\text{I}(n)} = P_{\text{I}}^{(n)}/P_{\text{I}}^{(n-1)}, \tag{10}$$

and

$$k_2^{\text{II}(n)} = P_{\text{II}}^{(n)}/P_{\text{II}}^{(n-1)}, \tag{11}$$

where

$$P_{\text{I}}^{(n-1)} = \int_{R_{\text{I}}} P^{(n-1)}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}, \tag{12}$$

$$P_{\text{II}}^{(n-1)} = \int_{R_{\text{II}}} P^{(n-1)}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}, \tag{13}$$

$$P_{\text{I}}^{(n)} = \int_{R_{\text{I}}} \boldsymbol{A}P^{(n-1)}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}, \tag{14}$$

$$P_{\text{II}}^{(n)} = \int_{R_{\text{II}}} \boldsymbol{A}P^{(n-1)}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}, \tag{15}$$

and $P^{(n-1)}(\boldsymbol{r})$ is the fission source distribution in the $(n-1)$th iteration. It is preferable to partition the space according to the sign of $P(\boldsymbol{r})$. For example, $P(\boldsymbol{r}) > 0$ in R_{I} and $P(\boldsymbol{r}) < 0$ in R_{II}. If a partitioned space consists of a positive and negative $P(\boldsymbol{r})$, cancellation occurs in the space integration, and part of the information on the fission source distribution is lost. This leads to loss of accuracy and stability of the Monte Carlo calculation for the second eigenfunction. How to partition the space, however, might be arbitrary.

The method utilizes the property that $k_2^{\text{I}(n)} = k_2^{\text{II}(n)} = k_2$ when $P(\boldsymbol{r}) \propto \varphi_2(\boldsymbol{r})$. When $k_2^{\text{I}(n)} > k_2^{\text{II}(n)}$, the component in the region R_{I} is growing faster than in the region R_{II} and vice versa. To keep the component growing at the same rate, Booth proposes that the fission source distribution for the next iteration $P^{(n)}(\boldsymbol{r})$ be modified as

$$P^{(n)}(\boldsymbol{r}) = \left(k_2^{\text{II}(n)}/k_2^{\text{I}(n)}\right)^{\alpha}\boldsymbol{A}P^{(n-1)}(\boldsymbol{r}) \quad \text{for } \boldsymbol{r}\in R_{\text{I}}, \tag{16}$$

or

$$P^{(n)}(\boldsymbol{r}) = \left(k_2^{\text{II}(n)}/k_2^{\text{I}(n)}\right)^{\alpha}\boldsymbol{A}P^{(n-1)}(\boldsymbol{r}) \quad \text{for } \boldsymbol{r}\in R_{\text{II}}, \tag{17}$$

where $\alpha > 1$. Then, after the modified fission source distribution $P^{(n)}(\boldsymbol{r})$ gets renormalized as in Eq. (4), they are used as $P(\boldsymbol{r})$ in the next iteration. (The notations and minor details are changed from Booth's paper to be consistent with the following discussions.) The approximate best value for α, which was obtained in the paper by Booth via long derivation with some assumptions, would be

$$\alpha = k_1/(k_1 - k_2). \tag{18}$$

Also, the range of α where convergence occurs is approximately given by