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Application of Inactive Cycle Stopping Criteria for Monte Carlo Wielandt Calculations

Hyung Jin Shim*
Korea Atomic Energy Research Institute
1045 Daedeokdaero, Yuseong-gu, Daejeon 305-353, Korea
shimhj@kaeri.re.kr

Chang Hyo Kim
Department of Nuclear Engineering
Seoul National University
599 Gwanakro, Gwanak-gu, Seoul 151-742, Korea
kchyo@snu.ac.kr

ABSTRACT

The Wielandt method is incorporated into Monte Carlo (MC) eigenvalue calculation as a way to speed up fission source convergence. To make the most of the MC Wielandt method, however, it is highly desirable to halt inactive cycle runs in a timely manner because it requires a much longer computational time to execute a single cycle MC run than the conventional MC eigenvalue calculations. This paper presents an algorithm to detect the onset of the active cycles and thereby to stop automatically the inactive cycle MC runs based on two anterior stopping criteria. The effectiveness of the algorithm is demonstrated by applying it to a slow convergence problem.

Key Words: Monte Carlo eigenvalue calculation, Monte Carlo Wielandt Method, fission source convergence, anterior stopping criteria, slow convergence problem

1. INTRODUCTION

A Monte Carlo (MC) Wielandt method for eigenvalue calculations has been proposed as a way to accelerate a fission source convergence [1,2]. Like its deterministic counterpart, the MC Wielandt method is found to achieve a faster convergence than the power method. In order to make the most of this and attain the desired computational efficiency, however, one needs to detect the onset of the stationary cycles and halt the inactive cycle MC runs automatically, in a timely manner. This is because the Wielandt method requires a much longer computational time to execute a single cycle MC run than the conventional power method [1].

As a way to check the convergence of the fission source distribution (FSD), Ueki and Brown [3] developed posterior diagnostic criteria based on the information theory. Richet, Jacquet, and Bay [4] proposed another posterior statistical method to adjust the onset of the active cycles based on the Brownian bridge theory. Wenner and Haghighat [5] suggested a complementary use of these two approaches for a more trustworthy detection of the fission source convergence. However,

* Corresponding author.

these methods have a drawback in common in that they are only applicable after all the active cycle runs are completed.

There have been some studies to develop anterior or on-the-fly convergence criteria which are designed to halt automatically inactive cycle MC runs when the FSD becomes converged. We [6] developed anterior stopping criteria which require comparing two FSDs L correlation cycle lengths apart. Ueki [7] presented step-refined source convergence diagnostics using progressive relative entropies. Dumonteil et al. [8] introduced a different approach to construct a criterion based on filtering the Boltzmann entropy signals.

The objective of this paper is to examine the efficiency of the anterior stopping criteria developed by us in the MC Wielandt calculations. In Chapter 2, the anterior stopping criteria are reviewed with their mathematical derivations. The MC Wielandt method is summarized in Chapter 3. The anterior stopping criteria are applied for a slow convergence problem in Chapter 4.

2. ANTERIOR STOPPING CRITERIA

2.1. Derivation of Stopping Criteria

In the MC power method, the cycle-by-cycle update of the FSD is achieved by

$$S^i = \frac{1}{k^{i-1}}\mathbf{H}S^{i-1} + \varepsilon^i \ , \ i = 1, 2, \cdots ; \tag{1}$$
$$S^i \equiv S^i(\mathbf{P}),\ \varepsilon^i \equiv \varepsilon^i(\mathbf{P}),$$
$$\mathbf{H}S^{i-1} = \int_\Gamma H(\mathbf{P}' \to \mathbf{P}) S^{i-1}(\mathbf{P}) d\mathbf{P}.$$

$\mathbf{P}$ stands for $(\mathbf{r}, E, \mathbf{\Omega})$, the 6-dimensional phase space vector representing a neutron state. The superscript i or i-1 is the cycle index. $S^t (t = i \text{ or } i-1)$ is the FSD generated at t-th cycle for the next cycle run, which is normalized by $\int_\Gamma S^t(\mathbf{P})d\mathbf{P} = 1$. k^{i-1} is the eigenvalue estimated at cycle i-1. Γ is the phase space volume of the nuclear system to be analyzed. $H(\mathbf{P}' \to \mathbf{P})$ is the number of first-generation fission neutrons born per unit phase space volume about $\mathbf{P}$, due to a parent neutron born at $\mathbf{P}'$. ε^i is the stochastic error component of S^i resulting from sampling of a finite number of histories per cycle. It is defined by

$$\varepsilon^i(\mathbf{P}) \equiv S^i(\mathbf{P}) - E[S^i(\mathbf{P}) \,|\, S^{i-1}(\mathbf{P})]. \tag{2}$$

Because a finite number of histories is simulated, $S^i(\mathbf{P})$ in Eq. (1) cannot be measured in a continuous form. Therefore, one may divide the whole region into small non-overlapping cells with a spatial volume, V_m (m=1, 2, $\cdots$, N_m), and define the cell-wise fission sources by

$$S_m^i = \int_{V_m}\int_E\int_{\mathbf{\Omega}} S^i(\mathbf{r}, E, \mathbf{\Omega}) d\mathbf{r} dE d\mathbf{\Omega}\,. \tag{3}$$

In view of the fact that, when the FSD is converged, the difference between two fission sources correlation cycle L apart, S_m^i and S_m^{i-L}, must be statistically indistinguishable, one can require that the following conditions must be met for all cells.

$$\left|\frac{S_m^i - S_m^{i-L}}{S_m^i}\right| < \kappa \cdot \sigma\left[\frac{S_m^i - S_m^{i-L}}{S_m^i}\right];\ m = 1, 2, \cdots, N_m. \tag{4}$$

σ is the standard deviation of the bracketed quantity. κ stands for an integer, say, 1 or 2 or 3.

Treating S_m^i and S_m^{i-L} as two independent random variables, one can approximate σ in Eq. (4) to the second order of the fluctuation of S_m^i and S_m^{i-L} by

$$\sigma^2\left[\frac{S_m^i - S_m^{i-L}}{S_m^i}\right] \cong \frac{2}{(S_m^i)^2} \cdot \left(\sigma^2\left[S_m^i\right] - \mathrm{cov}\left[S_m^i, S_m^{i-L}\right]\right). \tag{5}$$

The substitution of Eq. (5) into Eq. (4) results in

$$\left|S_m^i - S_m^{i-L}\right| < \kappa\sqrt{2(\sigma^2[S_m^i] - \mathrm{cov}[S_m^i, S_m^{i-L}])};\ m = 1, 2, \cdots, N_m. \tag{6}$$

Because of the statistical behavior of $(S_m^i - S_m^{i-L})$, there can be cells whose fission sources do not satisfy Eq. (6). To use Eq. (6) as a convergence criterion, one needs to take into account the presence of such cells. Thus Eq. (4) is augmented by the following condition;

$$\frac{\text{the number of cells not satisfying Eq. (7)}}{\text{the total number of cells}} < C(\kappa). \tag{7}$$

Equations (6) and (7) form the type-A convergence criterion. $C(\kappa)$ depends on κ as well as the distribution function of the relative differences, $(S_m^i - S_m^{i-L})/S_m^i$, for all m. Under an assumption that $(S_m^i - S_m^{i-L})/S_m^i$ follows the normal distribution, $C(\kappa=1) \approx 32\%$, $C(\kappa=2) \approx 4.6\%$, and $C(\kappa=3) \approx 0.3\%$.

Another criterion can be derived from Eq. (4) by assuming that the relative difference of the cell-wise fission sources, $(S_m^i - S_m^{i-L})/S_m^i$ (m=1, 2, ⋯, N_m) is a set of N_m independent normal random variables. Under this assumption, the square sum of the normalized relative differences, Z, given by

$$Z = \sum_{m=1}^{N_m} \left\{ \frac{\left(\frac{S_m^i - S_m^{i-L}}{S_m^i} \right) - \overline{\frac{S_m^i - S_m^{i-L}}{S_m^i}}}{\sigma\left[\frac{S_m^i - S_m^{i-L}}{S_m^i} \right]} \right\}^2 \tag{8}$$

Z is regarded as the random variable that follows a chi-square distribution with N_m degrees of freedom. Then a stopping criterion can be given by

$$Z < \chi^2(N_m, \alpha) \tag{9}$$

$\chi^2(N_m,\alpha)$ denotes the value ν that satisfies probability $\{Z>\nu\} = \int_\nu^\infty p_Z(z)dz = \alpha$ in which $p_Z(z)$ is the chi-square distribution of N_m degrees of freedom. Noting $\overline{\frac{S_m^i - S_m^{i-L}}{S_m^i}}=0$ and substituting Eq. (5) into Eq. (8), one finds that Eq. (9) is expressed as

$$\sum_{m=1}^{N_m} \frac{(S_m^i - S_m^{i-L})^2}{2(\sigma^2[S_m^i] - \mathrm{cov}[S_m^i, S_m^{i-L}])} < \chi^2(N_m, \alpha) \tag{10}$$

This is called the type-B or χ^2 criterion.

2.2. Estimation of $\sigma^2[S_m^i]$, $\mathrm{cov}[S_m^i, S_m^{i-L}]$, and L

The application of the stopping criteria discussed in the above requires the way to estimate $\sigma^2[S_m^i]$, $\mathrm{cov}[S_m^i, S_m^{i-L}]$ and the correlation length L. We found the cycle-by-cycle stochastic error propagation model [9, 10] useful. According to this model, the inter-cycle covariance between the fission sources l cycles apart in stationary cycles, $\mathrm{cov}[S_m^i, S_{m'}^{i+l}]$, is expressed as

$$\mathrm{cov}[S_m^i, S_{m'}^{i+l}] = \sum_{t=0}^{\infty} \sum_{n=1}^{N_m} \sum_{n'=1}^{N_m} a_{mn}^t a_{m'n'}^{t+l} \, \mathrm{cov}[\varepsilon_n, \varepsilon_{n'}]\,. \tag{11}$$

a_{mn}^t is the m-th row and n-th column element of matrix $\mathbf{A}^t$ in which $\mathbf{A}$ is defined by

$$\mathbf{A} = \frac{1}{k_0}\left(\mathbf{H} - \mathbf{S}_0 \cdot \boldsymbol{\tau}^T \cdot \mathbf{H}\right);$$
$$\boldsymbol{\tau}^T = N_m \text{ dimensional row vector } (1,1,\cdots,1). \tag{12}$$

H is the fission matrix. k_0 and $\mathbf{S}_0$ denote the main mode eigenvalue and eigenvector of the matrix **H**, respectively. $\mathrm{cov}[\varepsilon_n, \varepsilon_{n'}]$ is the covariance of the cell-wise stochastic error components which are assumed to be independent of the cycle index for stationary cycles.

Assuming that the stationary cycle starts after the (i-L)-th cycle, one can obtain the following equations for $\sigma^2[S_m^i]$ and $\mathrm{cov}[S_m^i, S_m^{i-L}]$ from Eq. (11);

$$\sigma^2[S_m^i] = \sum_{t=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m} a_{mn}^t a_{mn'}^t \,\mathrm{cov}[\varepsilon_n, \varepsilon_{n'}], \tag{13}$$

$$\mathrm{cov}[S_m^i, S_m^{i-L}] = \sum_{t=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m} a_{mn}^t a_{mn'}^{t-L} \,\mathrm{cov}[\varepsilon_n, \varepsilon_{n'}]. \tag{14}$$

By definition, the covariance of the cell-wise stochastic error components at cycle i can be estimated by

$$\begin{aligned} \mathrm{cov}_S[\varepsilon_n^i, \varepsilon_{n'}^i] &= \frac{1}{M(M-1)}\sum_{j=1}^{M}((S_n^i)_j - \overline{S_n^i})\cdot((S_{n'}^i)_j - \overline{S_{n'}^i}); \\ \overline{S_m^i} &= \frac{1}{M}\sum_{j=1}^{M}(S_m^i)_j \quad (m = n \text{ or } n'), \end{aligned} \tag{15}$$

where M is the number of histories per cycle. $(S_n^i)_j$ is the fission sources of cell n generated by the j-th history at cycle i.

In ref. 6, it is shown that $\mathrm{cov}[\varepsilon_n, \varepsilon_{n'}]$ for the stationary cycles can be estimated using $\mathrm{cov}_S[\varepsilon_n^i, \varepsilon_{n'}^i]$ for the non-stationary cycles as

$$\mathrm{cov}[\varepsilon_n, \varepsilon_n] = \sigma^2[\varepsilon_n] \cong \frac{S_{0n}(1 - S_{0n})}{\overline{S_n^i}(1 - \overline{S_n^i})}\mathrm{cov}_S[\varepsilon_n^i, \varepsilon_n^i], \tag{16}$$

$$\mathrm{cov}[\varepsilon_n, \varepsilon_{n'}] \cong \frac{S_{0n}\cdot S_{0n'}}{\overline{S_n^i}\cdot\overline{S_{n'}^i}}\mathrm{cov}_S[\varepsilon_n^i, \varepsilon_{n'}^i] \;\; (n \neq n'). \tag{17}$$

where S_{0n} is the n-th component of the fundamental FSD vector $\mathbf{S}_0$.

As for the correlation length L, it can be inferred from an estimation of the correlation coefficient of two FSDs L cycle apart, $\rho[S_m^i, S_m^{i-L}]$, which is defined by

$$\rho[S_m^i, S_m^{i-L}] = \frac{\mathrm{cov}[S_m^i, S_m^{i-L}]}{\sigma[S_m^i]\cdot\sigma[S_m^{i-L}]} = \frac{\mathrm{cov}[S_m^i, S_m^{i-L}]}{\sigma^2[S_m^i]}. \tag{18}$$

The second equality is due to the stationary cycle assumption. The substitution of equations (13) and (14) into Eq. (18) leads to

$$\rho[S_m^i, S_m^{i-L}] = \frac{\sum_{t=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m} a_{mn}^t a_{mn'}^{t-L} \operatorname{cov}[\varepsilon_n, \varepsilon_{n'}]}{\sum_{t=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m} a_{mn}^t a_{mn'}^{t} \operatorname{cov}[\varepsilon_n, \varepsilon_{n'}]}. \quad (19)$$

Then, the correlation length, L, can be set as the minimum cycle distance l which makes the N_m-cell average of $\rho[S_m^i, S_m^{i-\ell}]$ less than a prescribed constant β. Mathematically, it is determined by

$$L = \min\left\{ l : \frac{1}{N_m}\sum_{m=1}^{N_m} \rho[S_m^i, S_m^{i-l}] < \beta \right\}. \quad (20)$$

β is a small positive number. Here, we set β=0.01 empirically.

3. Monte Carlo Wielandt Method

The Wielandt method is characterized in an operator notation as

$$\mathbf{T}\psi - \frac{1}{k_e}\mathbf{F}\psi = \left(\frac{1}{k} - \frac{1}{k_e}\right)\mathbf{F}\psi . \quad (21)$$

k and k_e denote the multiplication factor and an estimated eigenvalue, respectively. The operators are defined as

$$\begin{aligned} \mathbf{T}\psi &= [\mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E)]\psi(\mathbf{r},E,\mathbf{\Omega}) \\ &\quad - \int dE' \int d\mathbf{\Omega}' \Sigma_s(\mathbf{r};E',\mathbf{\Omega}' \to E,\mathbf{\Omega})\psi(\mathbf{r},E',\mathbf{\Omega}'), \\ \mathbf{F}\psi &= \chi(E)\int dE' \int d\mathbf{\Omega}' \nu(E')\Sigma_f(\mathbf{r};E')\psi(\mathbf{r},E',\mathbf{\Omega}'), \end{aligned} \quad (22)$$

where

$\psi(\mathbf{r},E,\mathbf{\Omega})$ = anglular flux,
$\Sigma_t(\mathbf{r},E)$ = total cross section,
$\Sigma_s(\mathbf{r};E',\mathbf{\Omega}' \to E,\mathbf{\Omega})$ = scattering cross section from $E',\mathbf{\Omega}'$ to $E,\mathbf{\Omega}$,
$\chi(E)$ = fission spectrum,
$\nu(E')$ = number of fission neutrons produced in a fission,
$\Sigma_f(\mathbf{r},E)$ = fission cross section.

Inverting $(\mathbf{T}-\mathbf{F}/k_e)$ and applying **F** on both sides of Eq. (21), one can obtain [11]

$$S=\frac{1}{k'}\mathbf{H}'S\,; \tag{23}$$

$$\frac{1}{k'}=\frac{1}{k}-\frac{1}{k_e}, \tag{24}$$

$$\mathbf{H}'=\mathbf{F}\left(\mathbf{T}-\frac{\mathbf{F}}{k_e}\right)^{-1}. \tag{25}$$

Using $\mathbf{H}=\mathbf{F}\mathbf{T}^{-1}$ [11], the operator $\mathbf{H}'$ can be written as

$$\mathbf{H}'=\mathbf{F}\left(\mathbf{T}-\frac{\mathbf{F}}{k_e}\right)^{-1}=\mathbf{F}\left[\left(1-\frac{\mathbf{H}}{k_e}\right)\mathbf{T}\right]^{-1}=\mathbf{F}\mathbf{T}^{-1}\left(1-\frac{\mathbf{H}}{k_e}\right)^{-1}=\mathbf{H}\left(1-\frac{\mathbf{H}}{k_e}\right)^{-1}. \tag{26}$$

Applying the power method to Eq. (23), the FSD is updated iteratively in the Wielandt method as

$$S^i=\frac{1}{k'^{i-1}}\mathbf{H}'S^{i-1}+\varepsilon^i\,. \tag{27}$$

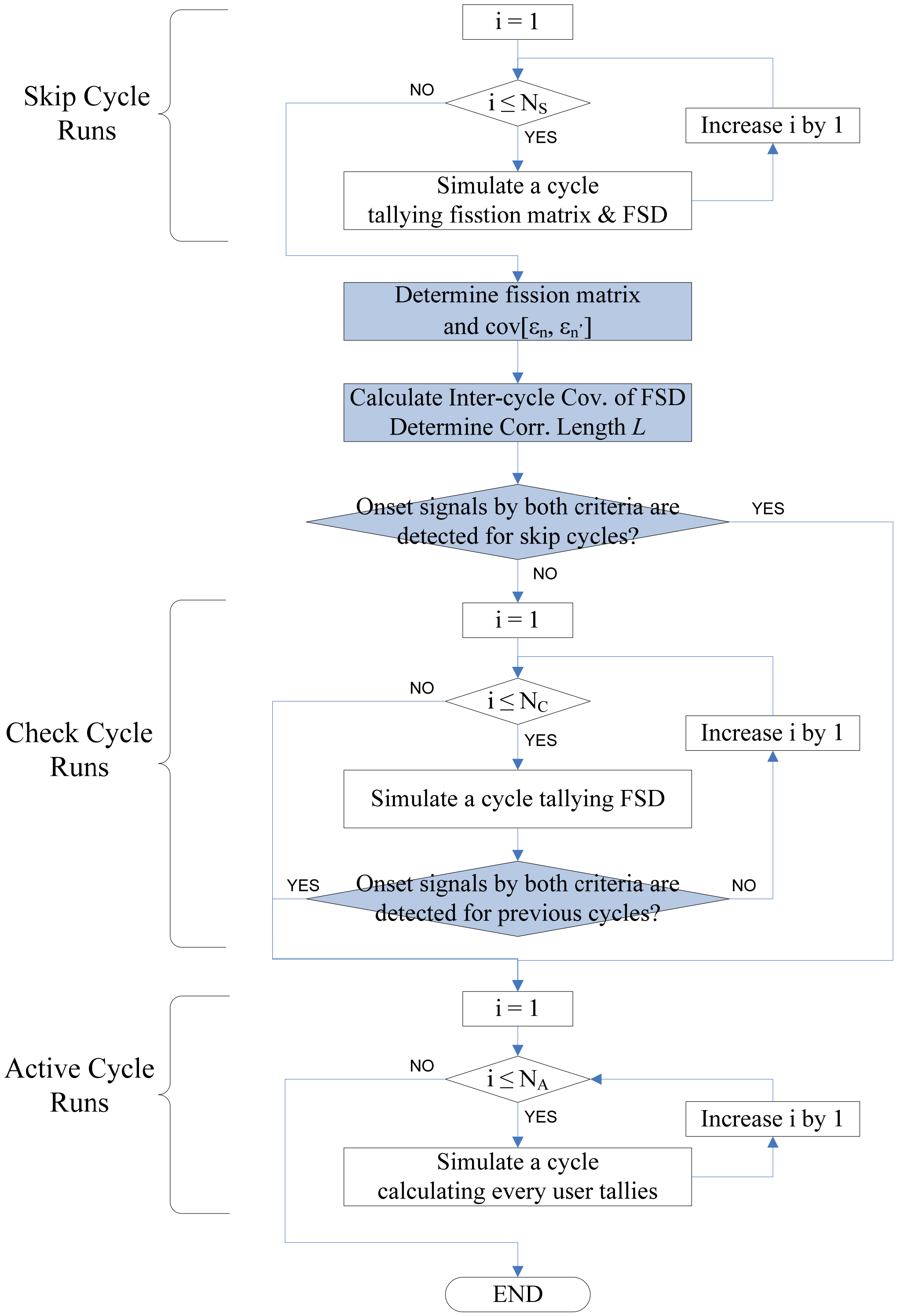
Comparing Eq. (27) with Eq. (1), one can observe that the only difference between the two methods is how to define the fission matrix operator. Therefore the anterior stopping criteria derived in the previous chapter can be applied for the MC Wielandt calculations without any modifications when the corresponding fission matrix is used.

4. NUMERICAL RESULTS

4.1. Algorithm

The type-A and B anterior stopping criteria were implemented in McCARD (Monte Carlo Code for Advanced Reactor Design) [12] and Figure 1 shows the algorithm. The MC eigenvalue calculation of McCARD is composed of three cycle runs; skip cycles, check cycles, and active cycles. The skip and check cycles are regarded as the inactive cycles.

The fission matrix and the FSD are tallied in the skip cycle runs. After the parameters required for the two criteria are prepared, they are applied to the skip cycles. If the FSD is not converged, the check cycle runs are performed until two criteria detect the onset of the stationary cycles.



N_S = number of skip cycles, N_C = max. number of check cycles, N_A = number of active cycles

Figure 1. Flowchart for the type-A and B anterior stopping criteria.

4.2. Fuel Storage Problem

The two anterior stopping criteria are applied to the MC Wielandt method calculations for a fuel storage facility problem [13] by varying k_e from ∞ to 0.95. Each MC calculation is performed for 100 skip cycles, 3,000 maximum check cycles, 1,000 active cycles with 100,000 histories per cycle and uniform initial source distribution over all the fuel bundles. Cells or bins for the fission matrix are allocated to one per fuel bundle horizontally and vertically.

Table I summarizes the results as a function of k_e. t_s is the cycle number at which the inactive cycle MC runs are halted by the stopping criteria. t_{UPM} denotes the cycle number signaling the onset of a stationary cycle estimated by Ueki's posterior source convergence diagnosis [3]. It is noteworthy to observe $t_s > t_{UPM}$ for all the test cases and this indicates that the two criteria adequately terminate the inactive cycle runs for the MC Wielandt calculations.

Table I. Stopped cycle number by the type-A and B criteria

k_e	L	t_{UPM}	t_s	
			*type-A**	*type-B***
∞	636	1298	1482	1612
10.0	576	1385	1438	1632
2.0	503	717	1048	1071
1.5	266	571	687	719
1.4	282	507	676	707
1.3	254	454	625	635
1.2	195	352	475	491
1.1	174	342	427	430
1.0	84	153	228	235
0.95	54	131	152	168

* $C(1)$= 31.7% is used.
** α=0.9 is taken.

5. CONCLUSIONS

The two anterior stopping criteria developed for conventional eigenvalue calculations are self-contained and free from empiricism. In this paper, we demonstrated an extended application of the criteria to the MC Wielandt method. We also demonstrated their effectiveness by applying them to a very slow convergence problem.

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REFERENCES

1. T. Yamamoto and Y. Miyoshi, "Reliable Method for Fission Source Convergence of Monte Carlo Criticality Calculation with Wielandt's Method," *J. Nucl. Sci. Technol.*, **41**, n. 2, pp. 99~107 (2004).
2. F. Brown, "Wielandt Acceleration for MCNP5 Monte Carlo Eigenvalue Calculations," M&C+SNA 2007, Monterey, CA, April 15-19 (2007).
3. T. Ueki and F. B. Brown, "Stationarity Modelling and Informatics-based Diagnostics in Monte Carlo Criticality Calculations," *Nucl. Sci. Eng.*, **149**, 38-50 (2005).
4. Y. Richet, O. Jacquet, and X. Bay, "Initialization Bias Suppression of an Iterative Monte Carlo Calculation," *Proc. Monte Carlo 2005 Topical Meeting,* Chattanooga, Tennessee (2005).
5. M. T. Wenner and A. Haghighat, "Study of Methods of Stationary Detection for Monte Carlo Criticality Analysis with KENO V.a," *Trans. Am. Nucl. Soc.*, **97**, pp.647-650 (2007).
6. H. J. Shim and C. H. Kim, "Stopping Criteria of Inactive Cycle Monte Carlo Calculations," *Nucl. Sci. Eng.*, **157**, pp. 132-141 (2007).
7. T. Ueki, "On-The-Fly Judgements of Monte Carlo Fission Source Convergence," *Trans. Am. Nucl. Soc.*, **98**, pp.512-514 (2008).
8. E. Dumonteil, A. Le Peillet, Yi-Kang Lee, O. Petit, C. Jouanne, and A. Mazzolo, "Source Convergence Diagnostics Using Boltzmann Entropy Criterion Application to Different OECD/NEA Criticality Benchmarks with the 3-D Monte Carlo Code Tripoli-4," *PHYSOR-2006*, *ANS Topical Meeting on Reactor Physics*, Vancouver, BC, Canada, September 10-14 (2006).
9. E. M. Gelbard and R. E. Prael, "Monte Carlo Work at Argonne National Laboratory," ANL-75-2 (NEACRP-L-118), p. 202, Argonne National Laboratory (1974).
10. H. J. Shim and C. H. Kim, "Real Variance Estimation Using an Inter-Cycle Fission Source Correlation for Monte Carlo Eigenvalue Calculations," *Nucl. Sci. Eng.* (will be published in May, 2009).
11. H. J. Shim and C. H. Kim, "Real Variance Estimation in Monte Carlo Wielandt Calculations," *PHYSOR 2008*, *International Conference on the Physics of Reactors*, Interlaken, Switzerland, September 14-19 (2008).
12. H. J. Shim and C. H. Kim, "Error Propagation Module Implemented in the MC-CARD Monte Carlo Code," *Trans. Am. Nucl. Soc.*, **86**, pp.325-327 (2002).
13. R. N. Blomquist and A. Nouri, "The OECD/NEA Source Convergence Benchmark Program," *Trans. Am. Nucl. Soc.*, **87**, pp.143-145 (2002).