Automatic Fission Source Convergence Criteria for Monte Carlo Criticality Calculations

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1. Introduction

The Monte Carlo criticality calculations for the multiplication factor and the power distribution in a nuclear system require knowledge of stationary or fundamental-mode fission source distribution (FSD) in the system. Because it is a priori unknown, so-called inactive cycle Monte Carlo (MC) runs are performed to determine it. The inactive cycle MC runs should be continued until the FSD converges to the stationary FSD. Obviously, if one stops them prematurely, the MC calculation results may have biases because the follow-up active cycles may be run with the non-stationary FSD. Conversely, if one performs the inactive cycle MC runs more than necessary, one is apt to waste computing time because inactive cycle MC runs are used to elicit the fundamental-mode FSD only.

In the absence of suitable criteria for terminating the inactive cycle MC runs, one cannot but rely on empiricism in deciding how many inactive cycles one should conduct for a given problem. Depending on the problem, this may introduce biases into Monte Carlo estimates of the parameters one tries to calculate. .

The purpose of this paper is to present new fission source convergence criteria designed for the automatic termination of inactive cycle MC runs.

2. Methods and Results

2.1 Derivation of Convergence Criteria

In deterministic methods, the convergence criterion for power distribution calculations is given by a maximum relative FSD difference in two successive cycles:

$$\max_m \left| \frac{S_m^p - S_m^{p-1}}{S_m^p} \right| < \varepsilon \qquad (1)$$

S_m^p is the fission source density of *m*-th cell at *p*-th iteration and ε is an upper limit guaranteeing the fission source convergence. Though used popularly in deterministic method, it has a couple of deficiencies as the convergence criterion for the MC power method. One is that, because of strong inter-cycle FSD correlation [2], the difference between two FSDs of successive cycles may not adequately represent the convergence of FSD. Considering the inter-cycle correlation, it is more appropriate to compare two FSDs that are *L(>1)* cycles apart, i.e., $(S_m^t(\mathbf{r}) - S_m^{t-L}(\mathbf{r}))$. The *L* here is called the correlation length.

Another is related to the fact that $S_m^t(\mathbf{r})$ and $S_m^{t-L}(\mathbf{r})$ are random or statistical variables associated with statistical uncertainties quantified by variances. It can be shown that $\left(S_m^t(\mathbf{r}) - S_m^{t-L}(\mathbf{r})\right) / S_m^t(\mathbf{r})$ has the variance:

$$\sigma^2\left[\frac{S_m^t - S_m^{t\text{-}L}}{S_m^t}\right] = \left(\frac{\bar{S}_m^{t\text{-}L}}{\bar{S}_m^t}\right)^2 \times \left(\frac{\sigma^2\left[S_m^t\right]}{\left(\bar{S}_m^t\right)^2} + \frac{\sigma^2\left[S_m^{t-L}\right]}{\left(\bar{S}_m^{t-L}\right)^2} - 2\frac{\operatorname{cov}\left[S_m^t, S_m^{t-L}\right]}{\bar{S}_m^t \bar{S}_m^{t-L}}\right) \qquad (2)$$

The bar sign designates the expected value.

If ε is set at a much smaller value than $\sigma\left[(S_m^t(\mathbf{r}) - S_m^{t-L}(\mathbf{r}))/S_m^t(\mathbf{r})\right]$, the criterion of Eq. (1) may hardly terminate the inactive cycle iterations even though FSD have converged to the stationary one. So it is proposed that the effective criterion of fission source convergence is given by

$$\left|\frac{S_m^t - S_m^{t-L}}{S_m^t}\right| < C_1 \sigma\left[\frac{S_m^t - S_m^{t-L}}{S_m^t}\right]. \qquad (3)$$

To take into account the presence of cases that do not meet Eq. (3), one may impose the following condition in parallel with Eq. (3):

$$\frac{\text{the number of cells that do not meet Eq. (3)}}{\text{the total number of cells}} < C_2 \qquad (4)$$

Because the cycles equal to or greater than $(t-L)$ is assumed to be stationary cycles, $\bar{S}_m^{t-L} = \bar{S}_m^t$ and $\sigma[S_m^{t-L}] = \sigma[S_m^t]$. Then, Equation (2) becomes

$$\sigma^2\left[\frac{S_m^t - S_m^{t\text{-}L}}{S_m^t}\right] = \frac{2\sigma^2\left[S_m^t\right] - 2\operatorname{cov}\left[S_m^t, S_m^{t-L}\right]}{\left(\bar{S}_m^t\right)^2}. \qquad (5)$$

The substitution of Eq. (5) into Eq. (3) leads to

$$\left|S_m^t - S_m^{t-L}\right| < C_1\sqrt{2\left(\sigma^2\left[S_m^t\right] - \operatorname{cov}\left[S_m^t, S_m^{t-L}\right]\right)}. \qquad (6)$$

Equation (6) is designated as the type-A criterion..

One can develop another convergence criterion by assuming that the relative differences between S_m^t and $S_m^{t\text{-}L}$ follow the normal distributions and that they are independent from one another. To show it, let us designate the square sum of the normalized relative differences by Z.

$$Z = \sum_{m=1}^{N_m}\left[\left\{\left(\frac{S_m^t - S_m^{t-L}}{S_m^t}\right) - \left(\frac{\bar{S}_m^t - \bar{S}_m^{t-L}}{\bar{S}_m^t}\right)\right\} \Big/ \sigma\left[\frac{S_m^t - S_m^{t-L}}{S_m^t}\right]\right]^2 \qquad (7)$$

N_m is the total number of cells in MC calculations.. Because of assumptions made on the relative differences of FSDs, Z is regarded as the random variable that follows a chi-square distribution with N_m

degrees of freedom, $\chi^2(N_m)$.

Noting again that the FSD's equal to or greater than t-L cycles are stationary, Eq. (7) becomes

$$Z=\sum_{m=1}^{N_m}\frac{\left(S_m^t-S_m^{t-L}\right)^2}{2\left(\sigma^2\left[S_m^t\right]-\mathrm{cov}\left[S_m^t,S_m^{t-L}\right]\right)}\,. \qquad (8)$$

When a random variable V follows the chi-square distribution with k degrees of freedom, $\chi^2(k,\alpha)$ denotes the value v satisfying

$$\text{Probability}\{V\ge v\}=\alpha\,.$$

Then, it can be used as convergence criteria that the value of Eq. (8) falls below $\chi^2(k,\alpha)$ as

$$\sum_{m=1}^{N_m}\frac{\left(S_m^t-S_m^{t-L}\right)^2}{2\left(\sigma^2\left[S_m^t\right]-\mathrm{cov}\left[S_m^t,S_m^{t-L}\right]\right)}<\chi^2(N_m,\alpha)\,. \qquad (9)$$

We call this criterion the χ^2 criterion or the type-B criterion.

2.2 FSD Variance and Covariance

From the fission matrix, the matrix eigenvalue equation of zone-wise FSD can be expressed as

$$\mathbf{S}=\frac{1}{k}\mathbf{HS}\,. \qquad (10)$$

where $\mathbf{H}$ and k are the fission matrix and the multiplication factor, respectively.

By the cycle-to-cycle error propagation model [1,2], the errors of FSD are shown to be expressed by

$$\mathbf{e}^t=\sum_{t'=0}^{t-1}(\mathbf{A_0})^{t'}\boldsymbol{\varepsilon}^{t-t'}+(\mathbf{A_0})^t\mathbf{e}^0 \qquad (11)$$

where

$\mathbf{e}^t$ = fluctuating component of FSD at t-th cycle

$\boldsymbol{\varepsilon}^t$ = stochastic errors generated at cycle number t.

$\mathbf{A_0}$ is defined by

$$\mathbf{A_0}=\frac{1}{k_0}\left[\mathbf{H}-\mathbf{S}_0\tau^T\right]. \qquad (12)$$

where $\tau^T=(1,1,\cdots,1)$ and k_0, $\mathbf{S}_0$ are a maximum eigenvalue and corresponding eigenvector of Eq. (10).

Then the covariance of FSDs l cycles apart can be written as

$$C_l\left[S_m,S_{m'}\right]=\sum_{t'=0}^{\infty}\sum_n\sum_{n'}a_{mn}^{t'}a_{m'n'}^{t'+l}\,\mathrm{cov}\left[\varepsilon_n,\varepsilon_{n'}\right] \qquad (13)$$

where $a_{mn}^{t'}$ is a m-th row and n-th column element of matrix $(\mathbf{A_0})^{t'}$.

From Eq. (13), the variance of S_m can be reduced as

$$\sigma^2[S_m]=\sum_{t'=0}^{\infty}\sum_n\sum_{n'}a_{mn}^{t'}a_{mn'}^{t'}\,\mathrm{cov}\left[\varepsilon_n,\varepsilon_{n'}\right]. \qquad (14)$$

The covariance of stochastic errors can be estimated from the simulation results of fission sources composing t-th cycle as

$$\mathrm{cov}_S\left[\varepsilon_n^t,\varepsilon_{n'}^t\right]=\frac{1}{M(M-1)}\sum_{i=1}^{M}\left(\left(S_n^t\right)_i-\bar{S}_n^t\right)\left(\left(S_{n'}^t\right)_i-\bar{S}_{n'}^t\right)$$
$$\bar{S}_m^t=\frac{1}{M}\sum_{t=1}^{N}\left(S_m^t\right)_i;\quad m=n\text{ or }n' \qquad (15)$$

where $(S_m^t)_i$ is the fission source density of m-th cell by i-th source at t-th cycle and M is the numbers of fission sources per cycle.

From Eq. (15), $\mathrm{cov}[\varepsilon_n,\varepsilon_{n'}]$ can be estimated as

$$\mathrm{cov}\left[\varepsilon_n,\varepsilon_{n'}\right]\approx\sqrt{\frac{S_{0n}}{S_n^{t-1}}}\sqrt{\frac{S_{0n'}}{S_{n'}^{t-1}}}\,\mathrm{cov}_S\left[\varepsilon_n^t,\varepsilon_{n'}^t\right]. \qquad (16)$$
$$t\in\{\text{inactive cycles}\}$$

2.3 Correlation Length And Numerical Results

The inter-cycle correlation length between FSDs l cycle apart can be reduced as

$$\rho\left[S_m,l\right]=\frac{\sum_{t'=0}^{\infty}\sum_n\sum_{n'}a_{mn}^{t'}a_{mn'}^{t'+l}\,\mathrm{cov}\left[\varepsilon_n,\varepsilon_{n'}\right]}{\sum_{t'=0}^{\infty}\sum_n\sum_{n'}a_{mn}^{t'}a_{mn'}^{t'}\,\mathrm{cov}\left[\varepsilon_n,\varepsilon_{n'}\right]}\,. \qquad (17)$$

Then, the correlation length, L, can be selected as the maximum value among cycle distances which are less than a prescribed constant, β:

$$L=\max\left\{l;\ \rho\left[S_m,l\right]<\beta\right\}. \qquad (18)$$

The convergence criteria of Eq. (6) and (9) were applied to the core problems varying the core radius. Table 1 shows the comparison of the converged cycle by the convergence criteria and Ueki's posterior method.

Table 1 Comparison of converged cycle

Core Radius (cm)	L (β=0.05)	Posterior Method	Eq. (6) With C_1=2	Eq. (9) With α=0.5
118	11	26	27	29
140	14	30	29	37
161	22	26	31	47
183	27	18	36	39
204	36	38	60	70

3. Conclusion

The fission source convergence criteria have been developed for the automatic termination of inactive cycle MC runs. From the numerical results, we demonstrated their effectiveness in terminating the inactive cycle MC runs. In particular, we showed that the initiation of the active cycle dictated by the proposed criteria agrees very well with those predicted by Ueki's posterior convergence test that can be determined only after stationary cycle calculations.

REFERENCES

[1] 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.

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