Efficiency Assessment of Monte Carlo Wielandt Method

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1. Introduction

Recently, a Monte Carlo (MC) Wielandt method for eigenvalue calculations was proposed to accelerate fission source convergence [1]. It was reported that the method has the potential to eliminate most of the variance bias for MC eigenvalue calculations [2]. However, not only the amount of the variance bias was not quantified but also the calculation efficiency was not estimated in terms of the real variance.

The objectives of this paper are to develop a real variance estimation method for the MC Wielandt calculations and to analyze the efficiency of the MC Wielandt method by the Figure of Merit (FOM) approach with the real variance. In addition, the MC algorithm for the Wielandt method is mathematically derived.

2. Estimation of Real Variance in MC Wielandt Calculations

2.1 Monte Carlo Algorithm for Wielandt Method

The time-independent Boltzmann transport equation for neutrons can be written in an operator notation as

$$\mathbf{T}\psi = \frac{1}{k}\mathbf{F}\psi \,. \tag{1}$$

k is the multiplication factor and the operators are defined as

$$\begin{aligned}\mathbf{T}\psi = &\left[\mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E)\right]\psi(\mathbf{r},E,\mathbf{\Omega}) \\ &- \int dE'\int d\mathbf{\Omega}'\Sigma_s(\mathbf{r};E',\mathbf{\Omega}'\to E,\mathbf{\Omega})\psi(\mathbf{r},E',\mathbf{\Omega}'),\end{aligned} \tag{2}$$

$$\mathbf{F}\psi = \chi(E)\int dE'\int d\mathbf{\Omega}'\nu(E')\Sigma_f(\mathbf{r},E')\psi(\mathbf{r},E',\mathbf{\Omega}'), \tag{3}$$

where

$\Sigma_t(\mathbf{r},E)$ = 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,
$\nu(E')$ = mean number of fission neutrons produced in a fission,
$\Sigma_f(\mathbf{r},E')$ = fission cross section.

By inverting **T** and operating with **F** on both sides of Eq. (1), we obtain the following form.

$$\mathbf{F}\psi = \frac{1}{k}\left[\mathbf{F}\mathbf{T}^{-1}\right]\mathbf{F}\psi \tag{4}$$

The fission source distribution (FSD), S and fission operator, **H** are defined as follows

$$S = \mathbf{F}\psi \,, \tag{5}$$

$$\mathbf{H} = \mathbf{F}\mathbf{T}^{-1} \,. \tag{6}$$

The fission operator $\mathbf{H}(\mathbf{r}',E',\mathbf{\Omega}'\to\mathbf{r},E,\mathbf{\Omega})$ denotes the number of first-generation fission neutrons born per unit volume about $(\mathbf{r},E,\mathbf{\Omega})$, due to a parent neutron born per unit volume at $(\mathbf{r}',E',\mathbf{\Omega}')$.

Inserting Eqs. (5) and (6) into Eq. (4) leads to the following eigenvalue equation.

$$S = \frac{1}{k}\mathbf{H}S \tag{7}$$

In the conventional MC eigenvalue calculations, the FSD and k are iteratively updated as

$$S^t = \frac{1}{k^{t-1}}\mathbf{H}S^{t-1}, \tag{8}$$

$$k^t = \frac{\int_V d\mathbf{r}\int dE\int d\mathbf{\Omega}\, S^t(\mathbf{r},E,\mathbf{\Omega})}{\frac{1}{k^{t-1}}\int_V d\mathbf{r}\int dE\int d\mathbf{\Omega}\, S^{t-1}(\mathbf{r},E,\mathbf{\Omega})} \,. \tag{9}$$

The superscript t and t-1 are iteration or cycle indices.

The Wielandt method is characterized by rewriting Eq. (1) as

$$\mathbf{T}\psi - \frac{1}{k_e}\mathbf{F}\psi = \left(\frac{1}{k}-\frac{1}{k_e}\right)\mathbf{F}\psi \,. \tag{10}$$

k_e is an estimated eigenvalue.

Inverting $\left(\mathbf{T}-\mathbf{F}/k_e\right)$ and applying **F** on both sides of Eq. (10), one can obtain

$$S = \left(\frac{1}{k}-\frac{1}{k_e}\right)\mathbf{H}'S \,, \tag{11}$$

$$\mathbf{H}' = \mathbf{F}\left(\mathbf{T}-\frac{1}{k_e}\mathbf{F}\right)^{-1} \,. \tag{12}$$

Applying the power method to Eq. (11), the FSD's are updated iteratively in the Wielandt method as

$$S^t = \left(\frac{1}{k}-\frac{1}{k_e}\right)\mathbf{H}'S^{t-1}. \tag{13}$$

Using Eq. (6), the fission operator $\mathbf{H}'$ in the Wielandt's method can be expressed as

$$\begin{aligned}\mathbf{H}' &= \mathbf{F}\left[\mathbf{T}-\frac{1}{k_e}\mathbf{F}\right]^{-1} = \mathbf{F}\left[\mathbf{T}-\frac{1}{k_e}\mathbf{H}\mathbf{T}\right]^{-1} \\ &= \mathbf{F}\left[\left(1-\frac{\mathbf{H}}{k_e}\right)\mathbf{T}\right]^{-1} = \mathbf{F}\mathbf{T}^{-1}\left(1-\frac{\mathbf{H}}{k_e}\right)^{-1} = \mathbf{H}\left(1-\frac{\mathbf{H}}{k_e}\right)^{-1}\end{aligned} \tag{14}$$

By the Taylor's series expansion, $\left(1-\mathbf{H}/k_e\right)^{-1}$ in Eq. (14) can be written as

$$\left(1-\frac{\mathbf{H}}{k_e}\right)^{-1}=1+\frac{\mathbf{H}}{k_e}+\left(\frac{\mathbf{H}}{k_e}\right)^2+\Lambda \tag{15}$$

Inserting Eq. (15) into Eq. (14) leads to

$$\mathbf{H}'=\mathbf{H}\left(1+\frac{\mathbf{H}}{k_e}+\left(\frac{\mathbf{H}}{k_e}\right)^2+\Lambda\right) \tag{16}$$

Substitution of Eq. (16) into Eq. (13) results in

$$\begin{aligned}S^t=&\left(\frac{1}{k^{t-1}}-\frac{1}{k_e}\right)\mathbf{H}S^{t-1}+\left(\frac{1}{k^{t-1}}-\frac{1}{k_e}\right)\mathbf{H}\left(\frac{\mathbf{H}}{k_e}\right)S^{t-1}\\&+\left(\frac{1}{k^{t-1}}-\frac{1}{k_e}\right)\mathbf{H}\left(\frac{\mathbf{H}}{k_e}\right)^2S^{t-1}+\Lambda\end{aligned} \tag{17}$$

The first term in the RHS of Eq. (17) means the number of the first fission sites sampled from the previous FSD. one can see that it is less than the RHS of Eq. (8) by as much as $\mathbf{H}S^{t-1}/k_e$, which means the number of first-generation fission sources to be simulated at the current iteration. In the course of the MC simulations, $\mathbf{H}S^{t-1}/k_e$ fission sources generate the second fission sites by as much as the second term in the RHS of Eq. (17). In the same way, the fission sites from all the generations are sampled.

2.2 Real Variance Estimation

The sample variance of a tallied nuclear parameter or a tally in the MC Wielandt calculations is biased because of the inter-cycle correlations of the FSD by Eq. (13). We have developed a real variance estimation method using FSD's inter-cycle correlation for the conventional MC eigenvalue calculations governed by Eq. (8) [3]. It can be directly applicable to the MC Wielandt calculations simply by replacing $\mathbf{H}$ by $\mathbf{H}'$.

The real variance of a tally denoted by Q, $\sigma_R^2\left[\overline{Q}\right]$ can be calculated by

$$\sigma_R^2\left[\overline{Q}\right]\cong\sigma_S^2\left[\overline{Q}\right]+\frac{1}{N}\cdot B'^{Q}(N), \tag{18}$$

$$B'^{Q}(N)=\frac{2}{N-1}\sum_{t=1}^{N-1}(N-t)\cdot C_t'^{Q}, \tag{19}$$

$$C_t'^{Q}=\sum_{m=1}^{N_m}\sum_{m'=1}^{N_m}R_m^Q R_{m'}^Q\left(\sum_{i'=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m}a_{mn}'^{i'}a_{m'n'}'^{i'+t}\operatorname{cov}\left[\varepsilon_n,\varepsilon_{n'}\right]\right). \tag{20}$$

N is the number of active cycles. $\sigma_S^2\left[\overline{Q}\right]$ is the sample variance of $\overline{Q}$ defined by

$$\sigma_S^2\left[\overline{Q}\right]=\frac{1}{N(N-1)}\sum_{i=1}^{N}\left(Q_i-\overline{Q}\right)^2,\ \overline{Q}=\frac{1}{N}\sum_{i=1}^{N}Q_i\ .$$

Q_i is an MC estimate of Q at an active cycle i. R_m^Q is the contribution to Q of a unit fission source in region m. $a_{mn}'^{i}$ is the m-th row and n-th column element of the matrix $\mathbf{A}'^{i}$ where matrix $\mathbf{A}'$ is defined by

$$\begin{aligned}&\mathbf{A}'=\left(\mathbf{H}'-\mathbf{S}_0\cdot\boldsymbol{\tau}^T\right)/k_0\ ;\\&\boldsymbol{\tau}^T=N_m\text{ dimensional row vector }(1,1,\Lambda\ ,1).\end{aligned} \tag{21}$$

k_0 and $\mathbf{S}_0$ denote the main mode eigenvalue and eigenvector. ε_n is the stochastic error at region n.

2.3 Efficiency Comparison

The efficiency of the MC calculation can be measured by FOM which is defined by

$$\text{FOM}=\frac{1}{R^2T}. \tag{22}$$

R is one standard deviation divided by the estimated mean value and T is the computing time.

The FOMs of the fission power tally for the fuel storage facility problem [4] are calculated as a function of the estimated eigenvalue k_e in the MC Wielandt calculations. The results are shown in Table 1. Note that k_e of ∞ in Table 1 corresponds to the conventional MC eigenvalue calculation. Note also that the FOM with k_e of 1.3 is 1.375 times greater than that of ∞.

Table 1. FOM for the fission power tally of the (1,3) assembly

k_e	CPU Time (min.)	power	est. real standard deviation	FOM
∞	534.2	5.91E-04	6.80E-02	0.40
10.0	584.5	6.14E-04	6.64E-02	0.39
2.0	1066.2	5.93E-04	5.62E-02	0.30
1.5	1600.4	6.63E-04	3.36E-02	0.55
1.4	1834.8	6.65E-04	3.23E-02	0.52
1.3	2200.1	6.46E-04	2.87E-02	0.55

3. Conclusion

A variance-bias estimation method for the MC Wielandt calculations is developed from that of the conventional MC eigenvalue calculations. From the FOMs using the real variance for the slow-convergence benchmark problem, one can see that the calculation efficiency of the MC Wielandt calculations is enhanced by 37.5%.

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