ESTIMATION OF ADJOINT-WEIGHTED KINETICS PARAMETERS IN MONTE CARLO WIELANDT CALCULATIONS

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ABSTRACT

The effective delayed neutron fraction, β_{eff}, and the prompt neutron generation time, Λ, in the point kinetics equation are weighted by the adjoint flux to improve the accuracy of the reactivity estimate. Recently the Monte Carlo (MC) kinetics parameter estimation methods by using the self-consistent adjoint flux calculated in the MC forward simulations have been developed and successfully applied for the research reactor analyses. However these adjoint estimation methods based on the cycle-by-cycle genealogical table require a huge memory size to store the pedigree hierarchy. In this paper, we present a new adjoint estimation in which the pedigree of a single history is utilized by applying the MC Wielandt method. The effectiveness of the new method is demonstrated in the kinetics parameter estimations for infinite homogeneous two-group problems and the Godiva critical facility.

1. Introduction

Reactor kinetics parameters such as the effective delayed neutron fraction, β_{eff}, and the prompt neutron generation time, Λ, in the point kinetics equation are weighted quantities. The self-consistent adjoint function (adjoint flux hereafter) from the solution to a relevant steady-state adjoint eigenvalue equation is preferred as a weighting function in order to improve the accuracy of the reactivity estimate in the point kinetics equation [1-3].

Recently, the Monte Carlo (MC) adjoint estimation techniques [4-6] which enables one to compute the adjoint flux in the MC forward calculations have been developed and successfully applied to the adjoint-weighted kinetics parameter estimation for research reactors. In these methods, the adjoint flux is interpreted as a distribution proportional to the number of fission neutrons or fissions produced in the *n*-th generation due to a unit source neutron as *n* approaches infinity, which is well known as the iterated fission probability (IFP) [7]. The inaccuracy problem in the MC kinetics parameter calculations caused by the constant source adjoint function [6] has been overcome by using the adjoint flux as the weighting function. However the current MC adjoint-weighted kinetics parameter estimation methods may require a huge memory size to store the genealogical table for all the neutron histories of the fission source generations as many as the adjoint convergence length, *n* as the number of histories per cycle or *n* increases.

In order to solve the huge memory consumption problem in the current methods, we present a new adjoint estimation in which the pedigree of a single history is utilized by applying the MC Wielandt method [8]. The Wielandt method allows the estimations of the adjoint flux and adjoint-weighted parameters within a single cycle neutron simulations. The effectiveness of the new method is demonstrated in the kinetics parameter estimations for infinite homogeneous two-group problems and the Godiva problem [9].

2. Adjoint Estimation in the MC Wielandt Method

2.1 Adjoint Estimation in the MC Eigenvalue Calculations

The steady-state neutron transport equation can be written in an operator notation as

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

ϕ is the angular flux and k is the eigenvalue. $\mathbf{T}$ and $\mathbf{F}$ denote the net loss operator and the fission production operator, respectively, which are defined by

$$\mathbf{T}\phi = \left[\mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E)\right]\phi(\mathbf{r},E,\mathbf{\Omega}) - \int dE'\int d\mathbf{\Omega}'\Sigma_s(E',\mathbf{\Omega}'\to E,\mathbf{\Omega}\,|\,\mathbf{r})\phi(\mathbf{r},E',\mathbf{\Omega}') , \tag{2}$$

$$\mathbf{F}\phi = \int dE'\int d\mathbf{\Omega}'\frac{\chi(E'\to E)}{4\pi}\nu(E')\Sigma_f(\mathbf{r},E')\phi(\mathbf{r},E',\mathbf{\Omega}') . \tag{3}$$

Σ_t, Σ_s, and Σ_f are the total, scattering and fission cross sections, respectively. ν is the mean number of fission neutrons produced from a fission reaction. χ is the energy spectrum of fission neutrons.

By operating $(1/k)\mathbf{F}\mathbf{T}^{-1}$ on both sides of Eq. (1), it can be expressed as

$$S = \frac{1}{k}\mathbf{H}S . \tag{4}$$

The fission source density (FSD), S and the fission operator, $\mathbf{H}$ are defined as

$$S \equiv \frac{1}{k}\mathbf{F}\phi , \tag{5}$$

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

When $\mathbf{P}$ denotes the state vector of a neutron in the six-dimensional phase space, $(\mathbf{r},E,\mathbf{\Omega})$, $\mathbf{H}S$ in Eq. (4) implies

$$\mathbf{H}S = \int d\mathbf{P}'H(\mathbf{P}'\to\mathbf{P})S(\mathbf{P}') , \tag{7}$$

where $H(\mathbf{P}'\to\mathbf{P})$ means the number of first-generation fission neutrons born per unit phase space volume about $\mathbf{P}$, due to a parent neutron born at $\mathbf{P}'$.

Corresponding to Eq. (1), the adjoint eigenvalue equation for the adjoint flux, $\phi^\dagger$ can be written as

$$\mathbf{T}^\dagger\phi^\dagger = \frac{1}{k}\mathbf{F}^\dagger\phi^\dagger , \tag{8}$$

where the adjoint operators are defined by

$$\mathbf{T}^\dagger\phi^\dagger = \left[-\mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E)\right]\phi^\dagger(\mathbf{r},E,\mathbf{\Omega}) - \int dE'\int d\mathbf{\Omega}'\Sigma_s(E,\mathbf{\Omega}\to E',\mathbf{\Omega}'\,|\,\mathbf{r})\phi^\dagger(\mathbf{r},E',\mathbf{\Omega}') , \tag{9}$$

$$\mathbf{F}^\dagger\phi^\dagger = \int dE'\int d\mathbf{\Omega}'\frac{\chi(E\to E')}{4\pi}\nu(E)\Sigma_f(\mathbf{r},E)\phi^\dagger(\mathbf{r},E',\mathbf{\Omega}') . \tag{10}$$

Then operating $\left(\mathbf{T}^\dagger\right)^{-1}$ on both sides of Eq. (8) gives

$$\phi^\dagger = \frac{1}{k}\mathbf{H}^\dagger\phi^\dagger . \tag{11}$$

By applying the power method to Eq. (11) and taking the unity as an initial distribution, the fundamental mode solution, $\phi_0^\dagger$ can be obtained by [10]

$$\phi_0^\dagger = \lim_{n\to\infty}\phi_{0,n}^\dagger ; \tag{12}$$

$$\phi_{0,n}^{\dagger}(\mathbf{P}) = \frac{1}{k_0{}^n}\int d\mathbf{P}' H^n(\mathbf{P} \to \mathbf{P}'). \tag{13}$$

k_0 is the fundamental mode eigenvalue. Note that $H^n(\mathbf{P} \to \mathbf{P}')$ is the number of the *n*-th generation fission neutrons born per unit phase space volume about $\mathbf{P}'$, due to a parent neutron born at $\mathbf{P}$ and that $\phi_{0,n}^{\dagger}(\mathbf{P})$ is normalized to satisfy $\int \phi_{0,n}^{\dagger}(\mathbf{P}) S_0(\mathbf{P}) d\mathbf{P} = 1$. Thus $\phi_0^{\dagger}(\mathbf{P})$ can be calculated by scoring the fission neutrons produced at the *n*-th generation starting from the fission source at $\mathbf{P}$ by using the genealogical table of fission sources, where *n* is named the convergence interval of the adjoint flux [10].

2.2 Adjoint Estimation in the MC Wielandt Calculations

Subtracting $(1/k_e)\mathbf{H}S$ from each side of Eq. (4) yields the eigenvalue equation of the Wielandt method as

$$\left(\mathbf{I} - \frac{1}{k_e}\mathbf{H}\right) S = \left(\frac{1}{k} - \frac{1}{k_e}\right)\mathbf{H}S, \tag{14}$$

where $\mathbf{I}$ is the identity operator and k_e is an estimated eigenvalue.

By operating $\left(\mathbf{I} - \mathbf{H}/k_e\right)^{-1}$ on both sides of Eq. (14), S can be expressed as

$$S = \left(\frac{1}{k} - \frac{1}{k_e}\right)\mathbf{H}'S; \tag{15}$$

$$\mathbf{H}' = \left(\mathbf{I} - \frac{\mathbf{H}}{k_e}\right)^{-1}\mathbf{H}. \tag{16}$$

The Taylor series expansion of $\mathbf{H}'$ of Eq. (16) can be written as [11]

$$\mathbf{H}' = \left[1 + \frac{\mathbf{H}}{k_e} + \left(\frac{\mathbf{H}}{k_e}\right)^2 + \cdots\right]\mathbf{H}. \tag{17}$$

In the MC eigenvalue calculations with the Wielandt method, the FSD is updated cycle-by-cycle as

$$S^{(i+1)} = \left(\frac{1}{k^{(i)}} - \frac{1}{k_e}\right)\mathbf{H}'S^{(i)} + \varepsilon^{(i+1)}. \tag{18}$$

i is the cycle index. $\varepsilon^{(i+1)}$ denotes the stochastic error component of $S^{(i+1)}$ [12].

Then the insertion of Eq. (17) into Eq. (18) yields

$$S^{(i+1)} = \left(\frac{1}{k^{(i)}} - \frac{1}{k_e}\right)\mathbf{H}'S^{(i)} = \sum_{i'=0}^{\infty}\left(\frac{1}{k^{(i)}} - \frac{1}{k_e}\right)\mathbf{H}S^{(i,i')}; \tag{19}$$

$$S^{(i,i')} = \left(\frac{\mathbf{H}}{k_e}\right)^{i'} S^{(i)}. \tag{20}$$

From Eq. (19), the MC Wielandt algorithm [8] can be interpreted as the fission source of the *i'*-th generation in cycle *i*, $S^{(i,i')}$ produces the next-cycle fission source as many as $\left(1/k^{(i)} - 1/k_e\right)\mathbf{H}S^{(i,i')}$ while $\left(1/k_e\right)\mathbf{H}S^{(i,i')}\left(= S^{(i,i'+1)}\right)$ is generated as the (*i'*+1)-th source for the current cycle simulations.

From Eqs. (19) and (20), we can clearly see that the generation-by-generation updates of the FSD are performed in a cycle of the MC Wielandt calculations. Therefore the adjoint flux based on Eq. (13) can be estimated within a single cycle by using a single history pedigree table.

Assuming that *n* is large enough to ensure the convergence of the adjoint flux, the number of the fission neutrons generated for the $(i'+n)$-th generation becomes the adjoint flux of a fission source neutron at generation i'. Therefore the adjoint flux at $\mathbf{P}$ from $S^{(i,i')}(\mathbf{P})$ can be calculated by

$$\begin{aligned}\phi_0^\dagger(\mathbf{P}) &= \frac{1}{W}\frac{\int d\mathbf{P}' S^{(i,i'+n)}\left(\mathbf{P}' \middle| S^{(i,i')}(\mathbf{P})\right)}{S^{(i,i')}(\mathbf{P})} \\ &= \frac{1}{W}\frac{\int d\mathbf{P}' \frac{1}{k_e^n} H^n(\mathbf{P}\to\mathbf{P}') S^{(i,i')}(\mathbf{P})}{S^{(i,i')}(\mathbf{P})} \\ &= \frac{1}{W}\frac{1}{k_e^n}\int d\mathbf{P}' H^n(\mathbf{P}\to\mathbf{P}'),\end{aligned} \tag{21}$$

where $S^{(i,i'+n)}\left(\mathbf{P}' \middle| S^{(i,i')}(\mathbf{P})\right)$ is the fission source distribution produced from $S^{(i,i')}(\mathbf{P})$ at n generations apart. W can be obtained from the normalization condition of the adjoint flux as

$$W = \frac{1}{k_e^n}\int\int H^n(\mathbf{P}\to\mathbf{P}') S(\mathbf{P}) \mathrm{d}\mathbf{P} d\mathbf{P}' . \tag{22}$$

By using Eq. (4) and the normalization condition of the FSD, $\int S(\mathbf{P}) d\mathbf{P} = 1$, *W* is obtained as

$$W = \left(\frac{k}{k_e}\right)^n \cancel{\int S(\mathbf{P}') d\mathbf{P}'} = \left(\frac{k}{k_e}\right)^n . \tag{23}$$

3. Adjoint-Weighted Kinetics Parameter Calculation

The developed adjoint estimation method for the MC Wielandt calculations is applied to estimate the adjoint-weighted kinetics parameters of infinite homogeneous two-group problems and the Godiva criticality problem.

3.1 Infinite Homogeneous Two-Group Problem

The kinetics parameters estimated by the proposed method are compared with the analytic solutions for the infinite homogeneous two-group problem. Table I describes two-group cross sections for this problem.

Table I. Two-group cross sections for the infinite homogeneous problems

	First Gr. (g=1)	Second Gr. (g=2)
Σ_t	0.50	0.50
Σ_f	0.025	0.175
ν	2.0	2.0
Σ_{sgg}	0.10	0.20
$\Sigma_{sg'g}$ (g'≠g)	0.312987	0.00
$\chi_{p,1}$	0.5375	0.5375
$\chi_{p,2}$	0.4625	0.4625
$\chi_{d,1}$	0.80	0.80
$\chi_{d,2}$	0.20	0.20
β_0 (= ν_d/ν)	0.006	0.006
1/v [sec/cm]	2.28626×10^{-6}	1.29329×10^{-6}

The MC Wielandt calculations for the kinetics parameter estimation are performed with varying the estimated eigenvalue, k_e and the convergence interval of the adjoint flux, *n*. The MC calculations are performed for 1,000 active cycles with changing the number of histories per cycle, N_{hist} to make the effective number of fission neutrons, $L\times N_{hist}$ constant as about 4,600,000, where *L* is the expected number of the fission neutrons for a history defined by

$$L = 1 + \frac{k_0}{k_e} + \left(\frac{k_0}{k_e}\right)^2 + \cdots = \frac{1}{1 - k_0/k_e}. \tag{24}$$

Figure I shows the comparison of β_{eff} and Λ calculated by the new method using *n* of 5 and different L's with the analytic solutions. From the figure, we can see that the MC results agree well with the references within 95% confidence intervals, which becomes very small when L is greater than 2. Figure II shows the sensitivity of the kinetics parameters to n for k_e of 1.4. From the figure, we can observe that the statistical uncertainty becomes larger as n bigger.

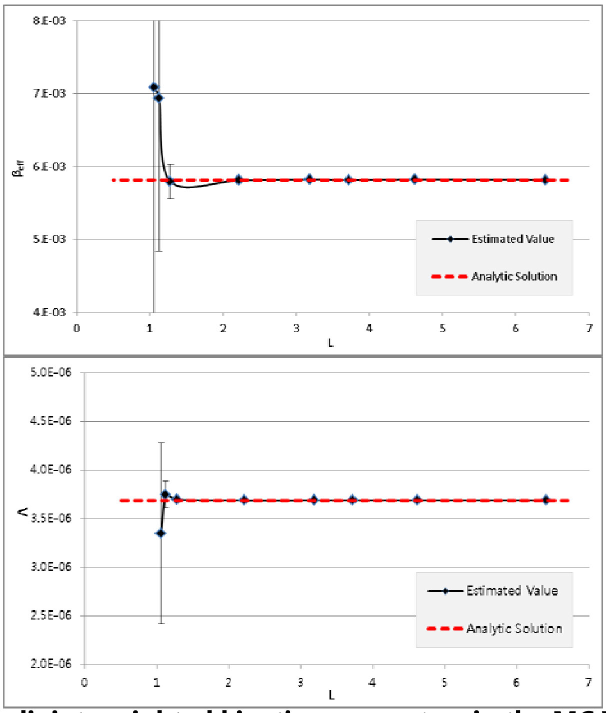

Figure I. Comparisons of adjoint-weighted kinetics parameters in the MC Wielandt calculations for the infinite homogeneous problems with varying *L*

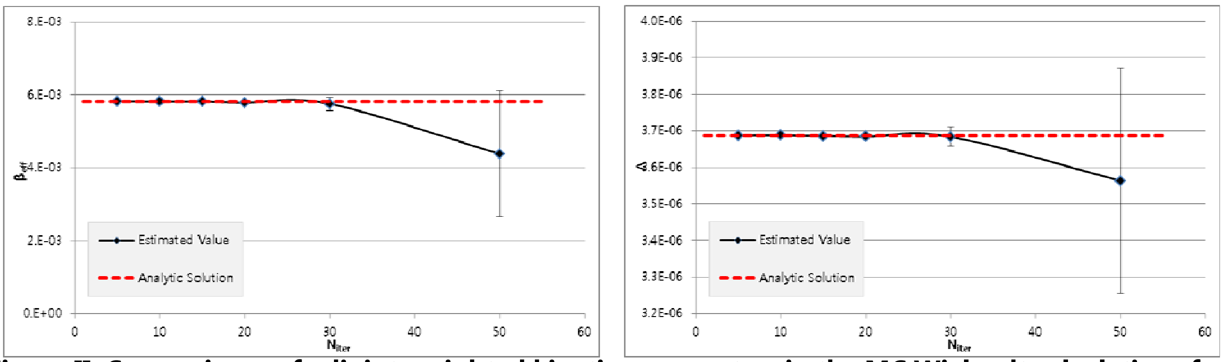

Figure II. Comparisons of adjoint-weighted kinetics parameters in the MC Wielandt calculations for the infinite homogeneous problems with varying the convergence interval of the adjoint flux

3.2 GODIVA Benchmark Problem

The adjoint-weighted kinetics parameters estimated by the new method are compared with the experimental data for the Godiva problem [9]. The calculations are performed with continuous energy cross section libraries produced from ENDF/B-VII.1. The MC calculations are performed for 1,000 active cycles with changing the number of histories per cycle, N_{hist} with the effective number of fission neutrons, $L \times N_{hist}$ of about 4,300,000

Figures III and IV show the comparison of β_{eff} and β_{eff}/Λ calculated by the new method changing L with n of 5 and n with k_e of 1.3, respectively, with experimental results. From the figures, we can observe that β_{eff} and β_{eff}/Λ from the new method agree well with the experimental data within errors of 1% and 3%, respectively, when when L is greater than 2 and n is less than 20.

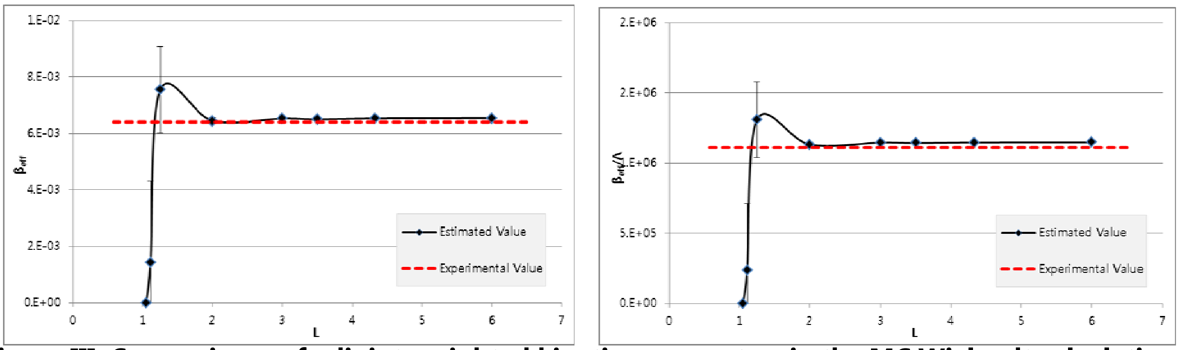

Figure III. Comparisons of adjoint-weighted kinetics parameters in the MC Wielandt calculations for Godiva problem with varying *L*

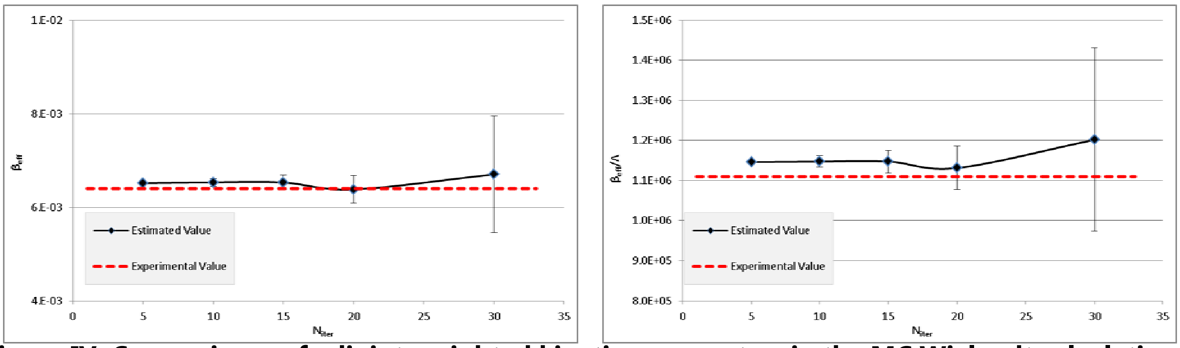

Figure IV. Comparisons of adjoint-weighted kinetics parameters in the MC Wielandt calculations for Godiva problem with varying the convergence interval of the adjoint flux

4. Conclusions

We have developed an efficient adjoint estimation method for the MC Wielandt calculations, which can significantly reduce the memory usage and applied the proposed method for the MC kinetics parameter estimations. From the comparisons with analytic solutions for the infinite homogeneous two-group problem, it is demonstrated that the new method can predict the effective delayed neutron fraction, β_{eff} and the prompt neutron generation time, Λ with great accuracy. For Godiva problem, it is demonstrated that β_{eff} and β_{eff}/Λ calculated by the new method agree well with the experiments within errors of 1% and 3%, respectively.

5. References

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