Adjoint Weighted Kinetics Parameter Estimation in the Monte Carlo Wielandt Calculations

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1. Introduction

Recently, the Monte Carlo (MC) adjoint estimation techniques [1-3] which enables one to compute the adjoint flux in the MC forward calculations have been developed and successfully applied to calculate the adjoint-weighted kinetics parameters of nuclear reactors. The adjoint flux in these methods is interpreted as the iterated fission probability (IFP) [4] and calculated by using a genealogical table for all the histories. However these methods require a huge amount of memories to store the genealogical table as the number of histories increases.

In order to eliminate this huge memory consumption in the current adjoint estimation method, we have developed a new method in which the pedigree of a single history is utilized by applying the MC Wielandt method [5]. 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 an infinite homogeneous two-group problem and the Godiva facility [6].

2. Methods

2.1 Adjoint Estimation in the MC Forward Simulations

The steady-state Boltzmann transport equation can be written by

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

where

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

$$\mathbf{F}\phi = \int dE' \int d\mathbf{\Omega}' \frac{1}{4\pi}\chi(E,E')\nu(E')\Sigma_f(\mathbf{r},E')\phi(\mathbf{r},E',\mathbf{\Omega}'). \tag{3}$$

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

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

In Eq. (4), the fission source density (FSD), S and the fission operator, $\mathbf{H}$ are defined as

$$S \equiv (1/k)\mathbf{F}\phi \tag{5}$$

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

The adjoint eigenvalue equation corresponding to the Eq. (1) can be written as

$$\mathbf{T}^{\dagger}\phi^{\dagger} = \frac{1}{k_0}\mathbf{F}^{\dagger}\phi^{\dagger}, \tag{7}$$

where the superscript of † denotes the adjoint of operator or the angular flux.

Then, operating $\left(\mathbf{T}^{\dagger}\right)^{-1}$ on both sides of Eq. (7) gives

$$\phi^{\dagger} = \frac{1}{k_0}\mathbf{H}^{\dagger}\phi^{\dagger}. \tag{8}$$

By applying the power method to Eq. (8), the physical meaning of the adjoint flux, a distribution proportional to the number of fission neutrons produced in the n-th generation due to a unit source neutron as n approaches infinity, is derived [3]. Thus, the adjoint flux can be estimated in the MC eigenvalue calculations by storing the genealogical table of all the neutron histories.

2.2 Monte Carlo Wielandt Method

Subtracting $(1/k_e)\mathbf{H}S$ from each side of Eq. (4) gives

$$\left[\mathbf{I} - \frac{\mathbf{H}}{k_e}\right]S = \left(\frac{1}{k} - \frac{1}{k_e}\right)\mathbf{H}S. \tag{9}$$

By operating $\left[\mathbf{I} - \mathbf{H}/k_e\right]^{-1}$ on both side of Eq. (9), it can be rewritten as

$$S = \left(\frac{1}{k} - \frac{1}{k_e}\right)\left[\mathbf{I} - \frac{\mathbf{H}}{k_e}\right]^{-1}\mathbf{H}S = \left(\frac{1}{k} - \frac{1}{k_e}\right)\mathbf{H}'S. \tag{10}$$

By the Taylor series expansion, $\mathbf{H}'$ can be written as [7]

$$\mathbf{H}' \equiv \left[\mathbf{I} - \frac{\mathbf{H}}{k_e}\right]^{-1}\mathbf{H} = \left[\mathbf{I} + \frac{\mathbf{H}}{k_e} + \left(\frac{\mathbf{H}}{k_e}\right)^2 + \cdots\right]\mathbf{H}. \tag{11}$$

Inserting Eq. (11) into Eq. (10) and applying the power method yield

$$S^{(i+1)} = \left(\frac{1}{k^{(i)}} - \frac{1}{k_e}\right)\mathbf{H}'S^{(i)} = \sum_{m=0}^{\infty}\left(\frac{1}{k^{(i)}} - \frac{1}{k_e}\right)\mathbf{H}S^{(i,m)}; \tag{12}$$

$$S^{(i,m)} = \left(\frac{\mathbf{H}}{k_e}\right)^m S^{(i)} \tag{13}$$

where the superscript (i+1) or (i) denotes the cycle index.

From Eq. (12), the MC Wielandt algorithm [5] can be interpreted as the fission source of the (n-1)-th generation in cycle i, $S^{(i,n-1)}$ produces the next-cycle fission source as many as $\left(1/k^{(i)} - 1/k_e\right)\mathbf{H}S^{(i,n-1)}$ while $(1/k_e)\mathbf{H}S^{(i,n-1)}\left(= S^{(i,n)}\right)$ is generated as the n-th source for the current cycle simulations.

2.3 Adjoint Weighted Kinetic Parameter Estimation in the MC Wielandt Calculations

From Eq. (13), we can see that the power method updates of the FSD are performed in the MC Wielandt single-cycle calculations. Therefore the number of fission neutrons produced in the *n*-th generation due to a unit source neutron can be readily estimated within a single cycle by using a single history pedigree table.

When adjoint flux are converged after *n*-th iteration, the amount of source used to estimate adjoint-weighted kinetics parameters can be written as

$$\sum_{m=n+1}^{\infty} S^{(i,m)} = S^{(i,n+1)} + S^{(i,n+2)} + \cdots = \frac{\left(k^{(i)}/k_e\right)^{n+1}}{1-k^{(i)}/k_e} S^{(i)}, \qquad (14)$$

which means that the adjoint-weighed kinetics parameters cumulated from the (*n*+1)-th generation should be normalized by the amount of Eq. (14) in MC Wielandt eigenvalue calculations.

3. Numerical Results

The adjoint-weighted kinetics parameter estimation method in the MC Wielandt calculations is implemented in an in-house continuous-energy MC code, McSIM. The kinetics parameters estimated by the new method are compared with the analytic solutions for the infinite homogeneous two-group problem and the experimental results for the Godiva problem.

Table I describes two-group cross sections for the infinite homogeneous problem. The MC calculations are performed on 1,000 active cycles with 10,000,000 histories per cycle. The adjoint convergence interval of 10 is used for the kinetics parameter estimation and k_e is set to 1.4 for the MC Wielandt calculations.

Table I: 2-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
$\chi_{d,1}$	0.20	0.20
β_0	0.006	0.006
$1/\nu$ [sec/cm]	2.28626×10^{-6}	1.29329×10^{-6}

Table II shows comparisons of the analytic solutions and the adjoint-weighted kinetics parameters estimated by the new method. From the table, we can see that the numerical results are agreed with the references within 95% confidence intervals.

Table II: Comparison of adjoint-weighted kinetics parameters for the infinite homogeneous 2-grp. problem

	Reference	**McSIM**	**Err.**
$\mathbf{k_{eff}}$	1.09725	1.09725 (0)*	0
$\boldsymbol{\beta_{eff}}$	5.81517×10^{-3}	5.81139×10^{-3} (42)	9
$\boldsymbol{\Lambda}$	3.68722×10^{-6}	3.68768×10^{-6} (7)	12

* ( ): Relative Standard Deviation [pcm]

For the GODIVA benchmark problem [6], the MC Wielandt calculations were performed with continuous energy cross section libraries from ENDF/B-VII.1. The MC calculations are performed on 1,000 active cycles with 100,000 histories per cycle. The adjoint convergence interval of 10 and k_e of 1.3 are applied.

Table III shows comparisons of experimental data of β_{eff} and $\beta_{\text{eff}}/\Lambda$ for GODIVA and those from the MC Wielandt calculations. From the table, we can observe that the results from the new method are well agreed with the experimental results.

Table III: Comparison of adjoint-weighted kinetics parameters for GODIVA benchmark problems

	Exp.	**McSIM**	**C/E**
$\mathbf{k_{eff}}$	1.00	1.00121 (13)*	1.00
$\boldsymbol{\beta_{eff}}$	0.00640	0.00647 (637)	1.01
$\boldsymbol{\beta_{eff}/\Lambda}$	1.11×10^{6}	1.15830×10^{6} (284)	1.04

* ( ): Relative Standard Deviation [pcm]

4. Conclusions

We have developed an efficient algorithm for the adjoint-weighted kinetics parameter estimation in the MC Wielandt calculations which can significantly reduce the memory usage. From the numerical applications, it is demonstrated that the new method can predict the kinetics parameters with great accuracy.

REFERENCES

[1] Y. Nauchi and T. Kameyama, "Development of Calculation Technique for Iterated Fission Probability and Reactor Kinetic Parameters Using Continuous-Energy Monte Carlo Method," *J. Nucl. Sci. Technol.*, Vol. 47, No. 11, p. 977 2010.

[2] B.C. Kiedrowski, F.B. Brown, P.P.H. Wilson, "Adjoint-Weighted Tallies for k-Eigenvalue Calculations with Continuous-Energy Monte Carlo," *Nucl. Sci. Eng.*, Vol. 168, p. 226, 2011.

[3] H. J. Shim, C. H. Kim, Y. H. Kim, "Estimation of Adjoint-Weighted Kinetics Parameters in Monte Carlo Forward Calculations," PHYSOR 2010, Pittsburgh, Pennsylvania, USA, May 9-14, 2010.

[4] H. Hurwitz, "Physical Interpretation of the Adjoint Flux: Iterated Fission Probability," *Naval Reactor Physics Handbook*, Vol. I, pp. 864-869, A. Radkowsky, Ed., U.S. Atomic Energy Commission, 1964.

[5] T. Yamamoto and Y. Miyoshi, "Reliable Method for Fission Source Convergence of Monte Carlo Criticality Calculation with Wielandt's Method," *J. Nucl. Sci. Technol.*, Vol. 41, No. 2, pp. 99-107, 2004.

[6] J. Blair Briggs (ed.), "International Handbook of Evaluated Criticality Safety Benchmark Experiments," NEA/NSC/DOC(95)03/I, Nuclear Energy Agency, Paris, 2004.

[7] H. J. Shim, C. H. Kim, "Tally Efficiency Analysis for Monte Carlo Wielandt Method," *Ann. Nucl. Energy*, Vol. 36, pp. 1694-1701, 2009.