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Reformulation and Efficient Implementation of the Generalized Perturbation Theory Suited for Monte Carlo Eigenvalue Calculations

2017년 2월

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Abstract

Sensitivity coefficients of reactor performance parameters, such as the effective multiplication factor, $k$, and power distribution to input parameters, are key factors in the fields of the sensitivity and uncertainty (S/U) analysis, safety assessments, nuclear data adjustments, etc. In order to estimate the $k$ sensitivity from the Monte Carlo (MC) particle transport calculations, the MC adjoint-weighted perturbation (AWP) methods based on the iterated fission probability (IFP) concept have been successfully applied for $k$ uncertainty quantifications due to the nuclear data uncertainty.

Recently, there have been several approaches to extend the MC AWP methods to estimate sensitivities of a ratio of responses in the form of ratios of linear or bilinear functions based on generalized perturbation theory (GPT). In addition, we derive a GPT formulation adequate to estimate sensitivities of general MC tallies such as volume flux, reaction rates, etc., not the form of a ratio of linear or bilinear functions by making the best of the fact that MC standard tally estimates are normalized to be per a fission source neutron in the MC eigenvalue calculations. From the generalized adjoint function equation with an adjoint source for the MC general tally, the physical meaning of the generalized adjoint function for a MC tally is derived. Next, it is shown that the derived MC GPT formulation can be used to estimate the $k$ sensitivity by comparing with the MC AWP $k$-sensitivity estimation formulation. As the equivalence of the AWP method and the first-order
DOS/FSP for the $k$ sensitivity estimation, it is proven that the derived GPT formulation is equivalent to the first-order DOS/FSP for the general tally.

However, the current MC adjoint-weighted tally techniques and the new proposed GPT-based MC AWP methods require a memory amount which is proportional to the numbers of the adjoint-weighted tallies and histories per cycle to store history-wise tally estimates during the convergence of the $k$-adjoint or the generalized adjoint function. Especially the MC adjoint-weighted perturbation (AWP) calculations for the nuclear data sensitivity and uncertainty (S/U) analysis suffer from the huge memory consumption to realize the IFP concept. In order to reduce the memory requirement drastically, we present a new adjoint estimation method of which the memory usage is irrelevant to the numbers of histories per cycle by applying the IFP concept for the MC Wielandt calculations.

The new algorithms for the adjoint-weighted kinetics parameter estimation and the AWP calculations in the MC Wielandt method are implemented in a Seoul National University MC code, McCARD and its validity is demonstrated in critical facility problems. From the comparison of the nuclear data S/U analyses, it is demonstrated that the memory amounts to store the sensitivity estimates in the proposed method become negligibly small.
Keyword :

Generalized Perturbation Theory (GPT)

Monte Carlo Eigenvalue Calculations

Sensitivity and Uncertainty (S/U) Analysis

Adjoint Weighted Perturbation (AWP) Method

Monte Carlo Wielandt Method

Student Number : 2009-23191
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Chapter 1. Introduction

1.1 Background

Sensitivity coefficients of reactor performance parameters, $Q$, such as the effective multiplication factor, $k$, and power distribution to input parameters, $x$, expressed by $(dQ/Q)/(dx/x)$, are key factors in the fields of the sensitivity and uncertainty (S/U) analysis, safety assessments, nuclear data adjustments, etc. In order to estimate a change of $Q$, denoted by $\Delta Q$, due to a variation of $x$, $\Delta x$, from the Monte Carlo (MC) particle transport calculations, two conventional stochastic perturbation techniques [1] such as the correlated sampling (CS) and the differential operator sampling (DOS) have been widely used. And Nagaya and Mori [2] augmented these conventional approaches with the fission source perturbation (FSP) method to take into account the perturbed source effect which is propagated generation-by-generation in the MC power iteration method [3]. The DOS method accompanied with the FSP method (DOS/FSP method hereafter) have been successfully applied for the MC nuclear data S/U analyses [4,5].

On the contrary to the MC perturbation approach using the fission source perturbation method [2], there have been recent noticeable advances [6-14] to estimate adjoint functions, which can be utilized to eliminate the perturbed source effect or the perturbation on the neutron flux distribution in the first-order perturbation theory [15,16], in the middle of the MC forward
neutron tracking. For the solution to the adjoint eigenvalue equation (shortly referred to as $k$-adjoint \cite{16} or $\phi^\dagger$), Nauchi and Kameyama \cite{6} and Kiedrowski et al. \cite{7} developed the $k$-adjoint weighted parameter estimation methods on the basis of its physical meaning, namely the iterated fission probability (IFP) \cite{17}. The MC adjoint-weighted perturbation (AWP) methods \cite{8,9} to estimate the $k$ sensitivity using the IFP concept have been successfully applied for $k$ uncertainty quantifications due to the nuclear data uncertainty. It is noteworthy that the AWP method is equivalent to the first-order DOS/FSP method for the $k$ sensitivity, as proven in Ref. \cite{8}. In order to extend the MC AWP methods to estimate sensitivities of a ratio of two reaction rates, Perfetti and Rearden \cite{10} devised a MC sensitivity calculation method with the generalized adjoint function, denoted by $\Gamma^\dagger$, by expressing it as the sum of the intra-generational and inter-generational effect terms. Aufiero et al. \cite{11} suggested the collision history-based approach to calculate sensitivities of responses in the form of ratios of linear or bilinear functions by applying the CS method for multi-generational collisions.

However, these MC adjoint-based sensitivity estimation methods may suffer from a huge memory consumption problem to save inter-generational contributions to $\phi^\dagger$ or $\Gamma^\dagger$ proportional to the number of the sensitivity tallies. In order to reduce memories required for the $k$-adjoint estimation, Perfetti et al. \cite{12} suggested the contribution-IFP hybrid method and Kiedrowski and Brown \cite{9} have applied a sparse data handling scheme. And present authors \cite{13} proposed a $k$-adjoint-weighted tallying method in
the MC Wielandt method [18] where multiple generations from a fission source neutron can be simulated in single history calculations. For the generalized adjoint function calculation, Qiu et al. [14] adopted the superhistory algorithm for the collision history-based method to reduce the memory requirement in the MC sensitivity estimation of a general response expressed by a ratio of two reaction rates.

1.2 Objective and Scope

In Chapter 2, we present a new adjoint estimation technique for the adjoint-weighted tallies to overcome the memory consumption problem by adopting the MC Wielandt method [18] where multiple generations of a fission source neutron can be simulated history-by-history within single cycle (or iteration) while one generation of each fission source neutron in a cycle of the conventional power iteration method. In Section 2.1, an IFP formulation for the MC Wielandt calculations is derived and it will be shown that the new adjoint estimation algorithm does not require saving the history-wise tally estimates. Formulations to estimate the adjoint flux in the MC Wielandt method are derived and the proposed MC adjoint estimation method is implemented into the Seoul National University MC code, McCARD [19]. Sections 2.2 and 2.3 provide algorithms and application results for the adjoint-weighted kinetics parameter calculations and the adjoint-weighted perturbation (AWP) calculations, respectively.
In Chapter 3, we derive a generalized perturbation theory (GPT) formulation adequate to estimate sensitivities of general MC tallies such as volume flux, reaction rates, etc., not the form of a ratio of linear or bilinear functions, by making the best of the fact that standard tally estimates are normalized to be per a fission source neutron in the MC eigenvalue calculations. From the generalized adjoint function equation with an adjoint source for the MC general tally, the physical meaning of the generalized adjoint function for a MC tally is derived. Next, it is shown that the derived MC GPT formulation can be used to estimate the $k$ sensitivity by comparing with the MC AWP $k$-sensitivity estimation formulation [8]. As the equivalence of the AWP method and the first-order DOS/FSP for the $k$ sensitivity estimation [8], it is proven that the derived GPT formulation is equivalent to the first-order DOS/FSP for the general tally. From the derived MC GPT formulation, a MC sensitivity calculation algorithm is derived for the MC Wielandt method to reduce the memory consumption. The proposed methods have been implemented into McCARD [19] and tested in two-group infinite homogeneous problems and Godiva critical assembly [24]. Finally, the memory efficiency is demonstrated in the S/U analysis for the TMI-1 pin cell problem in the OECD benchmarks for uncertainty analysis modeling (UAM) for design, operation, and safety analysis of LWRs [20].
Chapter 2. $k$-Adjoint Weighted Tallies in the Monte Carlo Wielandt Method

2.1 Adjoint Estimation in the MC Wielandt Method

The time-independent neutron transport equation can be written in an operator notation as

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

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

$$T\phi = [\Omega \cdot \nabla + \Sigma_t(r,E)]\phi(r,E,\Omega) - \int dE' \int d\Omega' \Sigma_s(r,E',\Omega' \rightarrow E,\Omega)\phi(r,E',\Omega'),$$

(2.2)

$$F\phi = \int dE' \int d\Omega' \frac{\chi(E' \rightarrow E)}{4\pi} \nu(E') \Sigma_f(r,E')\phi(r,E',\Omega')$$

(2.3)

$\Sigma_t$, $\Sigma_s$, and $\Sigma_f$ are the total, scattering and fission cross sections, respectively. $\nu$ is the mean number of fission neutrons produced from a fission reaction. $\chi$ is the energy spectrum of fission neutrons.

By operating $(1/k)FT^{-1}$ on both sides of Eq. (2.1), one can
obtain

\[ S = \frac{1}{k} HS , \quad (2.4) \]

where the fission source density (FSD), \( S \), satisfying \( \int S(P) dP = 1 \), and the fission operator, \( H \), are defined as

\[ S = \frac{1}{k} F \phi , \quad (2.5) \]

\[ H = FT^{-1} \quad (2.6) \]

When \( P \) denotes the state vector of a neutron in the six-dimensional phase space, \((r, E, \Omega)\), \( HS \) in Eq. (2.4) can be written as

\[ HS = \int dP' H(P' \to P) S(P') , \quad (2.7) \]

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

And the fundamental mode adjoint flux, \( \phi_0^\dagger \), of the IFP concept can be derived as [8]

\[ \phi_0^\dagger = \lim_{n \to \infty} \phi_{0,n}^\dagger ; \quad (2.8) \]

\[ \phi_{0,n}^\dagger (P) = \frac{1}{k_0^n} \int dP' H''(P \to P') , \quad (2.9) \]
where $k_0$ is the fundamental mode eigenvalue. $H^n(P \rightarrow P')$ means the number of the $n$-th generation fission neutrons born per unit phase space volume about $P'$, due to a parent neutron born at $P$ and $\phi_{0,n}(P)$ is normalized to satisfy $\int \phi_{0,n}^{\dagger}(P)S_0(P)dP = 1$ where $S_0$ denotes the fundamental mode FSD. Thus $\phi_{0,n}^{\dagger}(P)$ can be calculated by scoring the fission neutrons produced at the $n$-th generation starting from the fission source at $P$ by using a genealogical table of fission sources. When $n$, named the adjoint convergence interval, is large enough to ensure the convergence of the fundamental mode adjoint flux, $\phi_{0,n}^{\dagger}(P)$ can be used for $\phi_0^{\dagger}$ in the adjoint-weighted tally calculations. Note that Eq. (2.9) is derived [8] by taking the unity as an initial distribution when applying the power iteration method for the adjoint eigenvalue equation corresponding to Eq. (2.4).

The Wielandt method can be characterized by subtracting $(1/k_e)HS$ from each side of Eq. (2.4) as

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

(2.10)

where $I$ is the identity operator and $k_e$ is an estimated eigenvalue.

By operating $(I - H/k_e)^{-1}$ on both sides of Eq. (2.10), $S$ can be expressed as
\[ S = \left( \frac{1}{k} - \frac{1}{k_e} \right) H'S; \quad (2.11) \]

\[ H' = \left( I - \frac{H}{k_e} \right)^{-1} H. \quad (2.12) \]

And the Taylor series expansion of \( (I - H/k_e)^{-1} \) in Eq. (2.12) yields [21]

\[ H' = \left[ 1 + \frac{H}{k_e} + \left( \frac{H}{k_e} \right)^2 + \cdots \right] H. \quad (2.13) \]

By applying the power iteration method for Eq. (2.11), the fundamental mode FSD is updated iteration-by-iteration as

\[ \hat{S}^{(i+1)} = \left( \frac{1}{k^{(i)}} - \frac{1}{k_e} \right) H'S^{(i)}, \quad (2.14) \]

where \( S^{(i)} \) is the FSD for iteration or cycle \( i \) satisfying \( \int S^{(i)} dP = 1 \) while \( \hat{S}^{(i+1)} \) denotes an unnormalized fission source distribution for cycle \( i+1 \), from which \( S^{(i+1)} \) can be obtained by

\[ S^{(i+1)}(P) = \hat{S}^{(i+1)}(P) / \int \hat{S}^{(i+1)}(P) dP. \quad (2.15) \]

\( k^{(i)} \) is the eigenvalue estimated at cycle \( i \).

The MC Wieland algorithm [18] can be derived by inserting Eq.
(2.13) into Eq. (2.14) as [21]

\[
\hat{S}^{(i+1)} = \left( \frac{1}{k^{(l)}} - \frac{1}{k_e} \right) \sum_{i'=0}^{\infty} \left( \frac{H}{k_e} \right)^{i'} H S^{(l)}
\]

\[
= \left( \frac{1}{k^{(l)}} - \frac{1}{k_e} \right) H \left( \sum_{i'=0}^{\infty} S^{(i,i')} \right);
\]

\[
S^{(i,i')} = \left( \frac{H}{k_e} \right)^{i'} S^{(l)} ,
\]

where \( S^{(i,i')} \) means the fission source distribution of \( i' \)-th generation estimated at cycle \( i \) in the Wielandt iterations. By setting \( S^{(i,0)} = S^{(i)} \), Eq. (2.17) can be expressed as

\[
S^{(i,i'+1)} = \frac{H}{k_e} S^{(i,i')} .
\]

Then Eqs. (2.16) and (2.18) say the MC algorithm as fission source neutrons represented by \( S^{(i,i')} \) produce the ‘next-cycle’ fission sources from the MC simulations of \( \left( 1/k^{(l)} - 1/k_e \right) H S^{(i,i')} \) by Eq. (2.16) while generating the ‘next-generation’ fission sources with a probability of \( \left( 1/k_e \right) H S^{(i,i')} \) at the current cycle by Eq. (2.18), which continues starting from \( S^{(i,0)} \) until no more fission neutrons are sampled at the \( i' \)-th generation.

Figure 2.1 shows a schematic diagram of this MC Wielandt algorithm. In the figure, the arrow sign indicates that a parent neutron generates a daughter
neutron by a fission reaction. The inside of the dotted box in Figure 2.1 shows an example of the genealogical table of a single history, from which it is clearly shown that multi-generational simulations of a fission source neutron are performed within a cycle of the MC Wielandt calculations.

Figure 2.2 Schematic view of the MC Wielandt algorithm

It is meaningful to define the expected number of fission neutrons generated from a single history simulation in the MC Wielandt method, $L$, as

$$L = \sum_{i=0}^{\infty} \int S^{(i,e)}(P)dP.$$  \hspace{1cm} (2.19)

By inserting Eq. (2.17) into Eq. (2.19) and using Eq. (2.4) and
the condition of \( \int S^{(i)} d\mathbf{P} = 1 \), one can obtain [21]

\[
L = \sum_{i=0}^{\infty} \frac{H}{k_c} \left( \frac{k_0}{k_c} \right)^i \cdot \int S^{(i)} d\mathbf{P} = \frac{1}{1 - k_0/k_c}. \tag{2.20}
\]

Because \( \phi_{0,n}^{\dagger}(\mathbf{P}) \) defined by Eq. (2.9) means the number of fission neutrons generated for the next \( n \)-th generation from a fission source neutron located at position \( \mathbf{P} \), therefore, \( \phi_{0,n}^{\dagger}(\mathbf{P}) \) corresponding to \( S^{(i,x)}(\mathbf{P}) \) can be calculated from the single-history simulations of the MC Wielandt method as

\[
\phi_{0,n}^{\dagger}(\mathbf{P}) = W_n \int d\mathbf{P}' S^{(i,x+n)}(\mathbf{P}' \mid S^{(i,x)}(\mathbf{P})) S^{(i,x)}(\mathbf{P}) \frac{S^{(i,x)}(\mathbf{P})}{S^{(i,x)}(\mathbf{P})}, \tag{2.21}
\]

where \( W_n \) is a normalization constant for the adjoint convergence interval of \( n \). \( S^{(i,x+n)}(\mathbf{P}' \mid S^{(i,x)}(\mathbf{P})) \) denotes the number of fission neutrons generated from \( S^{(i,x)}(\mathbf{P}) \) after \( n \) generations at \( \mathbf{P}' \), which can be defined, from Eq. (2.18), as

\[
S^{(i,x+n)}(\mathbf{P}' \mid S^{(i,x)}(\mathbf{P})) = \frac{1}{k_c} H^n(\mathbf{P} \rightarrow \mathbf{P}') S^{(i,x)}(\mathbf{P}). \tag{2.22}
\]

The normalization constant, \( W_n \), can be obtained by inserting Eq. (2.22) into Eq. (2.21).
\[ \phi_{0,n}^+(P) = W_n \cdot \frac{1}{k_e^n} \int \frac{dP'H^n(P \rightarrow P') S^{(i,r)}(P)}{S^{(i,r)}(P)} \]

\[ = W_n \cdot \frac{1}{k_e^n} \int dP'H^n(P \rightarrow P'). \quad (2.23) \]

Then by applying Eq. (2.23) for the normalization condition of
\[ \int \phi_{0,n}^+(P) S_0(P) dP = 1 \] or simply comparing Eq. (2.23) with Eq. (2.9), \( W_n \) becomes

\[ W_n = \left( \frac{k_e}{k_0} \right)^n. \quad (2.24) \]

Let us suppose that a \( p' \)-th collision of \( j' \)-th fission neutron of \( i' \)-th generation in \( j \)-th history simulation at cycle \( i \) of the MC Wielandt calculations produces \( \nu/k_e \) fission neutrons having their weights of \( w^{j',j',p'} \) for the \((i'+1)\)-th generation with a probability of \( \frac{\Sigma_{j'}^{j',j',p'}}{\Sigma_{j'}^{j',j',p'}} \) where \( w^{j',j',p'} \), \( \Sigma_{j'}^{j',j',p'} \) and \( \Sigma_{j'}^{j',j',p'} \) are the neutron weight, \( \Sigma_f \) and \( \Sigma_i \), respectively, for the collision. Then the adjoint flux for state \( P \) of the collided neutron at the \( i' \)-th generation, \( \phi_{0,n}^+(P_{j',j',p'}) \), can be estimated by summing up the number of fission neutrons scored at every collision site of \((i'+n-1)\)-th generation progeny \((n \geq 2)\) as
\( \phi_0^{+}(\mathbf{P}_{i,j,i'j'p'}) = \left( \frac{k_e}{k_{i-1}} \right)^n \sum_{j'' \in \Gamma_{i,j,i'j'p'}} \sum_{p''} \frac{1}{k_e} \frac{1}{\Sigma_f} \frac{\nu \phi_{i,j,i'j'p'}^{+}}{\nu \phi_{i,j,i'j'p'}^{+}} \), \quad (2.25)

where \( \Gamma_{i,j,i'j'p'} \) denote a set of progeny from the \( p' \)-th collision of \( j' \)-th fission neutron of \( i' \)-th generation in \( j \)-th history simulation at cycle \( i \). \( p'' \) is the collision index of fission neutron \( j'' \) included in the progeny set of \( \Gamma_{i,j,i'j'p'} \).

Note that \( \left( \frac{k_e}{k_{i-1}} \right)^n \) in the right hand side of Eq. (2.25) is the normalization constant defined by Eq. (2.24), in which the fundamental mode eigenvalue estimated at the previous cycle, \( k_{i-1} \), is used for \( k_0 \). From Eq. (2.25), one can see that the adjoint flux at \( \mathbf{P}_{i,j,i'j'p'} \), \( \phi_0^{+}(\mathbf{P}_{i,j,i'j'p'}) \), is calculated within the fixed history \( j \) at cycle \( i \) so that history-wise tally estimates do not have to be stored for the adjoint-weighting in the MC Wielandt method. And this makes the memory amount required for the adjoint estimation independent of the number of histories per cycle.
2.2 Adjoint-Weighted Kinetics Parameter Calculations

2.2.1 Kinetics Parameter Calculation Algorithm in MC Wielandt Method

Assuming that the angular flux and the cross-sections are time-independent, the prompt neutron generation time, $\Lambda$, and the effective delayed neutron fraction, $\beta_{\text{eff}}$, in the point kinetics equation are defined with the adjoint weighting by

$$\beta_{\text{eff}} = \frac{\langle \phi_0^+, S_d \rangle}{\langle \phi_0^+, F \phi_0 \rangle} = \frac{1}{k_0} \frac{\langle \phi_0^+, S_d \rangle}{\langle \phi_0^+, F \phi_0 \rangle}, \quad \text{(2.26)}$$

$$\Lambda = \frac{\langle \phi_0^+, \frac{1}{v} \phi_0 \rangle}{\langle \phi_0^+, F \phi_0 \rangle} = \frac{1}{k_0} \frac{\langle \phi_0^+, \frac{1}{v} \phi_0 \rangle}{\langle \phi_0^+, F \phi_0 \rangle}; \quad \text{(2.27)}$$

$$\hat{S}_d = \int dE' \int d\Omega' \frac{\chi_d(E' \rightarrow E)}{4\pi} v_d(E') \Sigma_f(r, E') \phi_0(r, E', \Omega'). \quad \text{(2.28)}$$

The angular bracket implies the inner product and $v$ is the neutron speed. $\phi_0$ denotes the fundamental mode angular flux. $\chi_d$ and $v_d$ are the energy spectrum and the mean emission number, respectively, of delayed neutrons from a fission reaction. The second equalities in Eqs. (2.26) and (2.27) are derived from a condition derived from the definition of $S$ given by Eq. (2.5) and the normalization condition of the adjoint flux, $\langle \phi_0^+, S_0 \rangle = 1$, as
\[ \langle \phi_0^\dagger, F \phi_0 \rangle = k_0 \langle \phi_0^\dagger, S_0 \rangle = k_0. \quad (2.29) \]

\( \beta_{\text{eff}} \) defined by Eq. (2.26) can be calculated by averaging the adjoint flux of the delayed neutrons divided by \( k_0 \) for the total number of fission neutrons \([6, 22]\) in the MC Wielandt calculations as

\[
\overline{\beta_{\text{eff}}} = \frac{1}{N M L} \sum_{i,j} \frac{1}{k_{i-1}} \sum_{i' = 0}^{\infty} \sum_{j' \in D} \phi_{0,n}^\dagger \left( \mathbf{P}_{i',j'} \right), \quad (2.30)
\]

where \( N \) and \( M \) are the numbers of active cycles and histories per cycle, respectively. \( L \) is the expected number of fission neutrons generated from a single history defined by Eq. (2.20). \( D \) denotes a set of delayed neutrons. \( \mathbf{P}_{i',j'} \) is the initial state vector of the \( j' \)-th neutron of \( i' \)-th generation in \( j \)-th history at cycle \( i \).

An insertion of Eq. (2.25) into Eq. (2.30) gives the \( \beta_{\text{eff}} \) calculation algorithm as

\[
\overline{\beta_{\text{eff}}} = \frac{1}{N M L} \sum_{i,j} \frac{1}{k_{i-1}} \left( \frac{k_e}{k_{i-1}} \right)^n \sum_{i' = 0}^{\infty} \sum_{j' \in D_{j',-n+1}} \sum_{p'} \frac{1}{k_e} w_{i',j'}^{p'} \frac{\Sigma_{j'}^{p'}}{\Sigma_{j'}^{p'}} \left( \mathbf{P}_{i',j'} \right), \quad (2.31)
\]

where \( D_{j',-n+1} \) denotes the set of delayed neutrons of \((i'-n+1)\)-th generation of \( j \)-th history at cycle \( i \).

And \( \Lambda \) defined by Eq. (2.27) can be calculated in the MC Wielandt calculations as
\[ \bar{\lambda} = \frac{1}{NML} \sum_{i,j} \frac{1}{k_{i-1}} \sum_{i'=0}^{\infty} \sum_{j'=0}^{j'_{p'}} \left( \frac{\Delta l_{ij}^{ij'}}{v_{ij'}^{ij'}} \right) \cdot \phi_{0,n}^+ \left( P_{ij,j'}^{ij'} \right), \] (2.32)

where \( \Delta l_{ij}^{ij'} \) and \( v_{ij'}^{ij'} \) are the track length and the neutron speed, respectively, between \((p'-1)\)-th and \(p'\)-th collisions of \(j'\)-th neutron of \(i'\)-th generation in \(j\)-th history at cycle \(i\).

An insertion of \( \phi_{0,n}^+ \left( P_{ij,j'}^{ij'} \right) \) of Eq. (2.25) into Eq. (2.32) gives

\[ \bar{\lambda} = \frac{1}{NML} \sum_{i,j} \frac{1}{k_{i-1}} \sum_{i'=0}^{\infty} \sum_{j'=0}^{j'_{p'}} \left( \frac{\Delta l_{ij}^{ij'}}{v_{ij'}^{ij'}} \right) \cdot \left( \frac{k_e}{k_{i-1}} \right)^n \sum_{j'=1}^{j_{p'}} \sum_{p'} \frac{1}{k_e} \sum_{j''_{n-1}}^{j_{n-1}} w_{ij',j''_{n-1}} \frac{V_{ij',j''_{n-1}}}{\Sigma_{ij',j''_{n-1}}} \right). \] (2.33)

Eq. (2.33) can be implemented by an algorithm calling the direct response of \( \Delta l/v \) before \(n-1\) generations while updating the adjoint responses in the \(i'\)-th generation simulations as

\[ \bar{\lambda} = \frac{1}{NML} \sum_{i,j} \frac{1}{k_{i-1}} \sum_{i'=0}^{\infty} \sum_{j'=0}^{j'_{p'}} \left( \frac{1}{k_e} w_{ij,j'} \frac{V_{ij,j'}}{\Sigma_{ij,j'}} \right) \cdot \left( \frac{\Delta l_{ij,(i'-n+1)}^{ij'}}{v_{ij,(i'-n+1)}^{ij'}} \right), \] (2.34)

where \( \Delta l_{ij,(i'-n+1)}^{ij'} \) is the direct response value of the \(p'\)-th collision of \(j'\)-th neutron of \((i'-n+1)\)-th generation in \(j\)-th history at cycle \(i\) from which the progenitor neutron of the \(j''\)-th neutron of \(i'\)-th generation in the same history is produced.
2.2.2 Numerical Results for Infinite Homogeneous Two-Group Problems

The proposed algorithms of Eqs. (2.31) and (2.34) have been implemented in McCARD [19] and tested for a homogeneous infinite medium problem characterized by two-group cross-sections given by Table 2.1 [22], with changing the differential scattering cross section. In the table, $\Sigma_{sg'g}$, $\chi_{g'g}$ and $\chi_{d,g'g}$ are the scattering cross section, energy spectrums of total fission neutrons, and delayed neutrons, respectively, from energy group $g$ to $g'$. In this study, $\Sigma_{s21}$ is set at 0.181905, 0.247143, or 0.312987 corresponding to the infinite multiplication factor, $k_{inf}$, of 0.9, 1.0, or 1.1.

Table 2.1 Two-group cross sections for the infinite homogeneous problems

<table>
<thead>
<tr>
<th>Cross-section</th>
<th>First Gr. ($g=1$)</th>
<th>Second Gr. ($g=2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma_{tg}$</td>
<td>0.50</td>
<td>0.50</td>
</tr>
<tr>
<td>$\Sigma_{fg}$</td>
<td>0.025</td>
<td>0.175</td>
</tr>
<tr>
<td>$\nu_{g}$</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>$\Sigma_{sgg}$</td>
<td>0.10</td>
<td>0.20</td>
</tr>
<tr>
<td>$\Sigma_{sg'g}$ ($g \neq g'$)</td>
<td>variable</td>
<td>0.00</td>
</tr>
<tr>
<td>$\chi_{1g}$</td>
<td>0.80</td>
<td>0.5</td>
</tr>
<tr>
<td>$\chi_{2g}$</td>
<td>0.20</td>
<td>0.5</td>
</tr>
<tr>
<td>$\chi_{d,1g}$</td>
<td>0.80</td>
<td>0.80</td>
</tr>
<tr>
<td>$\chi_{d,2g}$</td>
<td>0.20</td>
<td>0.20</td>
</tr>
<tr>
<td>$\beta_{lg}$ ($=v_d/v$)</td>
<td>0.006</td>
<td>0.006</td>
</tr>
<tr>
<td>$1/\nu_{g}$ [sec/cm]</td>
<td>$2.28626 \times 10^{-10}$</td>
<td>$1.29329 \times 10^{-6}$</td>
</tr>
</tbody>
</table>
The MC Wielandt calculations are performed varying $L$ by changing the $k_e$ value according to Eq. (2.20) at a fixed value of the adjoint convergence interval, $n$, of 10 or changing $n$ with fixing $L$ by 10. The eigenvalue calculations are performed on 1,000 active cycles with changing the number of histories per cycle, $M$, to make the effective number of fission neutrons, i.e. $M \times L$, constant as about 1,000,000. Tables 2 and 3 show comparisons of $\beta_{\text{eff}}$ and $\Lambda$, respectively, calculated by the proposed method with the analytic solutions. In the tables, RSD denotes the relative standard deviation, which is defined as the standard deviation (SD) divided by the mean value. From the tables, we can see that the results of the proposed method agree well with the analytic solutions within 95% confidence intervals. Also, it is noteworthy that the statistical uncertainties become larger as $n$ bigger or $L$ smaller. And this behavior of the statistical uncertainty can be explained by introducing the expected number of fission neutrons used to estimate the adjoint flux in a single history simulation in the MC Wielandt method, $L_{\text{adj}}$. In the same way to derive $L$ as Eq. (2.20), $L_{\text{adj}}$ can be obtained by summing the number of fission neutrons from generation $(n-1)$ as

$$L_{\text{adj}} = \sum_{i=n-1}^{\infty} \left( \frac{H}{k_e} \right)^i S^{(i)} d\mathbf{P} = \left( \sum_{i=n-1}^{\infty} \left( \frac{k_0}{k_e} \right)^i \right) \cdot \int S^{(i)} d\mathbf{P} = \left( \frac{k_0/k_e}{1 - k_0/k_e} \right)^{n-1} = L \left( 1 - \frac{1}{L} \right)^{n-1}. \tag{2.35}$$

The last equality in Eq. (2.35) is derived by using Eq. (2.20), i.e. $k_0/k_e = 1 - 1/L$. Then from Eq. (2.35) under necessary conditions that $L > 1$
and \( n \geq 1 \) for the adjoint estimation, it is obvious that \( L_{adj} \) decreases, which means the statistical uncertainty increases, as \( n \) is larger for a given \( L \) or \( L \) smaller with a fixed \( n \).
Table 2.2 Comparisons of $\beta_{\text{eff}}$’s for the infinite homogeneous two-group problem with varying $L$ and $n$

| $k_{\text{inf}}$ | $(\beta_{\text{eff}})_{\text{ref}}$ | \begin{tabular}{c} \textbf{n=10} \end{tabular} & \begin{tabular}{c} \textbf{L=10} \end{tabular} |
|------------------|----------------------------------|---------------------------------|-----------------|
|                  | \begin{tabular}{c} \textbf{L} \textbf{ $\overline{\beta}_{\text{eff}}$ } \textbf{(RSD [%])} \end{tabular} | \begin{tabular}{c} \textbf{L} \textbf{ $\overline{\beta}_{\text{eff}}$ } \textbf{(RSD [%])} \end{tabular} |
| 0.9              | $4.9977 \times 10^{-3}$          | \begin{tabular}{c|c} 2 & 5.0019 $\times 10^{-3}$ (1.25) \hline 5 & 5.0001 $\times 10^{-3}$ (0.20) \\ 10 & 4.9975 $\times 10^{-3}$ (0.14) \\ 15 & 4.9980 $\times 10^{-3}$ (0.14) \\ 20 & 4.9980 $\times 10^{-3}$ (0.12) \end{tabular} | \begin{tabular}{c|c} 5 & 4.9982 $\times 10^{-3}$ (0.09) \hline 10 & 4.9975 $\times 10^{-3}$ (0.14) \\ 15 & 4.9983 $\times 10^{-3}$ (0.20) \\ 20 & 4.9943 $\times 10^{-3}$ (0.23) \\ 50 & 5.0018 $\times 10^{-3}$ (1.36) \end{tabular} |
| 1.0              | $5.4353 \times 10^{-3}$          | \begin{tabular}{c|c} 2 & 5.4403 $\times 10^{-3}$ (1.20) \hline 5 & 5.4328 $\times 10^{-3}$ (0.19) \\ 10 & 5.4353 $\times 10^{-3}$ (0.12) \\ 15 & 5.4355 $\times 10^{-3}$ (0.11) \\ 20 & 5.4348 $\times 10^{-3}$ (0.10) \end{tabular} | \begin{tabular}{c|c} 5 & 5.4347 $\times 10^{-3}$ (0.07) \hline 10 & 5.4353 $\times 10^{-3}$ (0.12) \\ 15 & 5.4340 $\times 10^{-3}$ (0.18) \\ 20 & 5.4336 $\times 10^{-3}$ (0.22) \\ 50 & 5.4214 $\times 10^{-3}$ (1.30) \end{tabular} |
| 1.1              | $5.7942 \times 10^{-3}$          | \begin{tabular}{c|c} 2 & 5.8079 $\times 10^{-3}$ (0.97) \hline 5 & 5.7961 $\times 10^{-3}$ (0.18) \\ 10 & 5.7940 $\times 10^{-3}$ (0.12) \\ 15 & 5.7935 $\times 10^{-3}$ (0.14) \\ 20 & 5.7944 $\times 10^{-3}$ (0.11) \end{tabular} | \begin{tabular}{c|c} 5 & 5.7935 $\times 10^{-3}$ (0.07) \hline 10 & 5.7940 $\times 10^{-3}$ (0.12) \\ 15 & 5.7935 $\times 10^{-3}$ (0.14) \\ 20 & 5.7935 $\times 10^{-3}$ (0.21) \\ 50 & 5.7823 $\times 10^{-3}$ (1.06) \end{tabular} |

a) $(\beta_{\text{eff}})_{\text{ref}}$ is the analytic solution of $\beta_{\text{eff}}$.

b) $\overline{\beta}_{\text{eff}}$ is the mean value of $\beta_{\text{eff}}$ estimated from the MC Wielandt calculations.
Table 2.3 Comparisons of $\Lambda$’s for the infinite homogeneous two-group problem with varying $L$ and $n$

<table>
<thead>
<tr>
<th>$k_{inf}$</th>
<th>$\Lambda_{ref}^{a)}$</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$n=10$</td>
<td>$L=10$</td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$L$</td>
<td>$\bar{\Lambda}^{b)}$ (RSD [%])</td>
<td>$n$</td>
<td>$\bar{\Lambda}^{b)}$ (RSD [%])</td>
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<td></td>
</tr>
<tr>
<td>0.9</td>
<td>4.5011×10⁻⁶</td>
<td>2</td>
<td>4.5016×10⁻⁶ (0.16)</td>
<td>5</td>
<td>4.5010×10⁻⁶ (0.01)</td>
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<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>5</td>
<td>4.5011×10⁻⁶ (0.03)</td>
<td>10</td>
<td>4.5011×10⁻⁶ (0.02)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>10</td>
<td>4.5011×10⁻⁶ (0.02)</td>
<td>15</td>
<td>4.5008×10⁻⁶ (0.03)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>15</td>
<td>4.5010×10⁻⁶ (0.03)</td>
<td>20</td>
<td>4.5005×10⁻⁶ (0.05)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>20</td>
<td>4.5010×10⁻⁶ (0.01)</td>
<td>50</td>
<td>4.4994×10⁻⁶ (0.43)</td>
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<td></td>
</tr>
<tr>
<td>1.0</td>
<td>4.0576×10⁻⁶</td>
<td>2</td>
<td>4.0593×10⁻⁶ (0.17)</td>
<td>5</td>
<td>4.0576×10⁻⁶ (0.01)</td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td>5</td>
<td>4.0575×10⁻⁶ (0.03)</td>
<td>10</td>
<td>4.0576×10⁻⁶ (0.02)</td>
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<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>10</td>
<td>4.0576×10⁻⁶ (0.02)</td>
<td>15</td>
<td>4.0574×10⁻⁶ (0.03)</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>15</td>
<td>4.0575×10⁻⁶ (0.01)</td>
<td>20</td>
<td>4.0570×10⁻⁶ (0.05)</td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td>20</td>
<td>4.0576×10⁻⁶ (0.01)</td>
<td>50</td>
<td>4.0535×10⁻⁶ (0.35)</td>
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<td></td>
</tr>
<tr>
<td>1.1</td>
<td>3.6967×10⁻⁶</td>
<td>2</td>
<td>3.6967×10⁻⁶ (0.14)</td>
<td>5</td>
<td>3.6966×10⁻⁶ (0.01)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>5</td>
<td>3.6968×10⁻⁶ (0.02)</td>
<td>10</td>
<td>3.6966×10⁻⁶ (0.01)</td>
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<tr>
<td></td>
<td></td>
<td>10</td>
<td>3.6966×10⁻⁶ (0.01)</td>
<td>15</td>
<td>3.6965×10⁻⁶ (0.03)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>15</td>
<td>3.6967×10⁻⁶ (0.01)</td>
<td>20</td>
<td>3.6958×10⁻⁶ (0.05)</td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td>20</td>
<td>3.6965×10⁻⁶ (0.01)</td>
<td>50</td>
<td>3.6951×10⁻⁶ (0.36)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

a) $\Lambda_{ref}$ is the analytic solution of $\Lambda$.

b) $\bar{\Lambda}$ is the mean value of $\Lambda$ estimated from the MC Wielandt calculations.
2.2.3 Numerical Results for Critical Facilities

The adjoint-weighted kinetics parameters calculated by the proposed method in the MC Wielandt calculations are compared with results by the conventional method [22] in the MC power iteration calculations as well as experimental results for three critical facilities – Godiva [24], the Tank-type Critical Assembly (TCA) [25,26], and the Static Experimental Critical Facility (STACY) [27]. The MC calculations are conducted with continuous energy cross section libraries produced from ENDF/B-VII.1 [28]. The adjoint convergence interval, $n$, is set to 10 which was suggested as the minimum value of the latent generations for the kinetics parameter calculations in a typical pressurized water reactor [7]. In the MC Wielandt calculations, $L$ is set at 10. The MC calculations are performed on 1,000 active cycles for Godiva and 200 active cycles for TCA and STACY with 10,000 histories per cycle for the Wielandt calculations and 100,000 histories per cycle for the standard eigenvalue calculation.

Table 2.4 shows comparisons of $\beta_{\text{eff}}$’s estimated in the conventional MC power iteration method and the MC Wielandt method with measurements for Godiva and TCA. Table 2.5 shows comparisons of $\beta_{\text{eff}}/\Lambda$ values estimated from the two MC calculations with experimental results for Godvia, TCA, and STACY. The experimental data in Tables 4 and 5 are taken from Ref. 7, 25, 26, 27 and 29. From the tables, we can see that $\beta_{\text{eff}}$ and $\beta_{\text{eff}}/\Lambda$ calculated by the proposed method agree well with the measurements within 2% and 4%
errors, respectively.
Table 2.4 Comparisons of $\beta_{\text{eff}}$’s for Critical Facilities

<table>
<thead>
<tr>
<th>Facility</th>
<th>Core Name</th>
<th>$(\beta_{\text{eff}})_{\text{exp}}$</th>
<th>Power Iteration Method</th>
<th>Wielandt Method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\beta_{\text{eff}}$ b)</td>
<td>RSD [%]</td>
</tr>
<tr>
<td>Godiva</td>
<td>-</td>
<td>0.00659</td>
<td>0.00652 0.44 0.99</td>
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<tr>
<td>TCA</td>
<td>1.50U</td>
<td>0.00771</td>
<td>0.00771 1.10 1.00</td>
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<tr>
<td></td>
<td>1.83U</td>
<td>0.00760</td>
<td>0.00771 0.92 1.01</td>
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<tr>
<td></td>
<td>2.48U</td>
<td>0.00765</td>
<td>0.00766 1.08 1.00</td>
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<tr>
<td></td>
<td>3.00U</td>
<td>0.00749</td>
<td>0.00760 0.91 1.01</td>
<td></td>
</tr>
</tbody>
</table>

a) $(\beta_{\text{eff}})_{\text{exp}}$ is the experimental result.

b) $\beta_{\text{eff}}$ is the mean value of $\beta_{\text{eff}}$ estimated from the MC calculations.

Table 2.5 Comparisons of $\beta_{\text{eff}}/\Lambda$’s for Critical Facilities

<table>
<thead>
<tr>
<th>Facility</th>
<th>Core Name</th>
<th>$(\beta_{\text{eff}}/\Lambda)_{\text{exp}}$ a)</th>
<th>Power Iteration Method</th>
<th>Wielandt Method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\beta_{\text{eff}}/\Lambda$ b)</td>
<td>RSD [%]</td>
</tr>
<tr>
<td>Godiva</td>
<td>-</td>
<td>$1.10 \times 10^6$</td>
<td>$1.15 \times 10^6$ 0.43 1.05</td>
<td></td>
</tr>
<tr>
<td>TCA</td>
<td>1.50U</td>
<td>219</td>
<td>214 1.12 0.98</td>
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</tr>
<tr>
<td></td>
<td>1.83U</td>
<td>201</td>
<td>195 0.95 0.97</td>
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<td>2.48U</td>
<td>175</td>
<td>171 1.06 0.98</td>
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<tr>
<td></td>
<td>3.00U</td>
<td>161</td>
<td>154 0.92 0.96</td>
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<tr>
<td>STACY</td>
<td>#30</td>
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<td>125.1 1.10 0.99</td>
<td></td>
</tr>
<tr>
<td></td>
<td>#33</td>
<td>116.7</td>
<td>112.8 1.05 0.97</td>
<td></td>
</tr>
</tbody>
</table>

a) $(\beta_{\text{eff}}/\Lambda)_{\text{exp}}$ is the experimental result.

b) $\beta_{\text{eff}}/\Lambda$ is $\beta_{\text{eff}}$ divided by $\Lambda$ which are estimated in the MC calculations.
2.3 Adjoint-Weighted Perturbation Calculations

2.3.1 AWP Algorithm in MC Wielandt Method

By the first-order AWP method [8], a change of the fundamental mode eigenvalue, $\Delta k$, due to a variation of an input parameter such as the number density and the microscopic cross section of an isotope, $\Delta x$, can be expressed as

\[
\Delta k \cong \left\langle \phi_0^+, \Delta H S_0 \right\rangle, \quad (2.36)
\]

where $\Delta H S_0$ is defined by

\[
\Delta H S_0 = \left( \Delta x \frac{\partial H}{\partial x} \right) S_0 = \Delta x \sum_{p=0}^{\infty} \int dE' \int d\Omega' \cdots \int dP_0 \int d\Omega_0 \int d\Omega' \cdots \int dP_0 \int d\Omega_0 \left\{ C_j (r'; E'', \Omega'' \rightarrow E, \Omega) \right\} \left\{ C_j (r'; E'', \Omega'' \rightarrow E, \Omega) \right\} \left\{ K_f (P_{p-1} \rightarrow r', E'', \Omega'') \cdots K_f (P_0 \rightarrow P_1) I (E_0, E_0, r' \rightarrow r_0) \right\} S_0 (r', E_0, \Omega_0); \quad (2.37)
\]

\[
u (r', E_0, \Omega_0 \rightarrow P) = u_f (r'; E'', \Omega'' \rightarrow E, \Omega) + u_k (P_{p-1} \rightarrow r', E'', \Omega'') + \sum_{k=0}^{p-2} u_k (P_k \rightarrow P_{k+1}) + u_r (E_0, \Omega_0, r' \rightarrow r_0), \quad (2.38)
\]

\[
u_f (r; E'', \Omega'' \rightarrow E, \Omega) = \frac{1}{C_f (r; E'', \Omega'' \rightarrow E, \Omega)} \frac{\partial C_f (r; E'', \Omega'' \rightarrow E, \Omega)}{\partial x}, \quad (2.39)
\]
\[ u_k(P_k \rightarrow P_{k+1}) = \frac{1}{K_s(P_k \rightarrow P_{k+1})} \frac{\partial K_s(P_k \rightarrow P_{k+1})}{\partial x}, \quad (2.40) \]

\[ u_T(E_0, \Omega_0; r' \rightarrow r_0) = \frac{1}{T(E_0, \Omega_0; r' \rightarrow r_0)} \frac{\partial T(E_0, \Omega_0; r' \rightarrow r_0)}{\partial x}. \quad (2.41) \]

And the fission collision, transition, scattering collision, and free flight kernels, denoted by \(C_f, K_s, C_s, \) and \(T,\) respectively, are defined as

\[ C_f(r; E', \Omega' \rightarrow E, \Omega) = \frac{\chi(E' \rightarrow E)}{4\pi} \frac{\nu(E') \Sigma_f(r, E')}{\Sigma_i(r, E')}, \quad (2.42) \]

\[ K_s(P' \rightarrow P) = T(E, \Omega; r' \rightarrow r) \cdot C_s(r'; E', \Omega' \rightarrow E, \Omega), \quad (2.43) \]

\[ T(E, \Omega; r' \rightarrow r) = \frac{\Sigma_i(r, E)}{|r - r'|^2} \exp \left[ -\int_0^{r-r'} \Sigma_i(r - s, \frac{r - r'}{|r - r'|}, E) ds \right] \delta \left( \Omega \cdot \frac{r - r'}{|r - r'|} - 1 \right), \quad (2.44) \]

\[ C_s(r'; E', \Omega' \rightarrow E, \Omega) = \sum_{r \in \text{pairs}} \nu_r \frac{\Sigma_i(r'; E', \Omega')}{\Sigma_i(r', E')} f_i(E', \Omega' \rightarrow E, \Omega). \quad (2.45) \]

Then \( \Delta k \) defined by Eq. (2.36) can be calculated in the MC Wielandt calculations as

\[ \overline{\Delta k} = \frac{1}{NML} \sum_{i,j} \sum_{f=0}^{\infty} \sum_{f'=0}^{\infty} (k_e \cdot \Delta x \cdot u^{ij;j'} P' \phi^2_{0,n}(P_{ij;i'+1} f' 0), \quad (2.46) \]

where \( u^{ij;j'} P' \) the \( u^p \) value of Eq. (2.38) calculated at the \( p' \)-th collision of
$j'$-th neutron of $i'$-th generation in $j$-th history at cycle $i$ from which the $j''$-th neutron of $(i'+1)$-th generation is produced. Note that $k_e$ is multiplied because fission neutrons as many as $\left\lceil \nu/k_e + \xi \right\rceil$, where $\left\lfloor x \right\rfloor$ denotes the largest integer not exceeding $x$ and $\xi$ is a uniform random number on the interval of $(0,1)$, from a fission reaction in the MC Wielandt method. In the same way to estimate the adjoint flux of the fission neutron in the $\beta_{eff}$ calculation, then, $\Delta k$ can be calculated by

$$
\Delta k = \frac{1}{N_{ML}} \sum_{i,j} \left( k_e \right) \sum_{l=n}^{\infty} \sum_{p^*} \left( \frac{1}{k_e} W_{ij,j''j'''}^{p^*} \frac{V_{ij,j''j'''}^{p^*}}{\sum_l V_{ij,j''j'''}^{p^*}} \right) \left( k_e \cdot \Delta x \cdot u_{ij,(i'-n),p^*}^{j'} \right),
$$

(2.47)

where $k_e \cdot \Delta x \cdot u_{ij,(i'-n),p^*}^{j'}$ is the direct response of $\Delta k$ at the $p'$-th collision of $j'$-th neutron of $(i'-n)$-th generation in $j$-th history at cycle $i$ from which the progenitor neutron of the $j''$-th neutron of $i'$-th generation in the same history is produced.

### 2.3.2 Numerical Results for Cross Section Perturbation Problems

The MC AWP algorithm of Eq. (2.47) for the Wielandt method has been implemented in McCARD [19] and its validity is examined in $^{235}$U microscopic perturbation problems for the Godiva critical assembly by comparing with results calculated by the direct subtractions and the MC AWP...
method in the conventional power iteration calculations [8]. The conventional MC AWP calculations are performed on 100 active cycles with 100,000 histories per cycle. The MC Wielandt AWP calculations are performed on 100 active cycles with 10,000 histories per cycle with $L$ of 10 which corresponds to the expected number of simulated histories per cycle of 100,000. The adjoint convergence interval, $n$, in both of the AWP calculations is set to 10 which was selected for the AWP calculations in the conventional power iteration method [8]. In order to obtain the reference $\Delta k$ by the direct subtractions, the MC eigenvalue calculations are performed on 1,000 active cycles with 100,000 histories per cycle.

Table 2.6 shows comparisons of $\Delta k$ estimates and their RSDs calculated for five problems with perturbing the $\nu$ values or the capture, fission, elastic scattering or inelastic scattering cross sections of $^{235}\text{U}$ in the whole neutron energy region by 1%. From the table, we can see that the $\Delta k$ values estimated by the proposed method agree well with those from the direct subtraction method and the MC power iteration method within one SD intervals. These results lead to the conclusion that the proposed method for the MC Wielandt calculations can provide equivalent results with the first-order AWP method in the MC power iteration method.
Table 2.6 Comparison of $\Delta k$’s due to $^{235}\text{U}$ cross section perturbations for Godiva

<table>
<thead>
<tr>
<th>Perturbation Type</th>
<th>Method</th>
<th>$\Delta k$ (RSD [%])</th>
<th>Rel. Err. [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu$, 1%</td>
<td>2 independent runs</td>
<td>$9.91400 \times 10^{-3}$ (0.28)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC AWP/ Power Method</td>
<td>$9.91800 \times 10^{-3}$ (0.03)</td>
<td>0.04</td>
</tr>
<tr>
<td></td>
<td>MC AWP/ Wielandt Method</td>
<td>$9.91758 \times 10^{-3}$ (0.24)</td>
<td>0.04</td>
</tr>
<tr>
<td>$(n,\gamma)$, 1%</td>
<td>2 independent runs</td>
<td>$-4.05606 \times 10^{-4}$ (6.86)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC AWP/ Power Method</td>
<td>$-4.04523 \times 10^{-4}$ (0.21)</td>
<td>-0.27</td>
</tr>
<tr>
<td></td>
<td>MC AWP/ Wielandt Method</td>
<td>$-4.05633 \times 10^{-4}$ (0.35)</td>
<td>0.01</td>
</tr>
<tr>
<td>$(n,f\text{is})$, 1%</td>
<td>2 independent runs</td>
<td>$6.56597 \times 10^{-3}$ (0.42)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC AWP/ Power Method</td>
<td>$6.58036 \times 10^{-3}$ (0.07)</td>
<td>0.22</td>
</tr>
<tr>
<td></td>
<td>MC AWP/ Wielandt Method</td>
<td>$6.58120 \times 10^{-3}$ (0.26)</td>
<td>0.23</td>
</tr>
<tr>
<td>$(n,\text{els})$, 1%</td>
<td>2 independent runs</td>
<td>$1.05111 \times 10^{-3}$ (2.57)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC AWP/ Power Method</td>
<td>$1.06183 \times 10^{-3}$ (1.68)</td>
<td>1.02</td>
</tr>
<tr>
<td></td>
<td>MC AWP/ Wielandt Method</td>
<td>$1.07250 \times 10^{-3}$ (1.69)</td>
<td>2.03</td>
</tr>
<tr>
<td>$(n,\text{inels})$, 1%</td>
<td>2 independent runs</td>
<td>$8.28735 \times 10^{-4}$ (3.31)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC AWP/ Power Method</td>
<td>$8.56424 \times 10^{-4}$ (0.98)</td>
<td>3.34</td>
</tr>
<tr>
<td></td>
<td>MC AWP/ Wielandt Method</td>
<td>$8.56163 \times 10^{-4}$ (1.18)</td>
<td>3.31</td>
</tr>
</tbody>
</table>
2.3.3 Application Results for Nuclear Data S/U Analysis

The $k$ uncertainty due to the nuclear covariance data can be estimated by the so-called sandwich equation as [8]

$$\sigma^2[k] \approx \sum_{m,r,g} \sum_{m',r',g'} \text{cov}[x^m_{r,g}, x^{m'}_{r',g'}] \left( \frac{\partial k}{\partial x^m_{r,g}} \right) \left( \frac{\partial k}{\partial x^{m'}_{r',g'}} \right),$$  \hspace{1cm} (2.48)

where $x^m_{r,g}$ is the $g$-th group microscopic cross section of reaction type $r$ of isotope $i$ and $\text{cov}[x^m_{r,g}, x^{m'}_{r',g'}]$ denotes the covariance between $x^m_{r,g}$ and $x^{m'}_{r',g'}$. For this nuclear data S/U analysis, $\text{cov}[x^m_{r,g}, x^{m'}_{r',g'}]$ in the LANL 30-group structure [30] produced by the ERRORR module in NJOY [30] from the covariance file in ENDF/B-VII.1 [28] is used.

The $k$ uncertainties due to the nuclear data uncertainties for the Godiva critical assembly are estimated by Eq. (2.48) using the $k$ sensitivities to the microscopic cross sections, i.e. $\frac{\partial k}{\partial x^m_{r,g}}$ estimated by the MC AWP method in the standard power iteration calculations [8] and the proposed method in the MC Wielandt calculations. The MC perturbation calculations are performed on 100 active cycles with 100,000 histories per cycle for the standard calculations and 10,000 histories per cycle for the Wielandt calculations. The adjoint convergence intervals are set at 10 and $L$ of 10 is applied for the MC Wielandt calculations.

Table 2.7 shows the contributions of $^{235}$U and $^{238}$U cross section
uncertainties to the standard deviation of $k$, $\sigma_{XX}(k)$, in the Godiva problem estimated by the MC AWP method in the MC Wielandt calculations in comparison with those from the standard power iteration method. From the table, we can see that $\sigma_{XX}(k)$ values estimated by the two AWP methods in the Wielandt and the standard calculations are almost identical. Table 2.8 summarizes the memory consumptions for the two MC S/U analyses with changing the number of histories per cycle from 1,000 to 100,000. From the table, we can see that the memory amount required for the MC Wielandt S/U analysis is almost the same as 27~28 Mbytes independently of the number of histories per cycle while those in the conventional method increase proportionally to the number of histories per cycle. And it is notable that the memory size of 28 Mbytes required for the sensitivity tallies in the MC Wielandt S/U analysis is negligibly small comparing to the memory amount of 26.6 Gbytes consumed for the conventional MC S/U analysis when the number of histories per cycle is 100,000.
Table 2.7 Comparison of $k$ uncertainties due to the covariance in $^{235}\text{U}$ and $^{238}\text{U}$

ENDF/B-VII.1 for the Godiva critical assembly

<table>
<thead>
<tr>
<th>Covariance Type</th>
<th>Power Iteration Method $\sigma_{XX}(k)$ (RSD [%])</th>
<th>Wielandt Method $\sigma_{XX}(k)$ (RSD [%])</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unc. due to $^{235}\text{U}$ [%]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\nu, \nu$</td>
<td>0.55 (0.03)</td>
<td>0.55 (0.27)</td>
</tr>
<tr>
<td>$(n,\gamma), (n,\gamma)$</td>
<td>0.89 (0.33)</td>
<td>0.88 (0.39)</td>
</tr>
<tr>
<td>$(n,\gamma), (n,n)$</td>
<td>0.25 (0.95)</td>
<td>0.25 (1.00)</td>
</tr>
<tr>
<td>$(n,\text{fis}), (n,\text{fis})$</td>
<td>0.27 (0.07)</td>
<td>0.27 (0.28)</td>
</tr>
<tr>
<td>$(n,\text{fis}), (n,n)$</td>
<td>-0.05 (0.70)</td>
<td>-0.05 (0.92)</td>
</tr>
<tr>
<td>$(n,n), (n,n)$</td>
<td>0.30 (1.42)</td>
<td>0.30 (1.67)</td>
</tr>
<tr>
<td>$(n,2n), (n,2n)$</td>
<td>0.01 (4.54)</td>
<td>0.01 (4.24)</td>
</tr>
<tr>
<td>Total</td>
<td>1.21 (0.35)</td>
<td>1.20 (0.41)</td>
</tr>
</tbody>
</table>

| Unc. due to $^{238}\text{U}$ [%] |                               |                                          |
| $\nu, \nu$      | 0.10 (0.45)                             | 0.10 (0.68)                                 |
| $(n,\gamma), (n,\gamma)$ | 0.42 (0.15)                         | 0.42 (0.40)                                 |
| $(n,\gamma), (n,n)$   | -0.02 (15.03)                           | -0.02 (19.18)                               |
| $(n,\text{fis}), (n,\text{fis})$ | 0.02 (0.92)                         | 0.02 (1.24)                                 |
| $(n,n), (n,n)$        | 0.02 (36.54)                            | 0.02 (41.42)                                |
| $(n,2n), (n,2n)$      | 0.02 (8.76)                             | 0.02 (11.42)                                |
Table 2.8 Comparisons of required memory amounts for the MC S/U analyses for the Godiva critical assembly

<table>
<thead>
<tr>
<th>Method</th>
<th>The number of histories per cycle</th>
<th>with S/U Analysis</th>
<th>w/o S/U Analysis</th>
<th>Memory for S/U Analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power Iteration Method</td>
<td>1,000</td>
<td>293 MB</td>
<td>25 MB</td>
<td>268 MB</td>
</tr>
<tr>
<td></td>
<td>10,000</td>
<td>2,688 MB</td>
<td>30 MB</td>
<td>2,658 MB</td>
</tr>
<tr>
<td></td>
<td>100,000</td>
<td>26,714 MB</td>
<td>81 MB</td>
<td>26,633 MB</td>
</tr>
<tr>
<td>Wielandt Method</td>
<td>1,000</td>
<td>52 MB</td>
<td>25 MB</td>
<td>27 MB</td>
</tr>
<tr>
<td></td>
<td>10,000</td>
<td>57 MB</td>
<td>30 MB</td>
<td>27 MB</td>
</tr>
<tr>
<td></td>
<td>100,000</td>
<td>109 MB</td>
<td>81 MB</td>
<td>28 MB</td>
</tr>
</tbody>
</table>
Chapter 3. Generalized Perturbation Theory in Monte Carlo Eigenvalue Calculations

3.1 MC GPT Formulation

3.1.1 Sensitivity of a General Tally

In the standard MC eigenvalue calculations [3], a tally estimate, denoted as $Q$, is calculated by summing its corresponding responses over all the sampled fission source neutrons and normalizing it to be an estimate per a fission source neutron as

$$Q = \frac{\langle R_Q^S \rangle}{\langle S \rangle}.$$  \hspace{1cm} (3.1)

The angular brackets $<>$ imply integration over the six-dimensional phase space, $(r,E,\Omega)$. $S$ is the fundamental-mode fission source distribution (FSD) because the tally estimations are assumed to be conducted after the FSD converges. $R_Q$ is a response operator of the tally $Q$ defined by

$$R_Q^S = \int dP' R_Q (P' \rightarrow P) S (P');$$  \hspace{1cm} (3.2)

$$R_Q (P' \rightarrow P) = \sum_{j=0}^{\infty} g_{Q,j} (P) \int d\tau_0 K_{s,j} (P_0 \rightarrow P) T (E',\Omega'; r' \rightarrow \tau_0).$$  \hspace{1cm} (3.3)

where $P$, $P'$ and $P_j$ ($j=0,1,\ldots$) denote the state vectors of neutron in the six-
dimensional phase space, \((r, E, \Omega)\), \((r', E', \Omega')\), and \((r_j, E_j, \Omega_j)\), respectively, and \(g_Q(P)\) is a response function of tally \(Q\) at \(P\). \(K_{s,j}\) is the \(j\)-th scattering kernel defined by

\[
K_{s,0}(P_0 \rightarrow P) = \delta(P_0 - P),
\]

(3.4)

\[
K_{s,1}(P_0 \rightarrow P) = K_s(P_0 \rightarrow P),
\]

(3.5)

\[
K_{s,j}(P_0 \rightarrow P) = \int dP_{j-1} \cdots \int dP_1 K_s(P_{j-1} \rightarrow P) \cdots K_s(P_0 \rightarrow P_1); j = 2, 3, \ldots,
\]

(3.6)

where \(K_s\) is the transition kernel defined by the product of the scattering collision kernel, \(C_s\), and the free flight kernel, \(T\), as Eq. (2.43).

Let us consider a small change of an input parameter \(x\) by \(\Delta x\). The input parameter \(x\) can be a microscopic cross section, a number density of nuclide or etc. This perturbation will lead to the perturbations \(\Delta R_Q\) in \(R_Q\) and \(\Delta S\) in \(S\). Expressing each of the response operator and the FSD of Eq. (3.1) in the perturbed system as the sum of its unperturbed value and its perturbation, the \(Q\) estimate for a perturbed system, \(Q^*\), is written as

\[
Q^* = \frac{\langle (R_Q + \Delta R_Q)(S + \Delta S) \rangle}{\langle S + \Delta S \rangle}.
\]

(3.7)

From Eqs. (3.1) and (3.7), the relative change of the tally \(Q\) estimate can be written as
\[
\frac{\Delta Q}{Q} = \frac{Q^* - Q}{Q} = \frac{\langle S \rangle}{\langle R^*_Q S \rangle} \left[ \frac{\langle R^*_Q S^* \rangle - \langle R^*_Q S \rangle}{\langle S^* \rangle - \langle S \rangle} \right]
\]
\[
= \frac{\langle S \rangle}{\langle R^*_Q S \rangle} \left[ \frac{\langle (R^*_Q + \Delta R^*_Q)(S + \Delta S) \rangle - \langle R^*_Q S \rangle}{\langle S + \Delta S \rangle - \langle S \rangle} \right]
\]
\[
= \frac{1}{1 + \langle \Delta S \rangle / \langle S \rangle} \left[ 1 + \frac{\langle \Delta R^*_Q S \rangle}{\langle R^*_Q S \rangle} + \frac{\langle R^*_Q \Delta S \rangle}{\langle R^*_Q S \rangle} + \frac{\langle \Delta R^*_Q \Delta S \rangle}{\langle R^*_Q S \rangle} \right] - 1.
\]

By neglecting \( \Delta R^*_Q \Delta S \) and taking the first-order Taylor’s expansion in the right hand side (RHS) of Eq.(3.8), one can obtain the relative change of the tally estimate, \( \Delta Q/Q \), expressed as

\[
\frac{\Delta Q}{Q} = \left( 1 - \frac{\langle \Delta S \rangle}{\langle S \rangle} + \frac{\langle \Delta S \rangle^2}{2 \langle S \rangle} \right) \left[ 1 + \frac{\langle \Delta R^*_Q S \rangle}{\langle R^*_Q S \rangle} + \frac{\langle R^*_Q \Delta S \rangle}{\langle R^*_Q S \rangle} + \frac{\langle \Delta R^*_Q \Delta S \rangle}{\langle R^*_Q S \rangle} \right] - 1
\]
\[
= \frac{\langle \Delta R^*_Q S \rangle}{\langle R^*_Q S \rangle} + \left( \frac{\langle R^*_Q \Delta S \rangle}{\langle R^*_Q S \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle} \right).
\]

(3.9)

The first term on the RHS of Eq. (3.9), \( \langle \Delta R^*_Q S \rangle / \langle R^*_Q S \rangle \), reflects the perturbed operator effect (POE) while the last two terms in the () parentheses, \( \langle R^*_Q \Delta S \rangle / \langle R^*_Q S \rangle - \frac{\langle \Delta S \rangle}{\langle S \rangle} \), are named the perturbed source effect (PSE). From the definition of the response operator of Eq. (3.2), one can imagine that the POE includes the indirect effect of the perturbation [16]
on the current neutron generation, known as the intra-generational effect [10],
in the conventional GPT theory for the deterministic S/U analysis as well as
the direct effect while the PSE implies the indirect effect from the next
generations, or the inter-generational effect [10].

3.1.2 Perturbed Operator Effect Formulation

The POE in the section 3.1.1 can be readily calculated by the
conventional MC perturbation techniques such as the DOS or CS method [1].
Using the first-order DOS method, one can show that $\Delta R_\Omega S$ is given by

$$
\Delta R_\Omega S = \left( \frac{\partial R_\Omega}{\partial x} \right) S
$$

= $\Delta x \sum_{j=0}^{\infty} \int d r_0 \int d E_0 \int d \Omega_0 \int d r' \frac{\partial}{\partial x} \left\{ g_\Omega (P) K_{s,j} (P_0 \rightarrow P) T (E_0, \Omega_0; r' \rightarrow r_0) \right\}
\times S (r', E_0, \Omega_0)

= $\Delta x \sum_{j=0}^{\infty} \int d r_0 \int d E_0 \int d \Omega_0 \int d r' u^Q (r', E_0, \Omega_0 \rightarrow P)
\times \left\{ g_\Omega (P) K_{s,j} (P_0 \rightarrow P) T (E_0, \Omega_0; r' \rightarrow r_0) \right\} S (r', E_0, \Omega_0);

(3.10)

$$

u^Q (r', E_0, \Omega_0 \rightarrow P) = u_k (P) + \sum_{k=0}^{j-1} u_k (P_k \rightarrow P_{k+1}) + u_T (E_0, \Omega_0; r' \rightarrow r_0),

(3.11)
\[ u_g(P) = \frac{1}{g_Q(P)} \frac{\partial g_Q(P)}{\partial x}. \] (3.12)

\( u_k \) and \( u_T \) are defined as Eqs. (2.40) and (2.41) [8].

### 3.1.3 Perturbed Source Effect Formulation

Derivation of a MC GPT theory formulation to calculate the PSE starts from the eigenvalue equation [8,13] expressed in an operator notation as

\[ SS\lambda = H; \quad (3.13) \]

\[ HS = \int dP'H(\mathbf{P}' \rightarrow \mathbf{P})S(\mathbf{P}') \] (3.14)

where \( H(\mathbf{P}' \rightarrow \mathbf{P}) \) means the number of first-generation fission neutrons born per unit phase space volume about \( \mathbf{P} \), due to a parent neutron born at \( \mathbf{P}' \). \( \lambda \) is the eigenvalue defined by \( 1/k \).

In the same way to derive Eq. (3.7) from the small input parameter change, the eigenvalue equation for the perturbed system with the perturbations \( \Delta S \), \( \Delta \lambda \), and \( \Delta H \) in \( S \), \( \lambda \), and \( H \), respectively, can be expressed as

\[ S + \Delta S = (\lambda + \Delta \lambda) \cdot (H + \Delta H) \cdot (S + \Delta S). \] (3.15)
By neglecting terms involving products of variations in Eq. (3.15), it can be written as

\[ (I - \lambda H) \Delta S = \Delta \lambda HS + \lambda \Delta HS, \]  

(3.16)

where \( I \) is the identity operator.

In order to express the PSE without explicit expressions of \( \Delta S \) using Eq. (3.16), the generalized adjoint function equation is introduced as

\[ (I - \lambda H^\dagger) \Gamma^\dagger = S^\dagger_{ex}, \]  

(3.17)

where \( \Gamma^\dagger \) denotes the generalized adjoint function and \( H^\dagger \) is the adjoint operator of \( H \) defined by \[8\]

\[ H^\dagger \Gamma^\dagger = \int dP' H(P \rightarrow P') \Gamma^\dagger(P'). \]  

(3.18)

Following the conventional definition of the adjoint source \( S^\dagger_{ex} \) [16] with the changing \( \phi \) derivative term to \( S \) derivative term and using the definitions of \( Q \) and \( R_Q \) of Eqs. (3.1) and (3.2), respectively, \( S^\dagger_{ex} \) can be written as
\[ S^\dagger_{ex} = \frac{1}{\mathcal{Q}} \frac{\partial \langle \mathbf{Q} \rangle}{\partial \mathcal{Q}} - \frac{\partial \langle \mathbf{R}_0 \mathbf{S} \rangle}{\partial \mathcal{S}} - \frac{\partial \langle \mathbf{S} \rangle}{\partial \mathcal{S}} \]

\[ = \frac{1}{\langle \mathbf{R}_0 \mathbf{S} \rangle} \frac{\partial}{\partial \mathcal{S}(\mathbf{P}')} \left\{ \int d\mathbf{P}' \mathbf{R}_0' (\mathbf{P} \rightarrow \mathbf{P}') \mathbf{S} (\mathbf{P}') \right\} - \frac{1}{\langle \mathbf{S} \rangle} \frac{\partial}{\partial \mathcal{S} (\mathbf{P})} \left\{ \int d\mathbf{P} \mathbf{S} (\mathbf{P}) \right\} \]

\[ = \frac{\mathbf{R}^\dagger_0 \tau}{\langle \mathbf{R}_0 \mathbf{S} \rangle} - \frac{\tau}{\langle \mathcal{S} \rangle}; \]

(3.19)

\[ \mathbf{R}^\dagger_0 = \int d\mathbf{P}' \mathbf{R}_0 (\mathbf{P} \rightarrow \mathbf{P}'), \quad (3.20) \]

\( \tau \) denotes a function with all components being 1.

By taking inner products on both sides of Eq. (3.13) with \( \mathbf{\Gamma}^\dagger \) and both sides of Eq. (3.17) with \( \mathbf{S} \), one can obtain a necessary condition for existence of a solution of Eq. (3.17), \( \langle \mathbf{S}, \mathbf{S}^\dagger_{ex} \rangle = 0 \) [15,16].

\[ \langle \mathbf{\Gamma}^\dagger, (\mathbf{I} - \lambda \mathbf{H}) \mathbf{S} \rangle = 0, \quad (3.21) \]

\[ \langle \mathbf{S}, (\mathbf{I} - \lambda \mathbf{H}^\dagger) \mathbf{\Gamma}^\dagger \rangle = \langle \mathbf{S}, \mathbf{S}^\dagger_{ex} \rangle. \quad (3.22) \]

By introducing the definition of \( \mathbf{S}^\dagger_{ex} \) as Eq. (3.19), one can see that the necessary condition is satisfied as

\[ \langle \mathbf{S}^\dagger_{ex}, \mathbf{S} \rangle = \frac{\langle \mathbf{R}^\dagger_0 \tau - \tau, \mathbf{S} \rangle}{\langle \mathbf{R}_0 \mathbf{S} \rangle} - \frac{\langle \tau, \mathbf{R}_0 \mathbf{S} \rangle}{\langle \mathbf{R}_0 \mathbf{S} \rangle} - \frac{\langle \tau, \mathbf{S} \rangle}{\langle \mathbf{S} \rangle} = \frac{\langle \mathbf{R}_0 \mathbf{S} \rangle}{\langle \mathbf{R}_0 \mathbf{S} \rangle} - \frac{\langle \mathbf{S} \rangle}{\langle \mathbf{S} \rangle} = 0. \quad (3.23) \]
Then, by taking inner products on both sides of Eq. (3.16) with $\Gamma^\dagger$ and both sides of Eq. (3.17) introducing Eq. (3.19) with $\Delta S$, two following equations can be obtained as,

$$\langle \Gamma^\dagger, (\mathbf{I} - \lambda \mathbf{H}) \Delta S \rangle = \Delta \lambda \langle \Gamma^\dagger, \mathbf{H} S \rangle + \lambda \langle \Gamma^\dagger, \Delta \mathbf{H} S \rangle, \quad (3.24)$$

$$\langle \Delta S, (\mathbf{I} - \lambda \mathbf{H}^\dagger) \Gamma^\dagger \rangle = \frac{\langle \mathbf{R}_0 \Delta S \rangle}{\langle \mathbf{R}_0 S \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle}. \quad (3.25)$$

By subtracting Eqs. (3.24) and (3.25), and using the property that

$$\langle \Gamma^\dagger, (\mathbf{I} - \lambda \mathbf{H}) \Delta S \rangle = \langle \Delta S, (\mathbf{I} - \lambda \mathbf{H}^\dagger) \Gamma^\dagger \rangle$$

the PSE, defined by

$$\frac{\langle \mathbf{R}_0 \Delta S \rangle}{\langle \mathbf{R}_0 S \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle},$$

can be expressed by

$$\frac{\langle \mathbf{R}_0 \Delta S \rangle}{\langle \mathbf{R}_0 S \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle} = \Delta \lambda \langle \Gamma^\dagger, \mathbf{H} S \rangle + \lambda \langle \Gamma^\dagger, \Delta \mathbf{H} S \rangle \quad (3.26)$$

Further simplifications of Eq. (3.26) is conducted by deriving a physical meaning of the generalized adjoint function for tally $Q$ in the following section.

### 3.1.4 Calculation of the Generalized Adjoint Function

By operating $\sum_{i=0}^n (\lambda \mathbf{H}^\dagger)^i$ on both side of Eq. (3.17), one can
obtain

\[
\sum_{i=0}^{n} \left( \lambda H^\dagger \right)^i \left( I - \lambda H^\dagger \right) \Gamma^\dagger = \sum_{i=0}^{n} \left( \lambda H^\dagger \right)^i S_{ex}^\dagger, \quad (3.27)
\]

The left hand side (LHS) of Eq. (3.27) can be expressed as

\[
\sum_{i=0}^{n} \left( \lambda H^\dagger \right)^i \left( I - \lambda H^\dagger \right) \Gamma^\dagger = \left\{ \Gamma^\dagger - \lambda H^\dagger \Gamma^\dagger \right\} + \left\{ \lambda H^\dagger \Gamma^\dagger - \left( \lambda H^\dagger \right)^2 \Gamma^\dagger \right\} + \cdots + \left\{ \left( \lambda H^\dagger \right)^n \Gamma^\dagger - \left( \lambda H^\dagger \right)^{n+1} \Gamma^\dagger \right\}
\]

\[
= \Gamma^\dagger - \left( \lambda H^\dagger \right)^{n+1} \Gamma^\dagger
\]

\[
= \Gamma^\dagger - c \phi_{0,n+1}^\dagger,
\]

where \( c \) denotes an arbitrary constant and \( \phi_{0,n+1}^\dagger \), defined by Eq.(2.9), denotes a fundamental mode \( k \)-adjoint function with \((n+1)\) convergence interval. By inserting Eq. (3.28) into Eq. (3.27) and moving the \( k \)-adjoint term to the right hand side (RHS), one can obtain the solution of Eq. (3.17) expressed as a sum of a homogeneous solution, \( \phi_0^\dagger \), and a particular solution as

\[
\Gamma^\dagger = c \lim_{n \to \infty} \phi_{0,n+1}^\dagger + \lim_{n \to \infty} \Gamma_{p,n}^\dagger = c \phi_0^\dagger + \Gamma_p^\dagger, \quad (3.29)
\]

where \( \Gamma_p^\dagger \) denotes the particular solution of Eq. (3.17) defined as

\[
\Gamma_p^\dagger = \lim_{n \to \infty} \Gamma_{p,n}^\dagger; \quad (3.30)
\]
If \( c \) is selected by 0, the generalized adjoint can be orthogonal to the fundamental-mode FSD, \( S \) as

\[
\langle \Gamma^\dagger, S \rangle = \lim_{n \to \infty} \sum_{i=0}^{n} \left( \lambda^\dagger \mathbf{H}^\dagger \right)^i S_{\text{ex}}^\dagger \left( \lambda^\dagger \mathbf{H}^\dagger \right)^i S_{\text{ex}} = \sum_{i=0}^{\infty} \left( \lambda^\dagger \mathbf{H}^\dagger \right)^i S_{\text{ex}}^\dagger S_{\text{ex}} = 0. 
\]

(3.32)

The solution of Eq. (3.17), can be obtain more easily by operating \((\mathbf{I} - \lambda \mathbf{H}^\dagger)^{-1}\) in Eq. (3.17), applying the Taylor series expansion for \((\mathbf{I} - \lambda \mathbf{H}^\dagger)^{-1}\) [21], and introducing Eq. (3.19) into the resulting equation as

\[
\Gamma^\dagger = \left( \mathbf{I} - \lambda \mathbf{H}^\dagger \right)^{-1} S_{\text{ex}}^\dagger = \lim_{n \to \infty} \Gamma^\dagger_n 
\]

(3.33)

\[
\Gamma^\dagger_n = \sum_{i=0}^{n} \left( \lambda \mathbf{H}^\dagger \right)^i S_{\text{ex}}^\dagger = \sum_{i=0}^{n} \left( \lambda \mathbf{H}^\dagger \right)^i \left( \frac{\mathbf{R}_0^\dagger \tau}{\langle \mathbf{R}_0 S \rangle} - \frac{\tau}{\langle S \rangle} \right) 
\]

(3.34)

Now, so called the “fundamental-mode contamination free” condition [15] that the generalized adjoint is to be orthogonal to the fundamental-mode FSD, namely, \( \langle \Gamma^\dagger, S \rangle = 0 \), can be derived by using Eqs. (3.33), (3.34), (3.13) and (3.23) and the property of adjoint operator as
\[
\langle \Gamma^\dagger, S \rangle = \left\langle \lim_{n \to \infty} \sum_{i=0}^{n} (\lambda \mathbf{H}^i)^\dagger S_{exi}, S \right\rangle = \sum_{i=0}^{\infty} \left\langle (\lambda \mathbf{H}^i)^\dagger S_{exi}, S \right\rangle = \sum_{i=0}^{\infty} \left\langle S_{exi}, (\lambda \mathbf{H})^i S \right\rangle = \sum_{i=0}^{\infty} \left\langle S_{exi}, S \right\rangle = 0. \tag{3.35}
\]

Because \( \langle \Gamma^\dagger, \mathbf{H}S \rangle = 0 \) by inserting Eq. (3.13) into the contamination free condition of Eq. (3.35) and using Eq. (3.33), the PSE of Eq. (3.26) becomes

\[
\frac{\langle \mathbf{R}_Q \Delta S \rangle}{\langle \mathbf{R}_Q S \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle} = \lim_{n \to \infty} \lambda \langle \Gamma^\dagger_n, \Delta \mathbf{H}S \rangle \tag{3.36}
\]

When \( n \) is large enough to ensure the convergence of \( \Gamma^\dagger_n \), Eq. (3.36) can be approximated as

\[
\frac{\langle \mathbf{R}_Q \Delta S \rangle}{\langle \mathbf{R}_Q S \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle} \approx \lambda \langle \Gamma^\dagger, \Delta \mathbf{H}S \rangle \tag{3.37}
\]

where \( n \) is called the adjoint convergence interval.

From the definitions of adjoint operators, \( \mathbf{H}^\dagger \) of Eq. (3.18) and \( \mathbf{R}_Q^\dagger \) of Eq. (3.20), Eq. (3.34) can be expressed as

\[
\Gamma_n^\dagger \left( \mathbf{P} \right) = \sum_{i=0}^{n} \left\{ \frac{1}{\langle \mathbf{R}_Q S \rangle} \int d\mathbf{P}' \int d\mathbf{P}' R_Q \left( \mathbf{P}' \to \mathbf{P}' \right) \cdot \lambda^i H^i \left( \mathbf{P} \to \mathbf{P}' \right) \right. \\
- \left. \frac{1}{\langle S \rangle} \int d\mathbf{P}' \lambda^i H^i \left( \mathbf{P} \to \mathbf{P}' \right) \right\}. \tag{3.38}
\]
Note that $H'(P \rightarrow P')$ in Eq. (3.38) means the number of the $i$-th generation fission neutrons born per unit phase space volume about $P'$, due to a parent neutron born at $P$ [21]. Then the terms of

$$\int dP' \int dP'R_Q (P' \rightarrow P'') \cdot \lambda^i H^i (P \rightarrow P')$$

and

$$\int dP' \lambda^i H^i (P \rightarrow P')$$

in the RHS of Eq. (3.38) indicate the $Q$-tally contribution produced, and the number of fission source neutrons generated, respectively, at generation $i$ from a source neutron at $P$ in the MC power iteration calculations [3] with the source normalization scheme [23] in which one fission source neutron is enforced to generate one next-generation neutron on average by multiplying the fission neutron generation probability by $\lambda$ or $1/k$ and the weight adjustment of fission source neutrons. Thus $\Gamma_n^{\dagger}$ expressed by Eq. (3.38) means sums of the relative $Q$-tally contributions minus the number of fission neutrons generated from a source neutron at $P$ until the $n$-th MC generations with the source normalization scheme. It is obvious that the values of

$$\int dP' \int dP'R_Q (P' \rightarrow P'') \cdot \lambda^i H^i (P \rightarrow P')$$

and

$$\int dP' \lambda^i H^i (P \rightarrow P')$$

become $\langle R_Q S \rangle$ and $\langle S \rangle$, respectively, as the generation index $i$ approaches infinity because the FSD starting from the point source at $P$ converges to the fundamental-mode FSD, $S$. Accordingly, the value of the relative $Q$-tally contribution minus the number of fission neutrons at generation $i$ converges to zero as $i$ approaches infinity and $\Gamma_n^{\dagger}$ converges to $\Gamma^{\dagger}$ as $n$ approaches infinity. In other words, the generalized adjoint function, $\Gamma^{\dagger}$, represents how much a unit fission source at current phase space influences a $Q$-tally from
now in the MC eigenvalue calculations.

Finally, an insertion of Eq. (3.34) into Eq. (3.37) yields a GPT formulation to estimate the PSE from the MC forward eigenvalue calculations as

\[
\frac{\langle R_Q \Delta S \rangle}{\langle R_Q S \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle} \approx \lambda \sum_{i=0}^{n} \left( \lambda \langle \text{H}^\dagger \rangle \left( \frac{R_Q^\dagger}{<R_Q S>} - \frac{I}{<S>}, \Delta H S \right) \right)
\]

\[
= \lambda \sum_{i=0}^{n} \left[ \frac{\langle \lambda \text{H}^\dagger, \Delta H S \rangle}{< R_Q S>} - \frac{\langle \lambda \text{H}^\dagger, \Delta H S \rangle}{<S>} \right]
\]  

\[
= \lambda \sum_{i=0}^{n} \left[ \frac{\langle R_Q (\lambda \text{H})^\dagger \Delta H S \rangle}{< R_Q S>} - \frac{\langle (\lambda \text{H})^\dagger \Delta H S \rangle}{<S>} \right]
\]  

\[
= \lambda \sum_{i=0}^{n} \left[ \frac{\langle R_Q (\lambda \text{H})^\dagger \Delta H S \rangle}{< R_Q S>} - \frac{\langle (\lambda \text{H})^\dagger \Delta H S \rangle}{<S>} \right]
\]

\[
3.1.5 \text{ Application of the MC GPT Formulation for } k \text{ Sensitivity Estimation}
\]

In this section, we apply the derived MC GPT formulations of Eqs. (3.9) and (3.39) for the \( k \) perturbation estimation. By replacing \( R_Q \) with \( H \) in Eq. (3.9) because \( k = \langle HS \rangle / \langle S \rangle \) for the \( k \) tally from Eq. (3.1), \( \Delta k/k \) can be expressed as

\[
\frac{\Delta k}{k} = \frac{\langle \Delta HS \rangle}{\langle HS \rangle} + \left( \frac{\langle H \Delta S \rangle}{\langle HS \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle} \right).
\]  

(3.40)
Then the PSE in the () parentheses of the RHS of Eq. (3.40) can be written by replacing $R_Q$ with $H$ in Eq. (3.39) as

$$\frac{\langle H\Delta S \rangle}{\langle HS \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle} \approx \lambda \sum_{i=0}^{n} \left[ \frac{\langle H (\lambda H)' \Delta HS \rangle}{\langle HS \rangle} - \frac{\langle (\lambda H)' \Delta HS \rangle}{\langle S \rangle} \right]$$

(3.41)

$$= \lambda \sum_{i=0}^{n} \left[ \frac{\lambda^i \langle H^{i+1} \Delta HS \rangle}{\langle HS \rangle} - \frac{\lambda^i \langle H' \Delta HS \rangle}{\langle S \rangle} \right].$$

Replacing $\langle HS \rangle$ of one of denominators of the RHS of Eq. (3.41) with $\langle S \rangle/\lambda$ by Eq. (3.13) and expanding the summations, one can obtain

$$\frac{\langle H\Delta S \rangle}{\langle HS \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle} \approx \lambda \sum_{i=0}^{n} \left[ \frac{\lambda^{i+1} \langle H^{i+1} \Delta HS \rangle}{\langle S \rangle} - \frac{\lambda^i \langle H' \Delta HS \rangle}{\langle S \rangle} \right]$$

$$= \frac{\lambda}{\langle S \rangle} \left[ \left( \lambda \langle H\Delta HS \rangle - \langle \Delta HS \rangle \right) + \left( \lambda^2 \langle H^2 \Delta HS \rangle - \lambda \langle H\Delta HS \rangle \right) + \cdots + \left( \lambda^{n+1} \langle H^{n+1} \Delta HS \rangle - \lambda^n \langle H^n \Delta HS \rangle \right) \right]$$

$$= \lambda \sum_{i=0}^{n+2} \frac{\lambda^{i+1} \langle H^{i+1} \Delta HS \rangle}{\langle S \rangle} - \lambda \frac{\langle \Delta HS \rangle}{\langle S \rangle}.$$

(3.42)

Inserting of Eq. (3.42) into Eq. (3.40) and using Eq. (3.13) and the relation that $\lambda = 1/k$, the $k$ perturbation is expressed as
\[ \frac{\Delta k}{k} = \frac{\langle \Delta HS \rangle}{\langle HS \rangle} + \lambda^{n+2} \frac{\langle H^{n+1} \Delta HS \rangle}{\langle S \rangle} - \lambda \frac{\langle \Delta HS \rangle}{\langle S \rangle} \]

\[ = \frac{\langle \Delta HS \rangle}{k \langle S \rangle} + \frac{1}{k^{n+2}} \frac{\langle H^{n+1} \Delta HS \rangle}{\langle S \rangle} - \frac{\langle \Delta HS \rangle}{k \langle S \rangle} \]

\[ = \frac{1}{k^{n+2}} \frac{\langle H^{n+1} \Delta HS \rangle}{\langle S \rangle}. \] (3.43)

When the FSD is normalized to satisfy \( \langle S \rangle = 1 \) as the AWP method for the \( k \) perturbation estimation is derived [8], \( \Delta k \) can be written as

\[ \Delta k = \frac{1}{k^{n+1}} \langle H^{n+1} \Delta HS \rangle \] (3.44)

By comparing Eq. (3.44) with the \( \Delta k \) estimation equation derived from the IFP concept [17], i.e. \( \Delta k = \frac{1}{k^n} \langle H^n \Delta HS \rangle \) [8], one can see that the two equations are the same except that the indices of \( (n+1) \) in Eq. (3.44) become \( n \) because the adjoint convergence interval \( n \) in Ref. [8] is defined by the generation number at which the fission neutrons due to a source neutron is counted for the \( k \)-adjoint estimation.

3.1.6 Equivalence of the AWP Method and the First-Order DOS/FSP Method

Shim and Kim [8] have ever proved that the MC AWP method is
equivalent to the conventional first-order DOS/FSP method for the $\Delta k$
estimation. Here we prove that the derived MC GPT method for a MC general
tally calculated by Eqs. (3.9) and (3.39) is equivalent to the first-order
DOS/FSP method in the same procedure as Ref. [8].

The standard MC power iteration method for the eigenvalue
equation of Eq. (3.13) updates the FSD cycle-by-cycle (or generation-by-
generation) as

$$S_i = \frac{1}{k_{i-1}} HS_{i-1};$$  \hspace{1cm} (3.45)

$$k_{i-1} = \langle HS_{i-1} \rangle,$$  \hspace{1cm} (3.46)

where $i$ is the cycle index and $S_\ell (\ell = i$ or $i-1)$ is the FSD used for the cycle
$\ell$ MC simulations. $k_i$ is the eigenvalue estimate at cycle $i$.

The $Q$ value estimated from the MC simulations at the $i$-th cycle,
$Q_i$, can be written, from Eq. (3.1), as

$$Q_i = \frac{\langle R_Q S_i \rangle}{\langle S_i \rangle} = \langle R_Q S_i \rangle.$$  \hspace{1cm} (3.47)

For the second equality of Eq. (3.47), $\langle S_i \rangle$ is set to unity for
simplicity of derivations reflecting the source normalization scheme [23].

From Eq. (3.47), the derivative of $Q$ with respect to the input
parameter $x$ can be expressed as

$$\frac{\partial Q_i}{\partial x} = \left< \frac{\partial R_{q}}{\partial x} S_i \right> + \left< R_{q} \frac{\partial S_i}{\partial x} \right>.$$  (3.48)

In the first-order DOS/FSP method, the first and second terms of the RHS of Eq. (3.48) are calculated by the first-order DOS method [1] and the FSP method [2], respectively.

Inserting Eq. (3.46) into Eq. (3.45) and taking derivatives with respect to $x$ on the both sides of the resulting equation, $\partial S_i/\partial x$ can be expressed as

$$\frac{\partial S_i}{\partial x} = \frac{1}{k_{i-1}} \left[ \frac{\partial H}{\partial x} S_{i-1} + H \frac{\partial S_{i-1}}{\partial x} - S_i \left( \left< \frac{\partial H}{\partial x} S_{i-1} \right> + \left< H \frac{\partial S_{i-1}}{\partial x} \right> \right) \right].$$  (3.49)

Applying the successive insertions of Eq. (3.49) until $\partial S_{i-n-1}/\partial x$ which is assumed to be zero and setting $S_i$’s and $k_i$’s to be the fundamental-mode FSD and eigenvalue, i.e. $S$ and $k$, respectively, in the MC tally estimation cycles, namely, active cycles, Eq. (3.49) can be written by [8]

$$\frac{\partial S_i}{\partial x} = \frac{1}{k} \left[ \sum_{j=0}^{n} \left( \frac{H}{k} \right)^j \frac{\partial H}{\partial x} S - S \left( \sum_{j=0}^{n} \left( \frac{H}{k} \right)^j \frac{\partial H}{\partial x} S \right) \right].$$  (3.50)

Then inserting Eq. (3.50) into Eq. (3.48) and using the condition that $S_i = S$ in the active cycles, one can obtain
\[
\frac{\partial Q_j}{\partial x} = \left< \frac{\partial R_{Qj}}{\partial x} S \right> + \frac{1}{k} R_{Qj} \left[ \sum_{j=0}^{n} \left( \frac{H}{k} \right)^j \frac{\partial H}{\partial x} S - S \left( \frac{H}{k} \right)^j \frac{\partial H}{\partial x} S \right]
\]

\[
= \left< \frac{\partial R_{Qj}}{\partial x} S \right> + \frac{1}{k} \sum_{j=0}^{n} \frac{R_{Qj} \left( \frac{H}{k} \right)^j \frac{\partial H}{\partial x} S}{\left< R_{Qj} S \right>} - \frac{\left< R_{Qj} S \right>}{k} \sum_{j=0}^{n} \left( \frac{H}{k} \right)^j \frac{\partial H}{\partial x} S
\] (3.51)

Because \( \Delta Q_i = (\frac{\partial Q_i}{\partial x}) \Delta x \) and \( \Delta H = (\frac{\partial H}{\partial x}) \Delta x \) in the first-order perturbation theory, by multiplying \( \Delta x / Q_i \) on the both sides of Eq. (3.51), the mean value of the relative \( Q \) perturbation calculated by the first-order DOS/FSP method at each cycle becomes

\[
\frac{\Delta Q_i}{Q_i} = \frac{\left< R_{Qj} S \right>}{\left< R_{Qj} S \right>} + \frac{1}{k} \sum_{j=0}^{n} \left[ \frac{\left< R_{Qj} \left( \frac{H}{k} \right)^j \Delta H S \right>}{\left< R_{Qj} S \right>} - \left< \left( \frac{H}{k} \right)^j \Delta H S \right> \right] \quad (3.52)
\]

By comparing the MC GPT formulations of Eqs. (3.9) and (3.39) with Eq. (3.52) with the condition that \( \left< S_j \right> = 1 \) in the standard MC eigenvalue calculations, one can observe that the perturbation of a general tally \( Q \) estimated by the first-order DOS/FSP is the same as that by the developed MC AWP method.
3.2 Generalized Adjoint Function Estimation in the MC Wielandt Calculations

In the MC Wielandt eigenvalue calculations [18], the cycle-by-cycle FSD update are conducted as Eq. (2.16) while the generation-by-generation FSD update are Eqs. (2.17) and (2.18) [13]. By applying the generation-by-generation FSD update of Eq. (2.17) obtained in the MC Wielandt calculations, the PSE, Eq. (3.39), can be rewritten as

\[
\frac{\left\langle R_Q \Delta S \right\rangle}{\left\langle R_Q S \right\rangle} - \frac{\left\langle \Delta S \right\rangle}{\left\langle S \right\rangle} \approx \frac{1}{k} \sum_{i=0}^{n} \left( \frac{k_i}{k} \right)^i \left[ \frac{\left\langle R_Q \left( \frac{H}{k} \right)^i \Delta HS \right\rangle}{\left\langle R_Q S \right\rangle} - \frac{\left\langle \left( \frac{H}{k} \right)^i \Delta HS \right\rangle}{\left\langle S \right\rangle} \right],
\]

(3.53)

where \( i' \) denotes a generation index mentioned in Section 2.1. Because Eq. (3.53) is independent of cycle and history index, the PSE can be estimate within 1 history’s simulation in the MC Wielandt calculations.
3.3 Numerical Results

3.3.1 Numerical Results for Infinite Homogeneous Two-Group Problems

The generalized sensitivity estimation method in the MC Wielandt method has been implemented in McCARD [19] and tested for infinite homogeneous problems characterized by two-group cross-sections given by Table 3.1 [22] where those infinite multiplication factors, \( k_{\text{inf}} \), are set to 0.9, 1.0 or 1.1.

Relative changes of the total fission reaction rate due to a 1.0\% perturbation of the first-group fission cross section are calculated by the proposed method. The MC Wielandt calculations are performed varying \( L \) by changing the \( k_e \) value according to Eq. (2.20) at a fixed value of the adjoint convergence interval, \( n \), of 10 or changing \( n \) with fixing \( L \) by 50 for the infinite homogeneous problem with \( k_{\text{inf}} \) of 0.9. The eigenvalue calculations are performed on 1,000 active cycles with changing the number of histories per cycle, \( M \), to make the effective number of fission neutrons, i.e. \( M \times L \), constant as about 10,000,000. Table 3.2 shows 6 pairs of \((M, k_e)\) values corresponding to \( L \) values.

Tables 3.3 and 3.4 show comparisons of the POE and the PSE calculated by the proposed method with analytic solutions. In the table, RSD means the relative standard deviation. From the table, the POE results of the proposed method have differences of about 0.060\% with the analytic
solutions, \((\Delta R_f/R_f)_{\text{ref}}\). These differences are caused from the first-order approximation of \(\Delta RS\) in the first equality of Eq. (3.10). From the table, we can see that the POE and PSE results estimated by the proposed method agree well with the analytic solution applied the first-order approximation within 95% confidence intervals.

Table 3.5 shows the comparisons of the relative fission reaction rate changes \((\Delta R_f/R_f)\) estimated in the MC power iteration method and the MC Wielandt method for the two-group problems with \(k_{\text{inf}}\) of 0.9, 1.0 or 1.1. The all calculations are performed on 1,000 active cycles with \(n\) of 10. The MC power iteration calculations are performed with 10,000,000 histories per cycle and the MC Wielandt calculations are performed with 200,000 histories per cycle and \(L\) of 50 to make the effective number of fission neutrons about 10,000,000. The used \(k_e\) values are shown as Table 3.2. From Table 3.5, we can see that the results estimated by the MC Wielandt method agree well with those from the MC power method within 95% confidence intervals. Although the MC results have the differences with the analytic solutions shown as Tables 3.3 and 3.4, these results lead to the conclusion that the proposed method for the MC Wielandt calculations can provide equivalent results with the method in the MC power iteration method.
Table 3.1 Two-group cross sections for the infinite homogeneous problem

<table>
<thead>
<tr>
<th>Cross Section</th>
<th>First Gr. (g=1)</th>
<th>Second Gr. (g=2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma_{tg}$</td>
<td>0.50</td>
<td>0.50</td>
</tr>
<tr>
<td>$\Sigma_{fg}$</td>
<td>0.025</td>
<td>0.175</td>
</tr>
<tr>
<td>$\nu_g$</td>
<td>2.00</td>
<td>2.00</td>
</tr>
<tr>
<td>$\Sigma_{s1g}$</td>
<td>0.10</td>
<td>0.00</td>
</tr>
</tbody>
</table>
| $\Sigma_{s2g}$| 0.181905 for $k_{inf}$ of 0.9  
                | 0.247143 for $k_{inf}$ of 1.0  
                | 0.312987 for $k_{inf}$ of 1.1  | 0.20 |
| $\chi_{1g}$  | 0.8            | 0.5             |
| $\chi_{2g}$  | 0.2            | 0.5             |

Table 3.2 The number of histories per cycle ($M$) and the $k_e$ value for the two-group problem in the MC Wielandt calculations

<table>
<thead>
<tr>
<th>$L$</th>
<th>$M$ a)</th>
<th>$k_{inf}$</th>
<th>$k_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>5,000,000</td>
<td>1.80000</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>2,000,000</td>
<td>1.12500</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>1,000,000</td>
<td>1.00000</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>500,000</td>
<td>0.9</td>
<td>0.94737</td>
</tr>
<tr>
<td>30</td>
<td>333,333</td>
<td>1.0</td>
<td>0.93103</td>
</tr>
<tr>
<td>50</td>
<td>200,000</td>
<td>1.1</td>
<td>0.91837</td>
</tr>
<tr>
<td>50</td>
<td>200,000</td>
<td>1.0</td>
<td>1.02041</td>
</tr>
<tr>
<td>50</td>
<td>200,000</td>
<td>1.1</td>
<td>1.12245</td>
</tr>
</tbody>
</table>

a) The number of histories per cycle
Table 3.3 Comparisons of the relative fission reaction rate changes ($\Delta R_f/R_f$) for the two-group problem with $k_{inf}$ of 0.9 in the MC Wielandt calculations varying $L$ with the fixed $n$ of 10

<table>
<thead>
<tr>
<th>Terms</th>
<th>Analytic Solution</th>
<th>$L$</th>
<th>McCARD (RSD [%])</th>
<th>Relative Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$(\Delta R_f/R_f)_{ref}$</td>
<td>$(\Delta R_f/R_f)_{ref,1st}^a$</td>
<td></td>
<td>$(\Delta R_f/R_f)_{ref}$</td>
</tr>
<tr>
<td>Perturbed Operator Effect</td>
<td>$4.86813 \times 10^{-4}$</td>
<td>$4.87117 \times 10^{-4}$</td>
<td>2</td>
<td>$4.87102 \times 10^{-4}$ (0.002)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5</td>
<td>$4.87109 \times 10^{-4}$ (0.002)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>10</td>
<td>$4.87108 \times 10^{-4}$ (0.002)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>20</td>
<td>$4.87137 \times 10^{-4}$ (0.002)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>30</td>
<td>$4.87122 \times 10^{-4}$ (0.002)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>50</td>
<td>$4.87119 \times 10^{-4}$ (0.002)</td>
</tr>
<tr>
<td>Perturbed Source Effect</td>
<td>$-1.15919 \times 10^{-4}$</td>
<td>$-1.15992 \times 10^{-4}$</td>
<td>2</td>
<td>$-1.15448 \times 10^{-4}$ (0.872)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5</td>
<td>$-1.15963 \times 10^{-4}$ (0.122)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>10</td>
<td>$-1.15991 \times 10^{-4}$ (0.082)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>20</td>
<td>$-1.15952 \times 10^{-4}$ (0.068)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>30</td>
<td>$-1.16021 \times 10^{-4}$ (0.064)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>50</td>
<td>$-1.16095 \times 10^{-4}$ (0.062)</td>
</tr>
</tbody>
</table>

$a$) $(\Delta R_f/R_f)_{ref,1st}$ is the analytic solution calculated by using the 1st-order approximations, $\Delta R_o S = \Delta x \left( \partial R_o / \partial x \right) S$ and $\Delta H S = \Delta x \left( \partial H / \partial x \right) S$.
Table 3.4 Comparisons of the relative fission reaction rate changes ($\Delta R_f / R_f$) for the two-group problem with $k_{inf}$ of 0.9 in the MC Wielandt calculations varying $n$ with the fixed $L$ of 50

<table>
<thead>
<tr>
<th>Terms</th>
<th>Analytic Solution</th>
<th>$n$</th>
<th>McCARD (RSD [%])</th>
<th>Relative Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$(\Delta R_f / R_f)_{ref}$</td>
<td>$(\Delta R_f / R_f)_{ref,1st}$</td>
<td></td>
<td>$(\Delta R_f / R_f)_{ref}$</td>
</tr>
<tr>
<td>Perturbed Operator Effect</td>
<td>4.86813×10^{-4}</td>
<td>4.87117×10^{-4}</td>
<td>2</td>
<td>4.87119×10^{-4}  (0.002)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5</td>
<td>4.87119×10^{-4}  (0.002)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>10</td>
<td>4.87119×10^{-4}  (0.002)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>20</td>
<td>4.87119×10^{-4}  (0.002)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>30</td>
<td>4.87119×10^{-4}  (0.002)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>50</td>
<td>4.87119×10^{-4}  (0.002)</td>
</tr>
<tr>
<td>Perturbed Source Effect</td>
<td>-1.15919×10^{-4}</td>
<td>-1.15992×10^{-4}</td>
<td>2</td>
<td>-1.15643×10^{-4} (0.025)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5</td>
<td>-1.16011×10^{-4} (0.042)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>10</td>
<td>-1.16095×10^{-4} (0.062)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>20</td>
<td>-1.15987×10^{-4} (0.093)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>30</td>
<td>-1.16021×10^{-4} (0.125)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>50</td>
<td>-1.15832×10^{-4} (0.197)</td>
</tr>
</tbody>
</table>

a) $(\Delta R_f / R_f)_{ref,1st}$ is the analytic solution calculated by using the 1st-order approximations, $\Delta R_f S = \Delta x \left( \partial R_f / \partial x \right) S$ and $\Delta H S = \Delta x \left( \partial H / \partial x \right) S$.
Table 3.5 Comparisons of the relative fission reaction rate changes ($\Delta R_f/R_f$) estimated in the MC power iteration method and the MC Wielandt method for the two-group problems

<table>
<thead>
<tr>
<th>$k_{inf}$</th>
<th>Terms</th>
<th>$(\Delta R_f/R_f)_{ref}$</th>
<th>MC power iteration method</th>
<th>MC Wielandt method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\Delta R_f/R_f$</td>
<td>Relative Error</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(SD [%])</td>
<td>(%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\Delta R_f/R_f$</td>
<td>Relative Error</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(SD [%])</td>
<td>(%)</td>
</tr>
<tr>
<td>0.9</td>
<td>Total</td>
<td>3.70894×10^{-4}</td>
<td>3.71098×10^{-4} (0.014)</td>
<td>0.055</td>
</tr>
<tr>
<td></td>
<td>POE</td>
<td>4.86813×10^{-4}</td>
<td>4.87110×10^{-4} (0.002)</td>
<td>0.061</td>
</tr>
<tr>
<td></td>
<td>PSE</td>
<td>-1.15919×10^{-4}</td>
<td>-1.16012×10^{-4} (0.046)</td>
<td>0.080</td>
</tr>
<tr>
<td>1.0</td>
<td>Total</td>
<td>3.15705×10^{-4}</td>
<td>3.15910×10^{-4} (0.015)</td>
<td>0.065</td>
</tr>
<tr>
<td></td>
<td>POE</td>
<td>3.74495×10^{-4}</td>
<td>3.74735×10^{-4} (0.002)</td>
<td>0.064</td>
</tr>
<tr>
<td></td>
<td>PSE</td>
<td>-5.87898×10^{-5}</td>
<td>-5.88247×10^{-5} (0.082)</td>
<td>0.059</td>
</tr>
<tr>
<td>1.1</td>
<td>Total</td>
<td>2.63321×10^{-4}</td>
<td>2.63411×10^{-4} (0.017)</td>
<td>0.034</td>
</tr>
<tr>
<td></td>
<td>POE</td>
<td>2.82800×10^{-4}</td>
<td>2.82979×10^{-4} (0.002)</td>
<td>0.063</td>
</tr>
<tr>
<td></td>
<td>PSE</td>
<td>-1.94786×10^{-5}</td>
<td>-1.95680×10^{-5} (0.224)</td>
<td>0.459</td>
</tr>
</tbody>
</table>
3.3.2 Numerical Results for Cross Section Perturbation Problems

The proposed GPT-based MC AWP method is examined in $^{235}$U microscopic perturbation problems for the Godiva critical assembly by comparing with results calculated by the direct subtractions and the MC AWP method in the conventional power iteration calculations [8]. The conventional MC AWP calculations are performed on 1,000 active cycles with 10,000,000 histories per cycle. The MC Wielandt AWP calculations are performed on 1,000 active cycles with 200,000 histories per cycle with $L$ of 50 which corresponds to the expected number of simulated histories per cycle of 10,000,000. The generalized adjoint convergence interval, $n$, in both of the AWP calculations is set to 10 which was selected for the AWP calculations in the conventional power iteration method [8]. In order to obtain the reference values by the direct subtractions, the MC eigenvalue calculations are performed on 1,000 active cycles with 10,000,000 histories per cycle.

Tables 3.6 and 3.7 shows comparisons of the relative errors of the fission reaction rate estimates ($\Delta R_f/R_f$) and those of the absorption reaction rate estimates ($\Delta R_a/R_a$) with their RSDs calculated for five problems with perturbing the $\nu$ values or the capture, fission, elastic scattering or inelastic scattering cross sections of $^{235}$U in the whole neutron energy region by 1%. From the tables, we can see that the $\Delta R_f/R_f$ values and the $\Delta R_a/R_a$ values estimated by the proposed method agree well with those from the direct subtraction method and the MC power iteration method within 2 SD intervals.
at most. These results lead to the conclusion that the proposed method for the MC Wielandt calculations can provide equivalent results with the direct subtraction method and the GPT-based first-order AWP method in the MC power iteration method.
Table 3.6 Comparison of the relative fission reaction rate changes ($\Delta R_f/R_f$) due to $^{235}$U cross section perturbations for Godiva

<table>
<thead>
<tr>
<th>Perturbation Type</th>
<th>Method</th>
<th>$\Delta R_f/R_f$ [%] (SD [%])</th>
<th>Rel. Err. [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu$, 1%</td>
<td>2 independent runs</td>
<td>0.00060 (237.231)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Power Method</td>
<td>0.00010 (11.672)</td>
<td>-83.952</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Wielandt Method</td>
<td>0.00009 (17.060)</td>
<td>-84.123</td>
</tr>
<tr>
<td>$(n,\gamma)$, 1%</td>
<td>2 independent runs</td>
<td>-0.04226 (3.346)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Power Method</td>
<td>-0.04250 (0.003)</td>
<td>0.573</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Wielandt Method</td>
<td>-0.04250 (0.004)</td>
<td>0.575</td>
</tr>
<tr>
<td>$(n,f_{is})$, 1%</td>
<td>2 independent runs</td>
<td>0.64822 (0.219)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Power Method</td>
<td>0.65028 (0.002)</td>
<td>0.318</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Wielandt Method</td>
<td>0.65028 (0.002)</td>
<td>0.319</td>
</tr>
<tr>
<td>$(n,\text{els})$, 1%</td>
<td>2 independent runs</td>
<td>0.10917 (1.296)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Power Method</td>
<td>0.10913 (0.024)</td>
<td>-0.038</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Wielandt Method</td>
<td>0.10915 (0.025)</td>
<td>-0.021</td>
</tr>
<tr>
<td>$(n,\text{inel})$, 1%</td>
<td>2 independent runs</td>
<td>0.09147 (1.547)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Power Method</td>
<td>0.09059 (0.016)</td>
<td>-0.954</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Wielandt Method</td>
<td>0.09061 (0.018)</td>
<td>-0.932</td>
</tr>
</tbody>
</table>
Table 3.7 Comparison of the relative absorption reaction rate changes ($\Delta R_a/R_a$) due to $^{235}\text{U}$ cross section perturbations for Godiva

<table>
<thead>
<tr>
<th>Perturbation Type</th>
<th>Method</th>
<th>$\Delta R_a/R_a$ [&quot;] (SD [&quot;]%)</th>
<th>Rel. Err. [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu$, 1%</td>
<td>2 independent runs</td>
<td>-0.00014 (1045.893)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Power Method</td>
<td>0.00014 (14.574)</td>
<td>-205.024</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Wielandt Method</td>
<td>0.00010 (30.402)</td>
<td>-172.491</td>
</tr>
<tr>
<td>$(n,\gamma)$, 1%</td>
<td>2 independent runs</td>
<td>0.87278 (0.163)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Power Method</td>
<td>0.87363 (0.000)</td>
<td>0.097</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Wielandt Method</td>
<td>0.87363 (0.000)</td>
<td>0.097</td>
</tr>
<tr>
<td>$(n,fis)$, 1%</td>
<td>2 independent runs</td>
<td>-0.45581 (0.310)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Power Method</td>
<td>-0.45711 (0.004)</td>
<td>0.284</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Wielandt Method</td>
<td>-0.45712 (0.005)</td>
<td>0.287</td>
</tr>
<tr>
<td>$(n,els)$, 1%</td>
<td>2 independent runs</td>
<td>0.17277 (0.819)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Power Method</td>
<td>0.17365 (0.028)</td>
<td>0.509</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Wielandt Method</td>
<td>0.17361 (0.030)</td>
<td>0.484</td>
</tr>
<tr>
<td>$(n,inels)$, 1%</td>
<td>2 independent runs</td>
<td>0.35979 (0.394)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Power Method</td>
<td>0.36032 (0.007)</td>
<td>0.147</td>
</tr>
<tr>
<td></td>
<td>MC GPT/Wielandt Method</td>
<td>0.36038 (0.008)</td>
<td>0.164</td>
</tr>
</tbody>
</table>
3.3.3 Memory Consumption for Nuclear Data S/U Analysis

The memory efficiency is demonstrated in the S/U analysis for the TMI-1 pin cell problem in the OECD benchmarks for uncertainty analysis modeling (UAM) for design, operation, and safety analysis of LWRs [20]. The specifications of the problem is given in Figure 3.1.

The fission reaction rate \( R_f \) uncertainty due to the nuclear covariance data can be estimated by the sandwich equation as Eq. (2.48) with the substitution of \( R_f \) for \( k \). For this nuclear data S/U analysis, \( \text{cov}[X_{r,g}^m, X_{r,g}^{m'}] \) in the LANL 30-group structure [30] produced by the ERRORR module in NJOY [30] from the covariance file in ENDF/B-VII.1 [28] is used.

The fission reaction rate uncertainty due to the nuclear data uncertainties for the Godiva critical assembly is estimated by Eq. (2.48) using the fission reaction rate sensitivities to the microscopic cross sections, i.e. \( \frac{\partial R_f}{\partial x_{r,g}^m} \) estimated by the GPT-based MC AWP method in the standard power iteration calculations and the proposed method in the MC Wielandt calculations. The MC perturbation calculations are performed on 1,000 active cycles with 100,000 histories per cycle for the standard calculations and 2,000 histories per cycle for the Wielandt calculations. The generalized adjoint convergence intervals are set at 10 and \( L \) of 50 is applied for the MC Wielandt calculations.

Table 3.8 shows the contributions of \( ^{235}U \) cross section uncertainties
to the standard deviation of the fission reaction rate, $\sigma_{XX}(Q)$, in the TMI-PWR unit cell benchmark estimated by the GPT-based MC AWP method in the MC Wielandt calculations in comparison with those from the standard power iteration method. From the table, we can see that $\sigma_{XX}(Q)$ values estimated by the two AWP methods in the Wielandt and the standard calculations are almost identical. Table 3.9 summarizes the memory consumptions for the two MC S/U analyses with changing the number of histories per cycle from 1,000 to 100,000. From the table, we can see that the memory amount required for the MC Wielandt S/U analysis is almost the same as about 93 Mbytes independently of the number of histories per cycle while those in the conventional method increase proportionally to the number of histories per cycle. And it is notable that the memory size of 93 Mbytes required for the sensitivity tallies in the MC Wielandt S/U analysis is negligibly small comparing to the memory amount of 27218 Mbytes consumed for the conventional MC S/U analysis when the number of histories per cycle is 100,000.
Figure 3.1 Configuration of TMI-PWR unit cell

<table>
<thead>
<tr>
<th>Color</th>
<th>Cell</th>
<th>Length [cm]</th>
<th>Temperature [K]</th>
<th>Material</th>
<th>Density [g/cm³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Red</td>
<td>Fuel pin</td>
<td>D_{fuel}=0.9391</td>
<td>900.0</td>
<td>UO₂ (4.85 w/o)</td>
<td>10.283</td>
</tr>
<tr>
<td>White</td>
<td>Air gap</td>
<td>D_{gap}=0.9582</td>
<td>600.0</td>
<td>He</td>
<td>0.001</td>
</tr>
<tr>
<td>Black</td>
<td>Cladding</td>
<td>D_{clad}=1.0928</td>
<td>600.0</td>
<td>Zircaloy-4</td>
<td>6.55</td>
</tr>
<tr>
<td>Blue</td>
<td>Moderator</td>
<td>Pitch=1.4427</td>
<td>562.0</td>
<td>H₂O</td>
<td>0.7484</td>
</tr>
</tbody>
</table>
Table 3.8 Comparison of the fission reaction rates ($R_f$) uncertainties due to the covariance in $^{235}$U and $^{238}$U ENDF/B-VII.1 for the TMI-1 PWR unit cell problem

<table>
<thead>
<tr>
<th>Covariance Type</th>
<th>Power Iteration Method $S_{XX}(R_f)$</th>
<th>Wielandt Method $S_{XX}(R_f)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Unc. due to $^{235}$U [%]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(n,$\gamma$), (n,$\gamma$)</td>
<td>0.220</td>
<td>0.219</td>
</tr>
<tr>
<td>(n,$\gamma$), (n,fis)</td>
<td>0.075</td>
<td>0.075</td>
</tr>
<tr>
<td>(n,$\gamma$), (n,n)</td>
<td>-0.006</td>
<td>0.002</td>
</tr>
<tr>
<td>(n,fis), (n,fis)</td>
<td>0.082</td>
<td>0.082</td>
</tr>
<tr>
<td>(n,fis), (n,n)</td>
<td>0.004</td>
<td>0.003</td>
</tr>
<tr>
<td>(n,n), (n,n)</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>Unc. due to $^{238}$U [%]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(n,$\gamma$), (n,$\gamma$)</td>
<td>0.299</td>
<td>0.299</td>
</tr>
<tr>
<td>(n,$\gamma$), (n,n)</td>
<td>-0.018</td>
<td>-0.018</td>
</tr>
<tr>
<td>(n,2n), (n,2n)</td>
<td>0.012</td>
<td>0.013</td>
</tr>
<tr>
<td>(n,fis), (n,fis)</td>
<td>0.012</td>
<td>0.012</td>
</tr>
<tr>
<td>(n,n), (n,n)</td>
<td>0.006</td>
<td>0.007</td>
</tr>
<tr>
<td>(n,n), (n,n')</td>
<td>-0.009</td>
<td>-0.010</td>
</tr>
<tr>
<td>(n,n'), (n,n')</td>
<td>0.088</td>
<td>0.089</td>
</tr>
<tr>
<td>Total</td>
<td>0.404</td>
<td>0.404</td>
</tr>
</tbody>
</table>
Table 3.9 Comparisons of required memory amounts for the MC S/U analyses with the covariance in $^{235}$U and $^{238}$U from ENDF/B VII.1 for the TMI-1 PWR unit cell benchmark

<table>
<thead>
<tr>
<th>Method</th>
<th>The number of histories per cycle</th>
<th>with S/U Analysis</th>
<th>w/o S/U Analysis</th>
<th>Memory for S/U Analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Power Iteration Method</strong></td>
<td>1,000</td>
<td>343.7 MB</td>
<td>72.0 MB</td>
<td>271.7 MB</td>
</tr>
<tr>
<td></td>
<td>10,000</td>
<td>2803.9 MB</td>
<td>90.3 MB</td>
<td>2713.6 MB</td>
</tr>
<tr>
<td></td>
<td>100,000</td>
<td>27498.1 MB</td>
<td>280.1 MB</td>
<td>27218.0 MB</td>
</tr>
<tr>
<td><strong>Wielandt Method</strong></td>
<td>1,000</td>
<td>165.9 MB</td>
<td>72.1 MB</td>
<td>93.8 MB</td>
</tr>
<tr>
<td></td>
<td>10,000</td>
<td>186.8 MB</td>
<td>93.1 MB</td>
<td>93.7 MB</td>
</tr>
<tr>
<td></td>
<td>100,000</td>
<td>376.6 MB</td>
<td>283.2 MB</td>
<td>93.4 MB</td>
</tr>
</tbody>
</table>
Chapter 4. Conclusions

In this thesis, a GPT formulation adequate to estimate sensitivities of general MC tallies such as volume flux, reaction rates, etc., not the form of a ratio of linear or bilinear functions was derived by making the best of the fact that MC standard tally estimates are normalized to be per a fission source neutron in the MC eigenvalue calculations. The perturbation of the response normalized by the fission source was expressed as the sum of the perturbed operator effect (POE) and perturbed source effect (PSE). The POE could be estimated by using the existing differential operator sampling (DOS) method, while the PSE could be obtained from the generalized adjoint-weighted perturbation (AWP) method. From the generalized adjoint function equation with an adjoint source for the MC general tally, the physical meaning of the generalized adjoint function for a MC tally is derived.

Next, it is shown that the derived MC GPT formulation can be used to estimate the $k$ sensitivity by comparing with the MC AWP $k$-sensitivity estimation formulation. As the equivalence of the AWP method and the first-order DOS/FSP for the $k$ sensitivity estimation, it is proven that the derived GPT formulation is equivalent to the first-order DOS/FSP for the general tally.

In order to overcome the memory consumption problem in the MC AWP methods, we present a new adjoint estimation method of which the memory usage is irrelevant to the numbers of histories per cycle by applying
the IFP concept for the MC Wielandt calculations.

The new algorithms for the GPT-based AWP calculations in the MC Wielandt method are implemented in a Seoul National University MC code, McCARD and its validity is demonstrated in infinite homogeneous two-group problem and Godiva critical assembly. As the results of the infinite homogenous two-group problem agree well with the analytic solution, it is demonstrated that the newly implemented method works well. From the numerical results in Godiva problem, we can see that the $\Delta k$, $\Delta R_f/R_f$ and $\Delta R_a/R_a$ values estimated by the proposed method agree well with those from the direct subtraction method and the MC power iteration method within 2 SD intervals at most. These results lead to the conclusion that the proposed method for the MC Wielandt calculations can provide equivalent results with the direct subtraction method and the GPT-based first-order AWP method in the MC power iteration method.

Also, the memory efficiency is demonstrated in the S/U analysis for the TMI-1 pin cell problem in the OECD benchmarks for uncertainty analysis modeling (UAM) for design, operation, and safety analysis of LWRs. From the comparison of the nuclear data S/U analyses in , it is demonstrated that the memory amounts to store the sensitivity estimates in the proposed method become negligibly small compared to the GPT-based AWP method in the MC power iteration method.
Reference


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초록

민감도/불확도 분석, 원자로 안전평가 또는 핵자료 평가와 같은 분야에서 입력인자에 대한 유효증배계수 $k$ 및 출력분포 등의 원자로 성능 파라미터들의 민감도 계수는 하나의 주요한 인자이다. 앞선 연구에서는 몬테카로 입자수송계산을 통한 $k$의 민감도를 측정을 위해 반복 핵분열 확률 개념을 적용한 몬테카로 수반핵가중 섭동법이 개발되어 핵자료 불확도에 의한 $k$의 불확도 측정에 성공적으로 적용되었다.

최근에는 일반섭동이론을 기반으로 몬테카로 수반핵가중 섭동법을 선행 또는 쌍선형 핵반응률의 비율에 대한 민감도 계수 측정에 적용하기 위한 여러 연구들이 수행되고 있다. 이에 반해 본 논문에서는 선행 또는 쌍선형 핵반응률의 형태가 아닌 중성자 속, 핵반응률과 같은 일반적인 몬테카로의 탈리에 대한 민감도 측정에 적용할 수 있는 일반섭동이론 수식을 유도하였다. 또한 몬테카로의 일반적인 탈리에 대한 일반 수반해 방정식을 통해 일반 수반해의 물리적 의미를 도출하였다. 새롭게 유도된 몬테카로 일반
섭동이론 수식은 $k$에 대하여 적용할 경우 기존에 개발된 $k$의 민감도 측정을 위한 수반해가중 섭동법과 동일함을 보였으며, 기존 핵분열중성자원의 섭동을 고려한 1차 미분연산자 샘플링법과 동등함을 증명하였다.

그러나 반복 핵분열 확률 개념을 적용한 기존의 $k$에 대한 몬테카로 수반해가중 섭동법 뿐 아니라 새롭게 제안된 일반섭동이론 기반 몬테카로 수반해가중 섭동법 또한 수반해가 수렴하는 동안의 중성자 가계도 및 수반해 가중 텔리에 필요한 정보들을 저장해야 하기 때문에, 핵자료에 대한 민감도/불확도 분석에 사용할 경우 매우 많은 컴퓨터 메모리공간을 필요로 한다. 여기에 필요한 메모리 공간을 줄이기 위해 본 논문에서는 몬테카로 빌란트법을 적용한 수반해 계산법을 제안하였다. 새롭게 제안된 수반해 계산법은 한 개의 히스토리 모사를 통해 여러 세대의 중성자를 모사하며 수반해를 계산할 수 있기 때문에 중성자 가계도를 저장할 필요가 없어 수반해 계산에 필요한 메모리가 크게 줄어들게 된다.
새로 제안된 빌란트법을 적용한 수반해 가중 동특성인자 계산법 및 수반해가중 섭동계산법은 서울대학교에서 개발한 몬테 칼로 코드인 McCARD에 장착되었고, 임계 시설 문제 및 가압경수로 핀셜문제를 통해 검증이 되었다. 또한 빌란트법을 적용한 민감도/불확도 분석시 기존 방법에 비해 매우 적은 컴퓨터 메모리 공간을 사용하는 것을 확인하였다.

주요어:

일반섭동이론

몬테칼로 고유치 계산

민감도/불확도 분석

수반해 가중 섭동법

몬테칼로 빌란트법

학번 : 2009-23191