

Development of an Adjoint Flux Calculation Technique for Exact Perturbation Theory in Monte Carlo Code MCS

Yunki Jo¹, and Deokjung Lee^{1,2*}

¹Department of Nuclear Engineering, Ulsan National Institute of Science and Technology, 50 UNIST-gil, Eonyang-eup, Ulju-gun, Ulsan, 44919, Republic of Korea

²Advanced Nuclear Technology and Services, 406-21 Jonga-ro, Jung-gu, Ulsan, 44429, Republic of Korea

Abstract. A calculation technique computing the adjoint flux of perturbed system is developed for the exact perturbation theory in Monte Carlo transport. By using a correlated sampling and iterated fission probability methods together, the adjoint flux of perturbed system is calculated during a forward Monte Carlo simulation of an unperturbed system. In the method, no additional particle simulation is required to compute the adjoint flux of perturbed system. The exact perturbation method is implemented in the Monte Carlo code MCS. The results of perturbation method for k -eigenvalue change are compared against differential operator sampling, adjoint-weighted perturbation, and direct perturbation methods for the Godiva benchmark and PLUS7 fuel assembly.

1 Introduction

The Monte Carlo method [1] is widely used for nuclear reactor analysis with the increase of computing power. It simulates particle histories by using pseudo-random numbers to achieve statistically converged results. It can use high-fidelity physics phenomena through stochastic particle simulations. In the Monte Carlo method, the exact model of problem geometry can be used with continuous energy cross section data. The reactor analysis requires computing the effect of small changes in input parameter. The number of perturbed reactor states can be more than a thousand depending on the range of interests. Unfortunately, the Monte Carlo method is too slow to run every perturbed reactor state. Additionally, the Monte Carlo method struggles to compute the effect of small perturbations due to its statistical uncertainty.

The Monte Carlo perturbation theory is used to solve this problem. By using perturbation methods, which are the differential operator sampling (DOS) and correlated sampling (CS) methods [2], it is possible to estimate the k -eigenvalue change in a perturbed system during a forward Monte Carlo calculation of an unperturbed system. However, it was observed that the neglect of perturbed fission source effect may cause a large error. To improve its accuracy, Nagaya and Mori presented perturbation methods calculating the perturbed source effect explicitly [3, 4]. Additionally, the first-order adjoint-weighted perturbation (AWP)

* Corresponding author: deokjung@unist.ac.kr

method was developed [5–9]. The AWP method uses the adjoint flux of unperturbed system as a weight function to consider a fission source perturbation effect implicitly. However, those conventional first-order perturbation methods still have a limitation of first-order accuracy. Therefore, the error of k -eigenvalue change estimated by the conventional first-order perturbation method becomes large for the perturbed system where product of perturbations is significant. It is because the product of perturbations is assumed to be negligible during a derivation of the conventional first-order perturbation methods. Examples showing large errors due to large perturbations are presented in Section 3. To overcome this problem, Truchet et al. [10, 11], and Tuya and Nagaya [12] presented perturbation methods based on the exact perturbation theory (EPT). However, their approach requires additional particle simulations in the perturbed system for $L+1$ generations, where L is the number of latent generations, to compute the adjoint flux of the perturbed system. The computational time increases by a factor of $L+2$ due to the computational burden of additional particle simulations.

In this work, a calculation technique named as a perturbation-included iterated fission probability (PIFP) method is developed to overcome the limitation of first-order accuracy in conventional perturbation methods and the computational burden of conventional exact perturbation (EP) methods. The PIFP method computes the adjoint flux of perturbed system for the EPT in Monte Carlo transport. The EP method is implemented in the Monte Carlo code MCS. In Section 2, the conventional perturbation theory and the PIFP method are presented. In Section 3, the results of perturbation methods for k -eigenvalue change are presented for the Godiva benchmark and PLUS7 fuel assembly.

2 Methodology and Computational Code

2.1 Perturbation Theory

In the perturbation theory, two reactor systems are considered. One is the unperturbed system (system 1), and the other is the perturbed system (system 2) where there is a change in input parameters. The steady-state Boltzmann transport equations for the unperturbed and perturbed systems are expressed as Eq. (1) and Eq. (2), respectively, with a subscript representing the system index.

$$(\mathbf{I} - \lambda_1 \mathbf{H}_1) S_1 = 0, \quad (1)$$

$$(\mathbf{I} - \lambda_2 \mathbf{H}_2) S_2 = 0, \quad (2)$$

where S is the fission source density, \mathbf{H} is the fission operator, and λ is the eigenvalue. Eq. (2) can be re-written as follows by using $\Delta\lambda = \lambda_2 - \lambda_1$, $\Delta\mathbf{H} = \mathbf{H}_2 - \mathbf{H}_1$, and $\Delta S = S_2 - S_1$.

$$(\mathbf{I} - (\lambda_1 + \Delta\lambda)(\mathbf{H}_1 + \Delta\mathbf{H}))(S_1 + \Delta S) = 0. \quad (3)$$

By taking inner product of Eq. (3) with the adjoint flux of unperturbed system ϕ_1^* and neglecting terms having product of perturbations through first-order approximation, one can obtain the first-order AWP equation for k -eigenvalue as follows:

$$\frac{\Delta k}{k_2} \cong \frac{\langle \phi_1^*, \lambda_1 \Delta \mathbf{H} S_1 \rangle}{\langle \phi_1^*, \lambda_1 (\mathbf{H}_1 + \Delta \mathbf{H}) S_1 \rangle}, \quad (4)$$

where the bracket denotes an integration over the phase space, which are position, direction, and energy. The first-order AWP equation also can be expressed as follows [5]:

$$\frac{\Delta k}{k_2} \cong - \frac{\langle \phi_1^*, (\Delta \mathbf{L} - \lambda_1 \Delta \mathbf{F}) \phi_1 \rangle}{\langle \phi_1^*, \lambda_1 (\mathbf{F}_1 + \Delta \mathbf{F}) \phi_1 \rangle}, \quad (5)$$

where \mathbf{L} and \mathbf{F} are the net loss and net fission production operators, respectively. ϕ is the neutron flux. The first-order AWP method has a limitation in its accuracy due to the first-order approximation used to neglect terms having product of perturbations. On the other hand, the EPT allows to estimate the perturbed k-eigenvalue exactly without applying any approximations. The EPT equation for k-eigenvalue is expressed as follows by taking inner product of Eq. (3) with the adjoint flux of perturbed system ϕ_2^* .

$$\frac{\Delta k}{k_2} = \frac{\langle \phi_2^*, \lambda_1 \Delta \mathbf{H} S_1 \rangle}{\langle \phi_2^*, \lambda_1 (\mathbf{H}_1 + \Delta \mathbf{H}) S_1 \rangle}. \quad (6)$$

The unknown term on the right-hand side of Eq. (6) is the adjoint flux of perturbed system ϕ_2^* which can be calculated by the PIFP method.

2.2 Perturbation-included Iterated Fission Probability Method

In the PIFP method, no additional particle simulation is required to compute the adjoint flux of perturbed system. By using CS and iterated fission probability (IFP) methods together, the adjoint flux of perturbed system is calculated during a forward Monte Carlo calculation of unperturbed system. In this section, the algorithm of PIFP method is presented. The $\mathbf{H}S$ term in Eq. (1) can be expressed as follows in terms of kernels:

$$\int d\mathbf{P}_0 \mathbf{H}(\mathbf{P}_0 \rightarrow \mathbf{P}) S(\mathbf{P}_0) = \sum_{n=0}^{\infty} \int d\mathbf{P}'_n \cdots \int d\mathbf{P}_0 C_f(\mathbf{P}'_n \rightarrow \mathbf{P}) T_{n+1}(\mathbf{P}_n \rightarrow \mathbf{P}'_n) \cdot C_{s,n}(\mathbf{P}'_{n-1} \rightarrow \mathbf{P}_n) T_n(\mathbf{P}_{n-1} \rightarrow \mathbf{P}'_{n-1}) \cdots C_{s,1}(\mathbf{P}'_0 \rightarrow \mathbf{P}_1) T_1(\mathbf{P}_0 \rightarrow \mathbf{P}'_0) S(\mathbf{P}_0), \quad (7)$$

where C_f is the fission collision kernel, T_i is the i -th transport kernel, $C_{s,i}$ is the i -th scattering collision kernel, and n is the number of scattering collisions before fission collision. In the Monte Carlo calculation, each kernel of Eq. (7) is defined as follows:

$$T_i(\mathbf{P}'_{i-1} \rightarrow \mathbf{P}'_{i-1}) = T_i(E_{i-1}, \boldsymbol{\Omega}_{i-1}; \mathbf{r}_{i-1} \rightarrow \mathbf{r}_i) = \exp(-\Sigma_t(\mathbf{r}_{i-1}, E_{i-1}) \ell_i), \quad (8)$$

$$C_{s,i}(\mathbf{P}'_{i-1} \rightarrow \mathbf{P}_i) = C_{s,i}(\mathbf{r}_i; E_{i-1}, \boldsymbol{\Omega}_{i-1} \rightarrow E_i, \boldsymbol{\Omega}_i) = \Sigma_s(\mathbf{r}_i, E_{i-1}) f_s(E_{i-1}, \boldsymbol{\Omega}_{i-1} \rightarrow E_i, \boldsymbol{\Omega}_i), \quad (9)$$

$$C_f(\mathbf{P}'_n \rightarrow \mathbf{P}) = C_f(\mathbf{r}_{n+1}; E_n, \boldsymbol{\Omega}_n \rightarrow E, \boldsymbol{\Omega}) = \frac{\chi(E_n \rightarrow E)}{4\pi} \nu(\mathbf{r}_{n+1}, E_n) \Sigma_f(\mathbf{r}_{n+1}, E_n), \quad (10)$$

where Σ_t , Σ_s and Σ_f are the total, scattering and fission cross sections, respectively. ℓ_i is the i -th neutron flight distance, $f_s(E_{i-1}, \boldsymbol{\Omega}_{i-1} \rightarrow E_i, \boldsymbol{\Omega}_i)$ is the scattering probability that a neutron with incident energy E_{i-1} and incident direction $\boldsymbol{\Omega}_{i-1}$ is scattered to the outgoing energy E_i and outgoing direction $\boldsymbol{\Omega}_i$. χ is the fission neutron energy spectrum, and ν is the average number of fission neutrons produced from a fission reaction. In the current implementation, the perturbation effect of scattering probability f_s is assumed to be neglected.

The $\Delta\mathbf{HS}$ term can be calculated by using one of DOS and CS methods. The DOS method computes the target response change by using Taylor series. By applying the first-order Taylor series of $\Delta\mathbf{HS}$ for Δx change in the input parameter x and simplifying phase space notations, the $\Delta\mathbf{HS}$ term is expressed as follows:

$$\Delta\mathbf{HS} = \sum_{n=0}^{\infty} \int d\mathbf{P}'_n \cdots \int d\mathbf{P}_0 \Delta x \left[\frac{1}{C_f} \frac{\partial C_f}{\partial x} + \frac{1}{T_{n+1}} \frac{\partial T_{n+1}}{\partial x} + \sum_{i=1}^n \left(\frac{1}{C_{s,i}} \frac{\partial C_{s,i}}{\partial x} + \frac{1}{T_i} \frac{\partial T_i}{\partial x} \right) \right] \cdot C_f T_{n+1} \prod_{i=1}^n (C_{s,i} T_i) S. \quad (11)$$

Eq. (11) represents that a derivative of fission operator \mathbf{H} can be estimated by scoring derivatives of each kernel, which are expressions in square brackets, during a forward Monte Carlo calculation of the unperturbed system. In the CS method, it is assumed that neutron histories in the perturbed system follows the neutron tracks in the unperturbed system. $\Delta\mathbf{HS}$ is computed by scoring the ratio of perturbed and unperturbed kernels as follows:

$$\Delta\mathbf{HS} = \left(\frac{\mathbf{H}_2}{\mathbf{H}_1} - 1 \right) \mathbf{H}_1 S = \sum_{n=0}^{\infty} \int d\mathbf{P}'_n \cdots \int d\mathbf{P}_0 \left[\frac{C_{f,2} T_{n+1,2} \prod_{i=1}^n (C_{s,i,2} T_{i,2})}{C_{f,1} T_{n+1,1} \prod_{i=1}^n (C_{s,i,1} T_{i,1})} - 1 \right] \cdot C_{f,1} T_{n+1,1} \prod_{i=1}^n (C_{s,i,1} T_{i,1}) S. \quad (12)$$

The numerator and denominator in square brackets consist of perturbed kernels and unperturbed kernels, respectively. The expression in square brackets is used as a weight adjusting factor to represent particle weights of the perturbed system during a forward Monte Carlo calculation of unperturbed system. The CS method has the advantage that no approximation is applied unlike the DOS method using n -th order Taylor series. However, as it was mentioned in the reference [2], the CS method should be carefully used since it may cause a large or unbounded variance of perturbed k -eigenvalue depending on the amount of perturbation. The result showing the large variance is presented in Section 3.

The adjoint flux of unperturbed system can be estimated as follows by using the power method and IFP interpretation [5, 7].

$$\phi_{1,n}^*(\mathbf{P}_0) = C \int d\mathbf{P}_n \frac{1}{k_1^n} H_1^n(\mathbf{P}_0 \rightarrow \mathbf{P}_n) \phi_0^*(\mathbf{P}_0), \quad (13)$$

where n is treated as the number of latent generations in the IFP method, and C is an arbitrary constant. $\phi_{1,n}^*$ is the n -th iterative solution of adjoint flux in the unperturbed system from the initial guess ϕ_0^* . As the number of latent generations increases, the iterative solution converges to the true solution of adjoint flux ϕ_1^* . By assuming $\phi_0^*(\mathbf{P}_0) = S(\mathbf{P}_0)$ in Eq. (13) as a reference [7], it can be expressed as

$$\phi_{1,n}^*(\mathbf{P}_0) = C \int d\mathbf{P}_n \cdots \int d\mathbf{P}_1 \prod_{i=0}^{n-1} \left[\frac{1}{k_1^{(i)}} H_1^{(i)}(\mathbf{P}_i \rightarrow \mathbf{P}_{i+1}) \right] S(\mathbf{P}_0), \quad (14)$$

where $k_1^{(i)}$ and $H_1^{(i)}$ are the k -eigenvalue and fission operator of the unperturbed system in i -th generation from the fission source density at phase space \mathbf{P}_0 , respectively. Eq. (14) represents the adjoint flux at phase space \mathbf{P}_0 is proportional to the number of progeny fission neutrons generated in the n -th generation from a unit source at \mathbf{P}_0 . The adjoint flux at phase space \mathbf{P}_0 in the perturbed system $\phi_{2,n}^*(\mathbf{P}_0)$ is expressed as

$$\phi_{2,n}^*(\mathbf{P}_0) = C' \int d\mathbf{P}_n \cdots \int d\mathbf{P}_1 \prod_{i=0}^{n-1} \left[\frac{1}{k_2^{(i)}} H_2^{(i)}(\mathbf{P}_i \rightarrow \mathbf{P}_{i+1}) \right] S(\mathbf{P}_0). \quad (15)$$

Eq. (15) also can be expressed as

$$\phi_{2,n}^*(\mathbf{P}_0) = C'' \int d\mathbf{P}_n \cdots \int d\mathbf{P}_1 \prod_{i=0}^{n-1} \left[\frac{1}{k_1^{(i)}} \left(H_1^{(i)}(\mathbf{P}_i \rightarrow \mathbf{P}_{i+1}) + \Delta H^{(i)}(\mathbf{P}_i \rightarrow \mathbf{P}_{i+1}) \right) \right] S(\mathbf{P}_0), \quad (16)$$

where $C'' = C' \prod_{i=0}^{n-1} (k_1^{(i)} / k_2^{(i)})$. Eq. (16) represents the adjoint flux of the perturbed system can be calculated during a forward Monte Carlo calculation of the unperturbed system by performing a cumulative product of perturbed fission operator ($\mathbf{H}_1 + \Delta\mathbf{H}$) during latent generations. The arbitrary constant C'' is unknown because it contains the k -eigenvalue of the perturbed system. However, it can be neglected since it will be cancelled out from the adjoint flux multiplied both in the numerator and denominator of Eq. (14). By substituting Eq. (12) and Eq. (16) into Eq. (6), one can obtain the estimation of k -eigenvalue change for the EP method as follows:

$$\left(\frac{\Delta k}{k_2} \right)^{(i+n)} = \frac{\sum_j \left\{ \prod_{l=0}^{n-1} \left[\frac{1}{k_1^{(i+1+l)}} \left(\mathbf{H}_1^{(i+1+l)} + \Delta\mathbf{H}^{(i+1+l)} \right) \right] \cdot \frac{1}{k_1^{(i)}} \Delta\mathbf{H}^{(i)} S_j^{(i)} \right\}}{\sum_j \left\{ \prod_{l=0}^{n-1} \left[\frac{1}{k_1^{(i+1+l)}} \left(\mathbf{H}_1^{(i+1+l)} + \Delta\mathbf{H}^{(i+1+l)} \right) \right] \cdot \frac{1}{k_1^{(i)}} \left(\mathbf{H}_1^{(i)} + \Delta\mathbf{H}^{(i)} \right) S_j^{(i)} \right\}}, \quad (17)$$

where the superscript represents the cycle index, j is a particle index, and l is the number of latent generations in IFP method. $(\Delta k/k_2)^{(i+n)}$ is the estimation of k -eigenvalue change calculated at cycle $(i+n)$. $k_1^{(i+1+l)}$ is the k -eigenvalue of unperturbed system calculated at cycle $(i+1+l)$. $\mathbf{H}_1^{(i)}$ and $\Delta\mathbf{H}^{(i)}$ are the fission operator of the unperturbed system and fission operator change at cycle (i) . $S_j^{(i)}$ is the j -th particle in cycle (i) .

2.3 Monte Carlo Code MCS

A Monte Carlo code MCS has been developed at Ulsan National Institute of Science and Technology (UNIST) since 2013 [13]. Both criticality and fixed-source modes are available in MCS for reactor analysis and shielding calculation. The criticality and multi-cycle depletion calculation capability of MCS has been verified and validated by solving various benchmark problems including the BEAVRS benchmark [13], and about 300 cases from the International Criticality Safety Benchmark Experimental Problems (ICSBEP) [14].

3 Perturbation Results for k -eigenvalue

This section presents numerical results of perturbation methods to estimate the k -eigenvalue change. A Monte Carlo code MCS is used with continuous energy ENDF/B-VII.1 nuclear data library. Godiva benchmark and PLUS7 fuel assembly are used for perturbation calculations. The reference result, which is the direct perturbation (DP) result, is calculated by running two independent inputs for unperturbed and perturbed systems. Results of four perturbation methods, which are DOS, AWP(DOS), AWP(CS) and EP, are compared against the reference DP results. The AWP(DOS), AWP(CS) and EP methods are implemented as Eq. (5), Eq. (4), and Eq. (6), respectively.

3.1 Godiva Benchmark

Godiva is a highly enriched uranium sphere of 8.7407 cm radius. The density of uranium is 18.74 g/cm³, and it consists of 1.02 wt% U-234, 93.71 wt% U-235, and 5.27 wt% U-238. For the Godiva benchmark, three density perturbation cases are considered as follows: 1) Density perturbation in the outermost shell region, 2) Density perturbation in the center sphere region, and 3) Density perturbation in the global region. The Godiva sphere is divided into 10 equi-volume regions. In the outermost shell region case, the density perturbation is applied only to the outermost shell region of 0.3016 cm thickness. In the center sphere region case, the density perturbation is applied to the center sphere of 4.0571 cm radius. In the global region case, the density perturbation is applied to the whole region of Godiva. The reference calculations for DP are performed by using 40 active cycles with 10 million histories per a cycle. The calculations for perturbation methods are performed by using 40 active cycles with 40 million histories per a cycle. The k -eigenvalue of base case is 0.99980 ± 0.00002 .

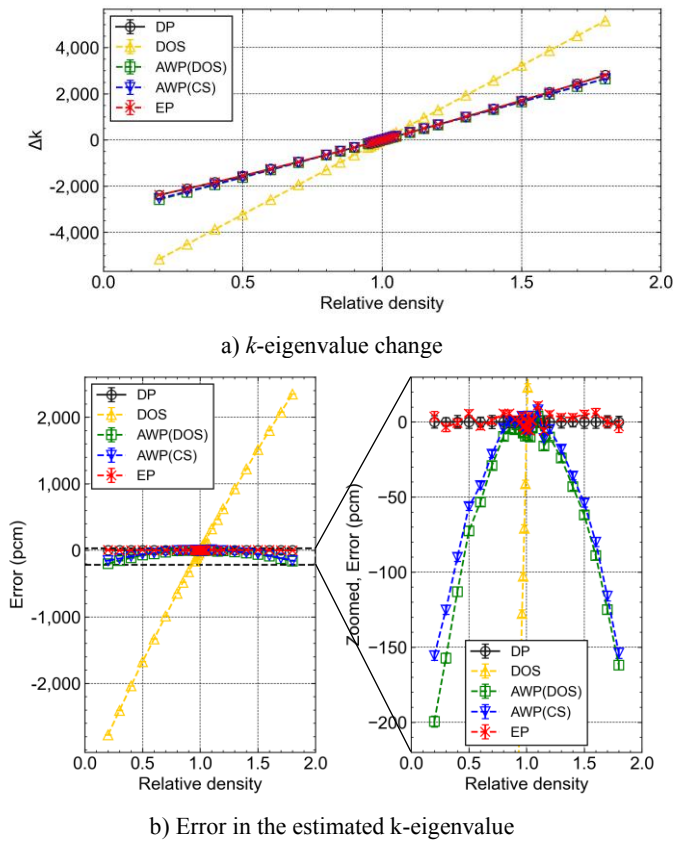


Fig. 1. Results of perturbation methods for local density change in the shell region of Godiva

The local density change ranging 0.2–1.8 of nominal density is considered in the outermost shell region. Figure 1 shows the results of perturbation methods for local density change in the outermost shell region of Godiva. The error bars represent $1-\sigma$ statistical errors. The k -eigenvalue changes -2400–2800 pcm depending on the local density change. The maximum error of DOS method is larger than 2000 pcm due to the neglect of the perturbed source effect. The AWP(DOS) and AWP(CS) methods shows maximum errors less than 200 pcm. On the other hand, the EP method shows the most accurate results with errors less than 10 pcm. This is because EP method is based on the EPT.

The local density change ranging 0.2–1.8 of nominal density is considered in the center sphere region. Figure 2 shows the results of perturbation methods for local density change in the center sphere region of Godiva. As it was observed in the outermost shell region case, large errors are observed in the DOS method due to the neglect of the perturbed source effect. The maximum errors of AWP(DOS) and AWP(CS) methods are -4083 pcm and -6219 pcm, respectively. Those large errors of AWP cases are due to the neglect of terms having product of perturbations. On the other hand, the maximum error of EP method is 397 pcm. For the density change ranging 0.2–1.5 of nominal density, the maximum error of EP method is 13 pcm. For cases having a density perturbation larger than 0.5 of nominal density, the statistical uncertainty of EP method becomes large or unbounded. As it was mentioned in the reference [2], this is due to the limitation of CS method using the same neutron track histories for the estimation of the perturbed system. In this work, no reset condition is applied for the CS method to prevent the large variance.

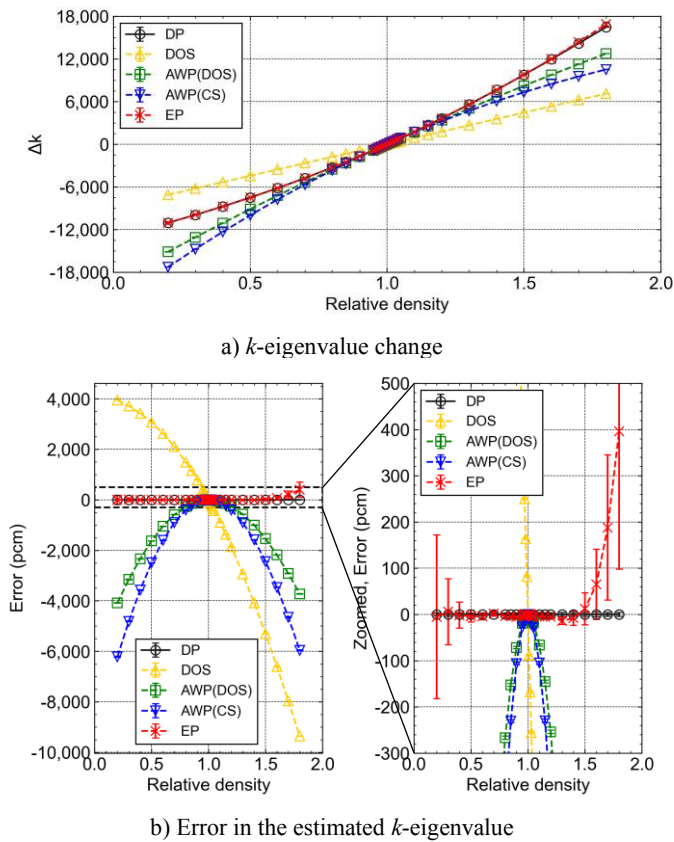


Fig. 2. Results of perturbation methods for local density change in center sphere region of Godiva

The global density change ranging 0.2–1.8 of nominal density is considered in the global region. Figure 3 shows the results of perturbation methods for global density change in Godiva. The maximum errors of DOS, AWP(DOS), and AWP(CS) methods are 14981, 7485 and -12002 pcm, respectively. The maximum error of EP method is -1203 pcm for the case having 1.8 of nominal density. For the density change ranging 0.5–1.4 of nominal density, the maximum error of EP method is 11 pcm. As it was observed in Figure 2, the statistical uncertainty of EP method becomes large or unbounded for the cases having a density perturbation larger than 0.5 of nominal density. The error of EP method for those cases also increases.

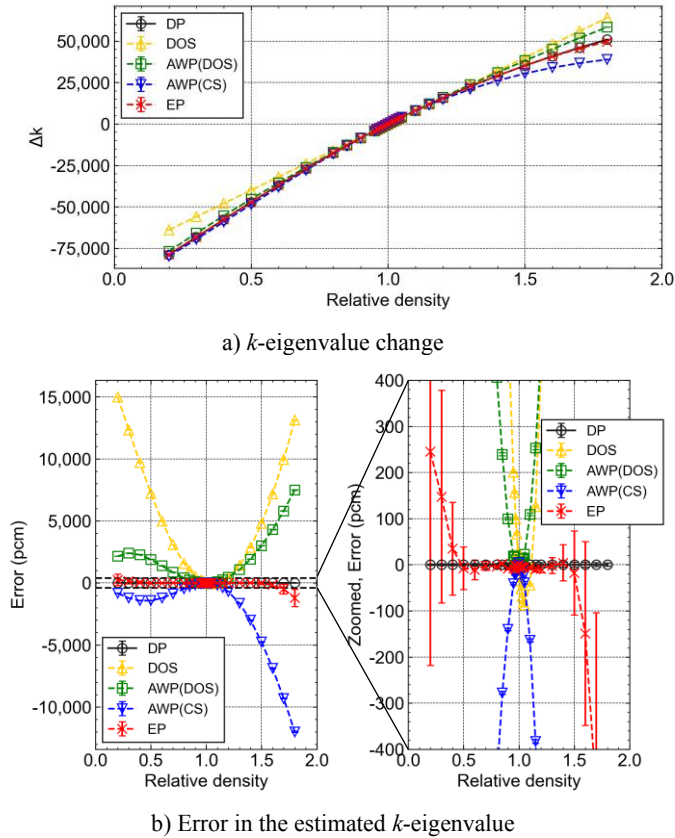


Fig. 3. Results of perturbation methods for global density change in Godiva

3.2 PLUS7 Fuel Assembly

A 2-D 16×16 PLUS7 fuel assembly model is used to check the effectiveness of EP method for a practical problem. A 16×16 PLUS7 fuel assembly contains 236 fuel rods and 5 large guide tubes. The fuel enrichments of normal and zoned fuel rods are 4.50 wt% and 4.00 wt%, respectively. The geometry specification is referred from the APR1400 benchmark [15]. The calculations are performed by using 25 active cycles with 8 million histories per a cycle. The k -eigenvalue of base case is 1.40896 ± 0.00005 .

The soluble boron concentration change ranging 0–5000 ppm is considered in PLUS7 fuel assembly. The boron concentration is 0 ppm in the unperturbed model. Figure 4 shows the results of perturbation methods for soluble boron concentration change in PLUS7 fuel assembly. Maximum errors of DOS, AWP(DOS) and AWP(CS) methods are -22015, -2246, and 9481 pcm, respectively. The EP method results show the significantly improved accuracy. The maximum error of EP method is 14 pcm.

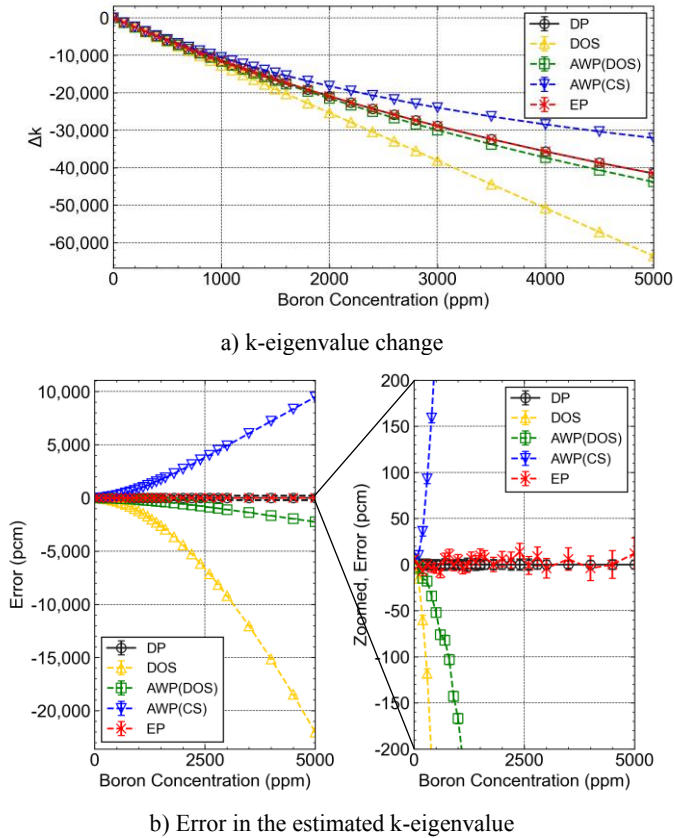


Fig. 4. Results of perturbation methods for boron concentration change in PLUS7 fuel assembly

The computational time of perturbation methods is compared for the soluble boron concentration change in PLUS7 fuel assembly. For the calculation, 28 perturbation cases shown in Figure 4 are considered. 155 processors of Intel Xeon Gold 6242R are used for the MPI parallel calculations. The DP case requires 29 Monte Carlo runs, and it takes 7.54 hours. When a perturbation method is used, one can obtain k -eigenvalue changes of 28 perturbation cases just by running a single unperturbed input as shown in Figure 4. The computational time of EP method is 0.50 hour which is 15.1 times faster than the DP case.

4 Conclusion

In this work, the PIFP method is developed for the EPT in Monte Carlo transport. It allows to use the EP method by computing the adjoint flux of perturbed system during a forward Monte Carlo calculation. The EP method is implemented in the Monte Carlo code MCS. For the Godiva and PLUS7 fuel assembly, k -eigenvalue change results of perturbation methods, which are DOS, AWP(DOS), AWP(CS), and EP, are compared against the reference DP result. The EP method result shows a significantly improved accuracy compared with the conventional perturbation methods. It is also observed that the EP method takes 15.1 times faster than the DP method to compute 29 boron concentration change cases in PLUS7 fuel assembly. For the future work, the perturbation effect of scattering probability f_s will be considered in the EP method.

This work was partially supported by the Energy Efficiency & Resources of the Korea Institute of Energy Technology Evaluation and Planning(KETEP) grant funded by the Ministry of Trade, Industry and Energy(No.20224B10100130). This work was partially supported by the Innovative Small Modular Reactor Development Agency grant funded by the Korea Government(MOTIE) (No. RS-2024-00407975).

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