Eigenvalue sensitivity analysis capabilities with the differential operator method in the superhistory Monte Carlo method

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A B S T R A C T

This paper applies the first-order differential operator method to the Monte Carlo k_{eff}-eigenvalue sensitivity analyses. The effect of the perturbed fission source distribution due to the change of a cross section on the sensitivity coefficients can be accurately estimated by introducing the source perturbation iteration method. However, a prohibitively huge memory is required for the source perturbation iteration method if a large number of sensitivity coefficients are calculated at the same time. For a reduction of the memory requirements, the superhistory method is applied to incorporate the effect of the source perturbation into the differential operator method for sensitivity analyses. In the superhistory method, one source particle and its progenies are followed over super-generations within one cycle calculation. It is not necessary to wait or store a large amount of information until all histories in each cycle are terminated. Although the superhistory method increases the variance of the sensitivity coefficients with the super-generation, the memory requirement can be dramatically reduced by introducing the superhistory method. The first-order differential operator method combined with the superhistory method is verified through some numerical examples where a localized cross section change significantly affects the sensitivity coefficients.

1. Introduction

There has been a growing interest in sensitivity and uncertainty analysis of k_{eff}-eigenvalue or neutron general responses performed with the Monte Carlo method. Additionally, there has been much research and techniques developed to date. The sensitivity analysis methods are now implemented into production-level Monte Carlo codes such as SCALE (Rearden, 2004; Perfetti, 2012; Perfetti and Rearden, 2016), MCNP (Kiedrowski et al., 2011; Kiedrowski and Brown, 2013), SERPENT (Aufiero et al., 2015), MORET (Jinaphanh et al., 2016), McCARD (Shim and Kim, 2011), and RMC (Qiu et al., 2015, 2016a,b). The calculation of the adjoint flux, which is necessary for sensitivity analysis, was considered difficult for the continuous-energy Monte Carlo. The iterated fission probability (IFP) method was developed for estimating the adjoint flux in the continuous energy Monte Carlo and the method is now implemented in many Monte Carlo codes (Truchet et al., 2015; Terranova and Zoia, 2017). The IFP method calculates the expected number of neutrons caused by a neutron at a location in phase space as the adjoint function. The contribution method, which was originally developed for shielding applications and is imple-

mented in the SCALE code, determines the importance of an event by simulating secondary particles at the site of the event and tracking the number of fission neutrons created by each secondary particle (Williams, 1977). A method implemented in the SERPENT code is based on the "collision-history based method" where all cross sections involved in the sensitivity calculations are artificially increased. Another method that this paper focuses on is the differential operator method (Rief, 1984; McKinney and Iverson, 1996; Densmore et al., 1997; Nagaya and Mori, 2005; Raskach, 2009, 2010; Jinaphanh et al., 2016). The unique feature of the differential operator method is that the calculation of the adjoint flux can be circumvented and the first derivative of k_{eff}-eigenvalue with respect to nuclear data can be estimated directly. Furthermore, the differential operator method is applicable to estimating responses of wide range of calculation characteristics: k_{eff}, reaction rates and their ratios both in the eigenvalue problem and in the problem of a subcritical system driven by an external neutron source (Raskach, 2010). On the other hand, the IFP method is applicable to computing k_{eff} derivatives and sensitivities only. The differential operator method has been previously implemented in the MCNP code. However, the differential operator method was replaced by another method; presumably, because it produces inaccurate sensitivity coefficient estimates for complex systems. The sensitivity coefficient is the first derivative of k_{eff}-eigenvalue

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or general responses. The first derivative is exactly sampled in the differential operator method. Nevertheless, the inaccuracy in the differential operator method is caused by neglecting the perturbation of the fission source distribution that cannot be taken into account unless a special technique is employed for considering the perturbation. A method for implementing the source perturbation effect was developed in (Nagaya and Mori, 2005, 2011; Nagaya et al., 2015; Raskach, 2009). However, the method requires the iteration procedure similar to IFP to obtain the converged perturbed fission source distribution. The iteration procedure is similarly required in the IFP method where the fission chain is tracked for a number of generations to compute the adjoint-weighted tallies. The iteration procedure in the differential operator method or in the IFP method results in an increase in the memory requirements if the sensitivity coefficients of many isotopes, reactions, and fine energy groups are calculated at the same time.

Several techniques for reducing the huge memory requirements have been developed and installed in the Monte Carlo codes. In MCNP, a sparse data handling scheme is employed, reducing the memory requirement by a factor of 10 to 100 for many problems (Kiedrowski and Brown, 2013). In McCARD (Shim and Kim, 2011; Choi and Shim, 2016a,b), a memory-efficient adjoint estimation method was developed by applying the IFP concept for the Monte Carlo Wielandt method (Yamamoto and Miyoshi, 2004). In RMC (Wang et al., 2015; Qiu et al., 2015; Qiu et al., 2016a,b), the superhistory method (Brissenden and Garlick, 1986) as well as the Wielandt method was adopted to reduce the memory consumption.

While the sensitivity analysis methods for generalized responses in the Monte Carlo method have been developed (Choi and Shim, 2016b; Qiu et al., 2016a; Perfetti and Rearden, 2016; Aufiero et al., 2016), the present paper focuses on the sensitivity analysis of k_{eff}-eigenvalue. This paper scrutinizes the source perturbation effect on a sensitivity coefficient due to the change of nuclear data through the multi-group Monte Carlo calculations. A method to include the source perturbation effect in the sensitivity coefficients and a memory reduction technique using the superhistory method are discussed in the following sections.

2. Methodology of k_{eff}-eigenvalue sensitivity calculation with the differential operator method

2.1. The differential operator method without perturbed source effect

This section presents a theory of k_{eff}-eigenvalue sensitivity calculation using the Monte Carlo differential operator method. The differential operator method for the perturbation calculation with the source perturbation being implemented was already established in previous research (Rief, 1984; Nagaya and Mori, 2005, 2011; Raskach, 2009; Jinaphanh et al., 2016). The capability of the differential operator method was expanded to the second and higher orders (Nagaya and Mori, 2011). In a Monte Carlo code, MVP (Nagaya et al., 2015), the order of the differential operator method was uniquely expanded to the 8th order. The reactivity change due to a local perturbation can be accurately obtained by the differential operator method by introducing the source perturbation and by expanding the higher order Taylor series. For sensitivity analyses, only the first-order derivatives are required. In this section, the method to calculate the sensitivity coefficient is repeatedly presented as follows; although, it is the duplication of the previously published papers. The formalism to calculate the first derivative of k_{eff}-eigenvalue with respect to a parameter was presented in detail in previous publications (e.g. Nagaya and Mori (2005)). This paper only presents the minimum explanations

for coding a Monte Carlo program to calculate the first derivative of k_{eff}-eigenvalue.

The differential operator method scores an estimate of each differential coefficient at each flight path or each collision point within a perturbed region. The estimates that are scored during the course of the random walk process are shown as follows. First, a particle starts from a fission source site $\mathbf{r}$. The angle is determined isotropically using a random number. The particle moves to a collision point $\mathbf{r}'$ that is determined by the transport kernel:

$$T(\mathbf{r} \rightarrow \mathbf{r}') = \Sigma_t \exp(-\Sigma_t s), \tag{1}$$

where Σ_t = the macroscopic total cross section, s = the flight distance. When the particle travels a distance s through the perturbed region and undergoes a collision, the weighting coefficient to be scored is

$$\frac{1}{T} \frac{\partial}{\partial a} T(\mathbf{r} \rightarrow \mathbf{r}') = \frac{1}{\Sigma_t} \frac{\partial \Sigma_t}{\partial a} - s \frac{\partial \Sigma_t}{\partial a}, \tag{2}$$

where a is a perturbation parameter. For simplicity, the variables for the energy and the direction are omitted. If the sensitivity coefficient with regard to a microscopic capture cross section of a nuclide i is sought, $a = \sigma_{c,i}$ and $\partial \Sigma_t / \partial a = N_i$ where $\sigma_{c,i}$ = the microscopic capture cross section of the nuclide i, N_i = the atom number density of the nuclide i. If a = the macroscopic capture cross section Σ_c, $\partial \Sigma_t / \partial a = 1$. If the particle passes through the perturbed region without undergoing a collision, only the second term on the right-hand side of Eq. (2), $-s \cdot \partial \Sigma_t / \partial a$, is scored.

Unless the particle is killed at the collision point, the particle undergoes a scattering reaction. The weighting coefficient for the scattering kernel Σ_s / Σ_t is

$$\frac{\Sigma_t}{\Sigma_s} \frac{\partial}{\partial a} \frac{\Sigma_s}{\Sigma_t} = \frac{1}{\Sigma_s} \frac{\partial}{\partial a} \Sigma_s - \frac{1}{\Sigma_t} \frac{\partial}{\partial a} \Sigma_t, \tag{3}$$

where Σ_s = the macroscopic scattering cross section.

The k_{eff}-eigenvalue is the sum of $\nu\Sigma_f \cdot w / \Sigma_t$ at each collision point in a cycle where w = the weight of the colliding particle, ν = the number of neutrons per fission, and Σ_f = the macroscopic fission cross section. Thus, the perturbation of $\nu\Sigma_f$ or Σ_t contributes to the change of k_{eff}. To include this effect in the sensitivity coefficient, the following weighting coefficient is scored at each collision:

$$\frac{\Sigma_t}{\nu\Sigma_f} \frac{\partial}{\partial a} \frac{\nu\Sigma_f}{\Sigma_t} = \frac{1}{\nu\Sigma_f} \frac{\partial}{\partial a} \nu\Sigma_f - \frac{1}{\Sigma_t} \frac{\partial}{\partial a} \Sigma_t. \tag{4}$$

The scorings of Eqs. (2), (3), and (4) are repeated at each flight and collision until the particle is discarded. As a result, the first derivative of the k_{eff}-eigenvalue with respect to the perturbation parameter a for the mth particle history is given by

$$\frac{\partial}{\partial a} k_{eff,NP,m} = \sum_i \frac{\nu\Sigma_{f,i}}{\Sigma_{t,i}} w_i w_{NP,i}, \tag{5}$$

where w_i = the particle weight of the ith collision, and

$$w_{NP,i} = \frac{1}{\nu\Sigma_{f,i}} \frac{\partial}{\partial a} \nu\Sigma_{f,i} - \frac{\delta_{a\Sigma_s}}{\Sigma_{t,i}} + \sum_{l=1}^{i} \frac{1}{\Sigma_{s,l}} \frac{\partial}{\partial a} \Sigma_{s,l} - \sum_k s_k \frac{\partial}{\partial a} \Sigma_{t,k}, \tag{6}$$

where $\delta_{a\Sigma_s} \{= 0$ if $a \neq \Sigma_s, = 1$ if $a = \Sigma_s\}$. The subscript NP denotes that Eq. (5) does not include the effect of the source perturbation caused by the change of the cross sections. The summation symbol on the right-hand side of Eq. (5) means that the summation is carried out at every collision point during the mth history. The second term on the right-hand side of Eq. (6) means the sum of $1/\Sigma_{s,l} \cdot \partial \Sigma_{s,l}/\partial a$ until the ith collision where $\Sigma_{s,l}$ is the macroscopic scattering cross section for the lth scattering. The last term on the right-hand side of Eq. (6) means the sum of $s_k \cdot \partial \Sigma_{t,k}/\partial a$ in the kth flight distance of the perturbed region until the ith collision. The