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Development of continuous-energy sensitivity analysis capability in OpenMC

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ABSTRACT

The iterated fission probability (IFP) method and the Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Track length importance CHaracterization (CLUTCH) method have been implemented in several Monte Carlo codes to perform sensitivity calculations. In this work the unified adjoint and generalized adjoint calculation framework combining the IFP method and the CLUTCH method is proposed, and corresponding capabilities for calculating nuclear data sensitivity to the effective multipilication factor and reaction rate ratios are implemented in OpenMC. Results are presented on Godiva, Jezebel and a PWR fuel pin system which demonstrate that OpenMC results agree well with reference direct perturbation sensitivity coefficients. In addition, two main problems of the IFP method related to the number of latent generations, namely convergence and statistical fluctuations are investigated theoretically and numerically. This paper further demonstrates that the fission matrix approach is better suited to generate the adjoint and generalized adjoint source distribution in the CLUTCH method to overcome the drawbacks of the IFP method.

1. Introduction

Due to the motivating need to calculate sensitivity coefficients of the effective multiplication factor and other reactor responses with regard to nuclear data for any fuel or reactor type with high fidelity, performing sensitivity and uncertainty analysis with continuous-energy Monte Carlo codes has been extensively studied in the past several years. This need is considered important for the development and analysis of the next-generation reactor technology such as high-temperature gas-cooled reactors. Several continuous-energy Monte Carlo codes, including McCARD (Shim and Kim, 2011; Choi and Shim, 2016a), MCNP6 (Kiedrowski and Brown, 2013), Serpent (Aufiero et al., 2015), the continuous-energy (CE) version of TSUNAMI-3D (Perfetti, 2012; Perfetti et al., 2016a), RMC (Qiu et al., 2016a,b), MORET (Jinaphanh et al., 2016) have developed sensitivity coefficients calculation capabilities of the effective multiplication factor to model geometrically complex systems. Moreover, some codes among those mentioned above, including CE TSUNAMI-3D (Perfetti and Rearden, 2016), McCARD (Choi and Shim, 2016b), Serpent (Aufiero et al., 2015) and RMC (Qiu et al., 2016c) have extended the calculation capability to generalized sensitivity coefficients.

For the effective multiplication factor sensitivity coefficient problem, also called the eigenvalue sensitivity coefficient problem, the iterated fission probability (IFP) method seems to be the most widely used method to calculate adjoint flux for calculating sensitivity coefficients in CE Monte Carlo applications. The IFP method originally developed by Hurwitz interprets the adjoint flux or importance of a neutron introduced at a location in phase space as the expected number of fission neutrons present in the system during some future generation that are progenies of the original neutron (Hurwitz, 1948), but it requires a large amount of computational memory due to its need to store related tallies for every neutron history (Perfetti et al., 2016a). Several improvements have been proposed, including adjoint superhistory method (Qiu et al., 2016a), adjoint Wielandt method (Choi and Shim, 2016a) and data decomposition method (Qiu et al., 2015). In addition, a new method named Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization (CLUTCH) has been proposed to solve the memory problem directly by utilizing a new interpretation of the adjoint flux rather than modifying the IFP method. CLUTCH is based on Contributon theory and determines the importance of a neutron introduced at a location in phase space by examining how many fission neutrons are created by that neutron (Perfetti et al., 2016a), and it needs pre-

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determined importance distribution function which can be obtained by the IFP method (Perfetti et al., 2016a) and the fission matrix method (Qiu et al., 2016b). In addition, there was an attempt to summarize the advances in Monte Carlo sensitivity methods (Kiedrowski, 2017).

For the generalized sensitivity coefficient problem, a first-of-its-kind method named GEAR-MC based on generalized perturbation theory has been implemented in CE TSUNAMI-3D (Perfetti and Rearden, 2016) for a set of neutronic responses which can be expressed as the ratio of reaction rates (Perfetti and Rearden, 2016). The GEAR-MC method breaks the generalized sensitivity coefficient into three terms, i.e. direct term, intra-generational term and inter-generational term. The original implementation of GEAR-MC requires a large amount of computational memory because an approach similar to the IFP approach has been utilized to estimate the inter-generational term. Similar to the situation in eigenvalue sensitivity coefficient problem, CLUTCH (Perfetti and Rearden, 2016) and the adjoint Wielandt method (Choi and Shim, 2016b) have been proposed to calculate the inter-generational term to overcome this huge memory burden. Instead of adopting generalized perturbation theory, a collision history-based method implemented in Serpent (Aufiero et al., 2015) utilizes the concept of accepted and rejected events to calculate the direct and indirect terms. In the collision history-based method, the scores of accepted and rejected events for the source neutrons should be passed to all their progeny for a sufficient number of generations similarly to IFP. In addition, this collision history-based method can also deal with the sensitivity coefficient problem of bilinear functions of both the forward and the adjoint flux. In addition, an approach called GPT-free method has been proposed to evaluate the sensitivity coefficients by capturing an effective functional subspace of the response function to preclude the burden of calculating general adjoint flux in GPT implementations, and this approach has been demonstrated to work efficiently in both deterministic (Kennedy et al., 2012) and Monte Carlo methods (Wu et al., 2012).

In this paper, the unified adjoint calculation framework combining the IFP method and the CLUTCH method is proposed for both the eigenvalue sensitivity coefficient problem and the generalized sensitivity coefficient problem, and the IFP approach and the fission matrix approach are utilized in CLUTCH to generate adjoint source distribution seperately. Corresponding sensitivity analysis capabilities have been implemented in OpenMC (Romano et al., 2015). The Green's function approach is utilized to construct the unified adjoint calculation framework. Some outstanding problems related to the determination of the number of latent generations are analyzed theoretically for the IFP approach leading to the recommendation of the fission matrix method to generate the importance function needed in CLUTCH for both the eigenvalue sensitivity coefficient problem and the generalized sensitivity coefficient problem. Finally, the calculation results of the IFP method and the CLUTCH method implemented in OpenMC are presented.

2. Sensitivity coefficient calculation theory

In the following sections, the calculation method based on first-order perturbation theory for eigenvalue sensitivity coefficients is described (Section 2.1) (Perfetti et al., 2016a). First-order generalized perturbation theory is utilized to compute the generalized sensitivity coefficients (Section 2.2) (Perfetti and Rearden, 2016).

2.1. Definition of eigenvalue sensitivity coefficient

The eigenvalue sensitivity coefficients describe the fractional change in the effective multiplication factor resulting from perturbations or uncertainties in nuclear data $x(r,E)$ such that

$$S_{k,x(r,E)} = \frac{\delta k/k}{\delta x(r,E)/x(r,E)}, \tag{1}$$

where k is the effective multiplication factor, $x(r,E)$ can be a cross section, a fission yield or a fission neutron emission function at position r and energy E, and δ is the differential perturbation operator.

First-order perturbation theory is typically utilized to get the differential perturbation in k due to the differential perturbation in nuclear data

$$\delta k = \frac{\langle \Phi^*, (\delta F - k\delta L)\Phi \rangle}{\langle \Phi^*, \frac{1}{k} F\Phi \rangle}, \tag{2}$$

where Φ is the neutron flux, Φ^* is the adjoint neutron flux, the fission neutron production operator F is given by

$$F\Phi = \frac{\chi(E)}{4\pi} \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' \nu\Sigma_f(\vec{r},E')\Phi(\vec{r},E',\hat{\Omega}'),$$

and the neutron loss operator L is given by

$$L\Phi = \hat{\Omega}\nabla\Phi(\vec{r},E,\hat{\Omega}) + \Sigma_t(\vec{r},E)\Phi(\vec{r},E,\hat{\Omega}) - \int_{4\pi} d\hat{\Omega}\prime \int_0^\infty dE\prime \Sigma_s(\vec{r},E\prime \to E, \hat{\Omega}\prime \to \hat{\Omega})\Phi(\vec{r},E\prime,\hat{\Omega}\prime)$$

Substituting Eq. (2) into Eq. (1), the eigenvalue sensitivity coefficient becomes

$$S_{k,x(r,E)} = x\frac{\langle \Phi^*, (\frac{1}{k}\frac{\delta F}{\delta x} - \frac{\delta L}{\delta x})\Phi \rangle}{\langle \Phi^*, \frac{1}{k} F\Phi \rangle}. \tag{3}$$

According to Eq. (3), calculating the eigenvalue sensitivity coefficient needs both the forward neutron flux and the adjoint neutron flux. The forward neutron flux can be obtained by solving the Boltzmann equation

$$L\Phi = \frac{F\Phi}{k}, \tag{4}$$

and the adjoint neutron flux can be obtained by solving the adjoint Boltzmann equation

$$L^*\Phi^* = \frac{F^*\Phi^*}{k}, \tag{5}$$

where the adjoint fission neutron production operator F^* is given by

$$F^*\Phi^* = \nu\Sigma_f(\vec{r},E) \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' \frac{\chi(E')}{4\pi} \Phi^*(\vec{r},E',\hat{\Omega}')$$

and the adjoint neutron loss operator L^* is given by

$$L^*\Phi^* = -\hat{\Omega}\nabla\Phi^*(\vec{r},E,\hat{\Omega}) + \Sigma_t(\vec{r},E)\Phi^*(\vec{r},E,\hat{\Omega}) - \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' \Sigma_s(\vec{r},E \to E', \hat{\Omega} \to \hat{\Omega}')\Phi^*(\vec{r},E',\hat{\Omega}')$$

2.2. Definition of generalized sensitivity coefficient

The generalized sensitivity coefficients describe the fractional change in a generalized response R resulting from perturbations or uncertainties in nuclear data $x(r,E)$ such that

$$S_{R,x(r,E)} = \frac{\delta R/R}{\delta x(r,E)/x(r,E)}. \tag{6}$$

In this work, only the response that can be expressed as a ratio of two reaction rates is considered, which can be expressed as

$$R = \frac{\langle \Sigma_1 \Phi \rangle}{\langle \Sigma_2 \Phi \rangle}, \tag{7}$$

where Σ_1 and Σ_2 are macroscopic cross sections.