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Development of sensitivity analysis capabilities of generalized responses to nuclear data in Monte Carlo code RMC

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ABSTRACT

Capabilities for nuclear data sensitivity and uncertainty analysis have been recently implemented in numerous continuous-energy Monte Carlo codes, including the Reactor Monte Carlo (RMC) code. Previous work developed the capability for RMC of computing sensitivity coefficients of the effective multiplication factor and related uncertainties, due to nuclear data. In this work, such capability was extended to generalized responses in the form of ratios of linear response functions of the forward flux based on the collision history-based approach as implemented in SERPENT2. The superhistory algorithm was also adopted in RMC to reduce memory consumption for generalized sensitivity calculations. These new capabilities of RMC were verified by comparing results of TSUNAMI-1D in SCALE6.1 code package, and SERPENT2 through Jezebel, Flattop and the UAM TMI PWR pin cell benchmark problems.

1. Introduction

In the past several years, there has been an increasing interest in performing sensitivity and uncertainty analysis with continuous-energy Monte Carlo codes. Several codes, including MCNP6 (Kiedrowski and Brown, 2013), SERPENT2 (Aufiero et al., 2015), the continuous-energy (CE) version of TSUNAMI-3D (Perfetti and Rearden, 2013) in SCALE6.2, MONK10 (Baker et al., 2015), McCARD (Shim and Kim, 2011), TRIPOLI4 (Truchet et al., 2015), and MORET5 (Jinaphanh et al., 2015), have developed capabilities of computing sensitivity coefficients of the effective multiplication factor with regard to nuclear data. Furthermore, some of these Monte Carlo codes—for example SERPENT2 (Aufiero et al., 2015) and CE-TSUNAMI-3D (Perfetti and Rearden, 2014)—have developed capabilities of computing generalized sensitivity coefficients based on different methods. As known, estimating generalized sensitivity coefficients requires two terms: the direct term which describes the perturbations of nuclear data to the response function, and the indirect term which describes the perturbations of nuclear data to flux or spectrum. Calculating the direct term is relatively easy, whereas computing the indirect term usually requires introducing generalized perturbation theory (GPT). CE-TSUNAMI-3D uses the GEAR-MC method (Perfetti and Rearden, 2014); such method further divides the indirect term into two terms: (1) the intra-generational term that describes how much importance a neutron produces in the current generation until its disappearance; (2) the inter-generational term that describes how much importance a neutron generates in the future generations (Perfetti and Rearden, 2014). Since the inter-generation term is computed using the iterated fission probability (IFP) method (Kiedrowski and Brown, 2013), the GEAR-MC method faces the challenge of huge memory requirements. Rather than solving the generalized perturbation equation explicitly, SERPENT2 uses the collision history-based method applying the concept of accepted and rejected events. Such method takes advantage of the Monte Carlo method itself and is relatively easy to implement.

In previous work, the Reactor Monte Carlo (RMC) code (Wang et al., 2015) acquired the capability of computing sensitivity coefficients of the effective multiplication factor with regard to nuclear data (Qiu et al., 2015). In this work, such capability of RMC was extended to generalized responses based on the collision history-based method (Aufiero et al., 2015) with the major difference that the collision history-based method implemented in SERPENT2 is based on delta-tracking technique, whereas the implementation in RMC is based on the ray-tracking technique. Furthermore, RMC relies on the superhistory algorithm (Qiu et al., 2016) to reduce memory consumption for the generalized sensitivity calculations. Section 2 of this manuscript presents the underlying theory for the collision history-based method, Section 3 describes the superhistory algorithm, and Section 4 provides a comparison of

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the results obtained using these newly-developed features in RMC with results of TSUNAMI-1D in SCALE6.1 code package (Oak Ridge National Laboratory, 2011) and SERPENT2 in three different benchmark problems.

2. Methodology

2.1. Generalized sensitivity coefficients

The sensitivity coefficient function is defined as the relative change in the response function, for example the effective multiplication factor divided by the relative change in nuclear data, and is expressed as

$$S_x^R = \frac{\delta R/R}{\delta x/x}, \tag{1}$$

where R is any kind of response functions and x is any nuclear data including microscopic cross sections, nubar, or scattering or fission energy transfer functions, etc.; x is in general function of position $\overrightarrow{r}$, incident and outgoing direction $\overrightarrow{\Omega}$ and $\overrightarrow{\Omega}'$, incident and outgoing energy E and E'. The energy-resolved sensitivity coefficients computed in this work are energy bin-integrated, in the form of

$$S_{x,g}^R = \int_{E_g}^{E_{g-1}} S_x^R(E)dE, \tag{2}$$

where g is the energy bin index and E_g and E_{g-1} are the lower and upper energies, respectively, in bin g. The energy-integrated sensitivity coefficients can be expressed in the form of

$$S_x^R = \int_0^{\infty} S_x^R(E)dE. \tag{3}$$

It should be noted that for microscopic cross sections and nubar, sensitivity coefficients are usually integrated over incident energy, whereas for scattering and fission energy transfer functions sensitivity coefficients are conventionally integrated over outgoing energy. Furthermore, for scattering transfer functions, sensitivity coefficients can also be expressed as a function of incident energy (also suitable for fission χ transfer function) and scattering cosine. In this work, the linear response function is assumed of the following form

$$R = \frac{\langle \Sigma_1, \Psi \rangle}{\langle \Sigma_2, \Psi \rangle}, \tag{4}$$

where Ψ is the neutron flux, Σ_1 and Σ_2 are any kind of macroscopic cross sections, and $\langle\ \rangle$ is an inner product over phase space. Using generalized sensitivity coefficients, one can conduct sensitivity and uncertainty analysis to different types of response functions. For example, setting $\Sigma_2 = 1$ allows to calculate sensitivity coefficients of one-group cross section obtained by Monte Carlo transport calculations, and these coefficients can be further used to study uncertainty propagation (Park et al., 2011) in depletion calculations. In this work, methods are restricted to first order perturbation theory; therefore, the perturbation of generalized response, δR, caused by perturbations of cross sections can be expressed as

$$\delta R = \left\langle \frac{\frac{d\Sigma_1}{dx}\Psi}{\Sigma_1\Psi} R\delta x - \frac{\frac{d\Sigma_2}{dx}\Psi}{\Sigma_2\Psi} R\delta x + \frac{\partial R}{\partial \Psi}\frac{\partial \Psi}{\partial x}\delta x \right\rangle. \tag{5}$$

Substituting Eq. (5) into Eq. (1), generalized response sensitivity coefficients can be expressed as

$$S_x^R = \left\langle \frac{\frac{d\Sigma_1}{dx}\Psi x}{\Sigma_1\Psi} - \frac{\frac{d\Sigma_2}{dx}\Psi x}{\Sigma_2\Psi} + \frac{\partial R}{\partial \Psi}\frac{\partial \Psi}{\partial x}\frac{x}{R} \right\rangle. \tag{6}$$

The first two terms on the right hand side of Eq. (6) are called the direct effect terms, which describe the impact of perturbations of cross sections on the generalized response. Scoring the direct effect terms in Monte Carlo transport calculations is relative easy to implement and can use standard Monte Carlo tally techniques (X-5 Monte Carlo Team, 2003). Considering the track length estimator, for example, a score for $\langle \Sigma_1\Psi \rangle$ is equal to

$$\langle \Sigma_1\Psi \rangle = \frac{1}{C_{tot}}\sum_{c=1}^{C_{tot}}\frac{1}{P_c w_0^c}\sum_{p=1}^{P_c}\sum_{\tau=1}^{L^{p,c}}\Sigma_1 \cdot w_\tau^{p,c} \cdot l_\tau^{p,c}, \tag{7}$$

where c is cycle index, C_{tot} is the total number of active cycles, p is particle index in cycle c, P_c is the total number of particles in cycle c, w_0^c is initial weight of every particle in cycle c, τ is track index for particle p in cycle c, $L^{p,c}$ is total number of tracks for particle p in cycle c, and $w_\tau^{p,c}$ and $l_\tau^{p,c}$ are the current weight and track length of particle p at track τ in cycle c; and a score for $\left\langle \frac{\partial \Sigma_1}{\partial x}\Psi x \right\rangle$ is given by

$$\left\langle \frac{\partial \Sigma_1}{\partial x}\Psi x \right\rangle = \frac{1}{C_{tot}}\sum_{c=1}^{C_{tot}}\frac{1}{P_c w_0^c}\sum_{p=1}^{P_c}\sum_{\tau=1}^{L^{p,c}} N_1 \cdot x \cdot \delta_{\sigma_1,x} \cdot w_\tau^{p,c} \cdot l_\tau^{p,c}, \tag{8}$$

where $\Sigma_1 = N_1\sigma_1$, N_1 is the number density, σ_1 is a microscopic cross section, $\delta_{\sigma_1,x}$ is the delta function and equals to one when $\sigma_1 = x$ or σ_1 contains x and zero otherwise. The last term in Eq. (6) is known as the indirect effect term, which describes the impact of perturbations of cross sections on the flux and can be computed by

$$\left\langle \frac{\partial R}{\partial \Psi}\frac{\partial \Psi}{\partial x}\frac{x}{R} \right\rangle = \frac{\left\langle \frac{\partial \Psi}{\partial x}\Sigma_1 x \right\rangle}{\langle \Sigma_1\Psi \rangle} - \frac{\left\langle \frac{\partial \Psi}{\partial x}\Sigma_2 x \right\rangle}{\langle \Sigma_2\Psi \rangle}. \tag{9}$$

Scoring the indirect term is more complicated than the direct effect term. TSUNAMI-3D in SCALE6.2 uses the GEAR method (Perfetti and Rearden, 2014) that is based on the generalized perturbation theory to compute the indirect term. SERPENT2 uses the collision-based history method based on the concept of accepted and rejected events (Aufiero et al., 2015) without relying on GPT.

2.2. Collision history-based method

According to Eq. (9), the key to compute the indirect term is to obtain scores for the numerators on the right hand side. Still taking the track length estimator as an example, one can obtain

$$\left\langle \frac{\partial \Psi}{\partial x}\Sigma_1 x \right\rangle = \frac{1}{C_{tot}}\sum_{c=1}^{C_{tot}}\frac{1}{P_c w_0^c}\sum_{p=1}^{P_c}\sum_{\tau=1}^{L^{p,c}}\Sigma_1 \cdot \frac{\partial w_\tau^{p,c}/w_\tau^{p,c}}{\partial x/x} \cdot w_\tau^{p,c} \cdot l_\tau^{p,c}. \tag{10}$$

In order to compute the relative change of particle weight $\partial w_\tau^{p,c}/w_\tau^{p,c}$ due to relative change of nuclear data $\partial x/x$, the collision history-based method (Aufiero et al., 2015) artificially increases all cross sections (Σ_G) involved in generalized sensitivity calculations by a factor of f_a. As a result, all the reactions G are accepted by a probability of $\frac{1}{f_a}$ and rejected by a probability of $1 - \frac{1}{f_a}$. This way, the distribution of particles is unchanged. Fig. 1 shows a neutron history of unperturbed system after all cross sections are increased by a factor of $f_a = 2$.

With accepted and rejected events, one can consider perturbation in neutron weight with the same neutron tracks as an unperturbed system by using biased sampling. The basic idea is quite similar to correlated sampling method (Bernnat, 1974; Nagaya, 2012). Assuming $p(S)$ is the probability density function at phase space S for the unperturbed system and $p^*(S)$ is the probability density function at phase space S for the perturbed system, one can obtain