Capability of computing sensitivity coefficients with regard to Legendre scattering moments implemented in RMC

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Abstract: In the past several years, different Monte Carlo codes have developed the capability of performing sensitivity and uncertainty analysis. Most of these Monte Carlo codes have focused on nuclear cross sections, fission neutron multiplicities and fission emission spectra. However, the angular scattering distributions would have a significant effect on the system where leakage is particularly important, and the scattering distributions are often represented by their Legendre moments; therefore, in this work, a capability of computing sensitivity coefficients of k_{eff} and different responses such as reaction rate ratios with regard to Legendre scattering moments is developed in the Reactor Monte Carlo (RMC) code. The new capability in RMC has been verified with SERPENT2 and a deterministic code, ERANOS, by two fast spectrum systems, *i.e.*, the Jezebel and flattop problems. Good agreement among RMC, SERPENT2 and ERANOS is observed.

Keyword: sensitivity coefficient; Legendre moment; Monte Carlo; RMC

1 Introduction

Recently, different Monte Carlo codes have developed the capability of performing sensitivity and uncertainty analysis. Although most of these Monte Carlo codes have the ability to compute sensitivity coefficients of the effective multiplication factor (k_{eff}), only few of them, *e.g.*, continuous-energy-TSUNAMI-3D[1] and SERPENT2[2], can calculate sensitivity coefficients of other response functions, which are known as generalized sensitivity coefficients. Recently, the Reactor Monte Carlo code RMC has developed such a capability of computing sensitivity coefficients of different response functions such as reaction rate ratios[3] and adjoint-weighted reaction rate ratios[4], to common nuclear data such as cross sections, fission spectrum and mean fission neutrons, based on the collision history-based method [2, 3]. In this work, this capability has been extended to sensitivity coefficients of Legendre scattering moments.

2 Method

2.1 Definition of sensitivity coefficients

Sensitivity coefficient is defined as the relative change in the response function, divided by the relative change in nuclear data, which can be expressed as

$$S_x^R = \frac{x}{R}\frac{dR}{dx}, \tag{1}$$

where x is any type of nuclear data such as cross sections, fission spectrum and mean fission neutrons, scattering cosine, Legendre scattering moments, *etc.* And R represents k_{eff} or ratio of reaction rates, which is defined as

$$R = \frac{\langle \Sigma_1 \Psi \rangle}{\langle \Sigma_2 \Psi \rangle}, \tag{2}$$

where
Ψ is the neutron flux,
Σ_1 and Σ_2 are two different cross sections, and
$\langle\ \rangle$ is integration over all space, angle, and energy variables.

2.2 Legendre moments

The scattering distribution $f^j(\mu|E)$ describes the probability density function of a neutron emerging with scattering cosine μ, conditioned to the incident energy E for some isotope and scattering reaction j. And $f^j(\mu|E)$ is often expressed in the form of Legendre polynomials

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$$f^j(\mu|E)=\sum_{l=0}^{\infty}\frac{2l+1}{2}P_l(\mu)f_l^j(E), \qquad (3)$$

where

$P_l(\mu)$ is the l^{th} Legendre polynomial and $f_l^j(E)$ is the l^{th} Legendre moment of the distribution $f^j(\mu|E)$. And $f_l^j(E)$ can be calculated by

$$f_l^j(E)=\int_{-1}^{1}P_l(\mu)f^j(\mu|E)d\mu, \qquad (4)$$

According to Eq. 1, sensitivity coefficients to $f_l^j(E)$ can be expressed as

$$S^R_{f_l^j(E)}=\frac{f_l^j(E)}{R}\frac{dR}{df_l^j(E)}. \qquad (5)$$

In order to calculate Eq. 5, two different methods have been proposed. The first method is a discretized approach that uses bin integrated unconstrained sensitivities and has been implemented in MCNP6[5]. The second method is a fully continuous method and has been implemented in SERPENT2[2]. The latter method was chosen for implementation in RMC.

According to this approach Eq. 5 can be expressed in the following way:

$$S^R_{f_l^j(E)}= \int_{-1}^{1}S^R_{f^j(\mu|E)}\cdot\frac{df^j(\mu|E)}{df_l^j(E)}\cdot f_l^j(E)\cdot\frac{1}{f^j(\mu|E)}d\mu, \qquad (6)$$

where $S^R_{f^j(\mu|E)}$ represents the unconstrained sensitivity coefficients of R to $f^j(\mu|E)$.

According to Eq. 3, the second term in Eq. 6 can be expressed in the form

$$\frac{df^j(\mu|E)}{df_l^j(E)}=\frac{2l+1}{2}P_l(\mu). \qquad (7)$$

The third term and the fourth term in Eq. 6 can be calculated directly from the nuclear data libraries. Take the elastic scattering distributions as an example. Elastic scattering distributions use tabular probability density function $f^j(\mu|E)$ and the cumulative density function $F^j(\mu|E)$, where

$$F^j(\mu|E)=\int_{-1}^{\mu}f^j(\mu'|E)d\mu'. \qquad (8)$$

For each incident neutron energy point E_i, there is a table of cosines $\mu_{i,k}$, and the corresponding probability density functions $f_{i,k}$ and cumulative density functions $F_{i,k}$, where i is the index of energy point and k is the index of the cosine point.

If the incident energy is between two energy points E_i and E_{i+1}, then the interpolation r is calculated by

$$r=\frac{E-E_i}{E_{i+1}-E_i}. \qquad (9)$$

A random number ξ_1 on the unit interval $[0,1)$ is generated to determine which energy point is going to be used. To be more specific, when $\xi_1>r$, E_i will be used otherwise E_{i+1} will. A second random number ξ_2 is used to sample a cosine from the cumulative density function $F_{i',k}<\xi_2<F_{i',k}$, where i' could be i or $i+1$, as discussed. Once the incident energy is determined, the third term in Eq. 6 can be calculated by

$$f_l^j(E)=(1-r)\cdot f_l^j(E_i)+r\cdot f_l^j(E_{i+1}), \qquad (10)$$

where $f_l^j(E_i)$ and $f_l^j(E_{i+1})$ can be pre-calculated based on Eq. 4. Once a cosine is sampled, the fourth term in Eq. 6 can be calculated by

$$f^j(\mu|E) =(1-r)\cdot f^j(\mu|E_i)+r\cdot f^j(\mu|E_{i+1}). \qquad (11)$$

Applying the collision history-based method[2], $S^R_{f^j(\mu|E)}$ can be obtained from the accepted scattering events in the collision history of the particles contributing to the response R. Since R can be obtained by the estimator $R=E[t_1]/E[t_2]$, then $S^R_{f_l^j(E)}$ can be estimated by

$$S^R_{f_l^j(E)}= \frac{\mathrm{cov}[t_1,\sum_{history}G_{f_l^j(E)}]}{E[t_1]}-\frac{\mathrm{cov}[t_1,\sum_{history}G_{f_l^j(E)}]}{E[t_1]}. \qquad (12)$$

2.3 Collision superhistory-based method

The collision history-based method[2] which was implemented in SERPENT2 is introduced briefly in this section.

In order to consider the perturbation of cross sections in a Monte Carlo simulation, all cross sections involved in sensitivity analysis are increased by a factor of f_a. To make the results unbiased, all the reactions relative to the perturbed cross sections are accepted by a probability of $\frac{1}{f_a}$ and rejected by

$1-\frac{1}{f_a}$. With these accepted and rejected events, the effect of the perturbation of the cross sections on the perturbation on the particle weight can be investigated[2]. Finally, sensitivity coefficients of different response functions, such as k_{eff}, to different nuclear data can be computed.

In order to consider the fission source perturbation effect, these accepted and rejected events have to be passed to the progeny neutrons for sufficient generations. Consequently, the memory consumptions used for storing these accepted and rejected events are proportional to the number of particle histories per cycle. For complexed systems, usually a large number of particles per cycle are used, which will consume considerable memory.

To reduce the memory consumption of sensitivity analysis, in RMC code, the collision history-based method was implemented in the superhistory[6,7,8] power iteration process rather than the standard power iteration process. And the combination of the collision history-based method and the superhistory method is called collision suphistory-based method in this paper. In the superhistory method, a source neutron and all its fission neutrons up to a specified number of generations (*e.g.*, λ) are simulated in the current cycle while the $\lambda+1$ generation fission neutrons of this source neutron are stored into the fission neutron bank for the next cycle. The history of a source neutron and all its progeny neutrons simulated in the current cycle is called a superhistory. Therefore, a score of sensitivity coefficients can be computed in every superhistory. And the tally used to store the collision information can be cleared in at the end of every superhistory rather the end of every cycle. Therefore, the memory consumption for sensitivity analysis can be reduced[3, 8].

Take Fig. 1 and Fig. 2 as examples. Assuming each neutron only produces one fission neutron, and three source neutrons are simulated for each cycle, it can be inferred the memory consumption of the standard Monte Carlo power iteration process (Fig. 1) is three times higher than that of the Monte Carlo power iteration process after adopting the superhistory method (Fig. 2).

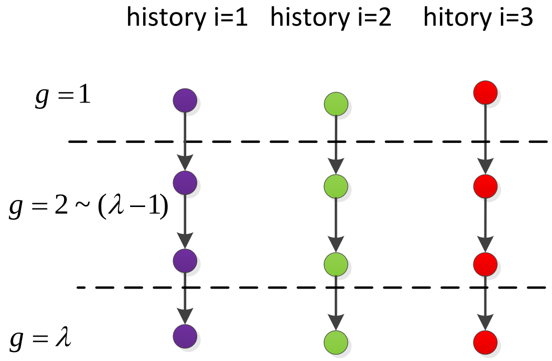

Fig.1 Standard Monte Carlo power iteration process.

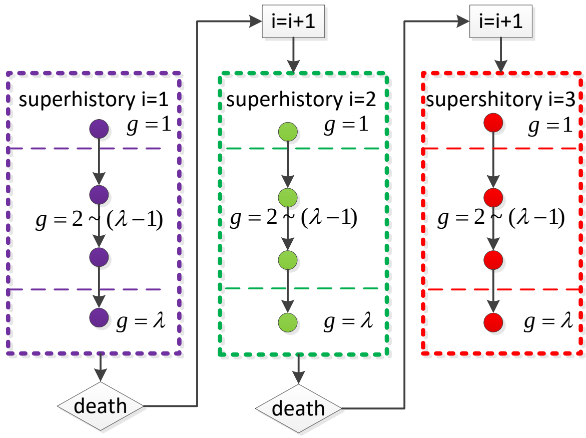

Fig.2 Monte Carlo power iteration process after adopting superhistory method.

3 Results and analysis

The newly developed capability of RMC has been verified by comparing with results computed by a deterministic code, ERANOS[9], and a Monte Carlo code, SERPENT2, through two different test problems: Jezebel and Flattop[10]. All calculations are based on ENDF/B-VII nuclear data library.

The Jezebel problem is a bare sphere of plutonium with a radius of 6.38493 cm. The Flattop problem is a plutonium sphere with a radius of 4.5332 cm reflected by 19.6088 cm of normal uranium (outer radius of 24.142cm). The isotopic composition and atom densities of the Jezebel and Flattop problems are listed in Table 1 and Table 2, respectively. As can been seen, the Jezebel problem contains five different isotopes while the Flattop contains eight.

In Tables 3 and 4, the energy-integrated k_{eff} sensitivities to the P1 moment of the elastic scattering distributions of the main isotopes are shown for Jezebel and Flattop, respectively. As shown, the three codes agree well with each other. These results are useful for the consideration of the angular distributions of secondary neutrons in nuclear data adjustment studies.

Table 1 Atom Densities in Jezebel.

Isotope	Atom Density (atoms/barn-cm)
^{239}Pu	3.7047E-02
^{240}Pu	1.7512E-03
^{241}Pu	1.1674E-04
^{69}Ga	8.2663E-04
^{71}Ga	5.4857E-04

Table 2 Atom Densities in Flattop.

Region	Isotope	Atom Density (atoms/barn-cm)
Core	^{239}Pu	3.6697E-02
	^{240}Pu	1.8700E-03
	^{241}Pu	1.1639E-04
	^{69}Ga	8.8692E-04
	^{71}Ga	5.8858E-04
Reflector	^{234}U	2.6438E-06
	^{235}U	3.4610E-04
	^{238}U	4.7721E-02

Table 3 Energy integrated k_{eff} sensitivity to the first Legendre moment of the elastic scattering distributions in Jezebel.

Isotope	SERPENT		ERANOS	RMC	
	Sensitivity	Rstd		Sensitivity	Rstd
^{239}Pu	-1.007E-01	0.1%	-1.006E-01	-1.000E-01	0.4%
^{240}Pu	-4.980E-03	0.2%	-4.970E-03	-4.960E-03	1.4%
^{241}Pu	-3.380E-04	0.6%	-3.500E-04	-3.200E-04	4.6%

Table 4 Energy integrated k_{eff} sensitivity to the first Legendre moment of the elastic scattering distributions in Flattop.

Isotope	SERPENT		ERANOS	RMC	
	Sensitivity	Rstd		Sensitivity	Rstd
^{235}U	-9.920E-04	0.3%	-1.000E-03	-9.628E-04	2.0%
^{238}U	-1.415E-01	0.1%	-1.433E-01	-1.410E-01	0.2%
^{239}Pu	-4.050E-02	0.1%	-4.060E-02	-4.055E-02	0.8%
^{240}Pu	-2.170E-03	0.5%	-2.180E-03	-2.242E-03	2.9%
^{241}Pu	-1.370E-04	1.5%	-1.360E-04	-1.253E-04	10.2%

In Fig. 3, the Jezebel k_{eff} energy-resolved sensitivities to the first third Legendre moments of the ^{239}Pu elastic scattering angular distribution are shown. For completeness, the sensitivity to the ^{239}Pu elastic scattering cross section (P0 moment), was additionally included in the Figure.

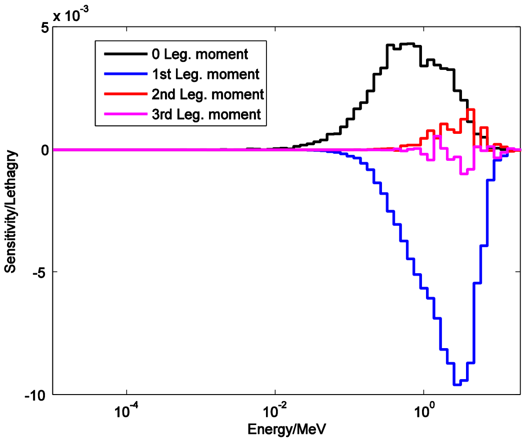

Fig.3 Jezebel k_{eff} sensitivity to the first three Legendre moments of the ^{239}Pu elastic scattering distribution.

In Fig. 4, the Flattop k_{eff} energy-resolved sensitivities to the first third Legendre moments of the ^{238}U elastic scattering angular distribution are shown.

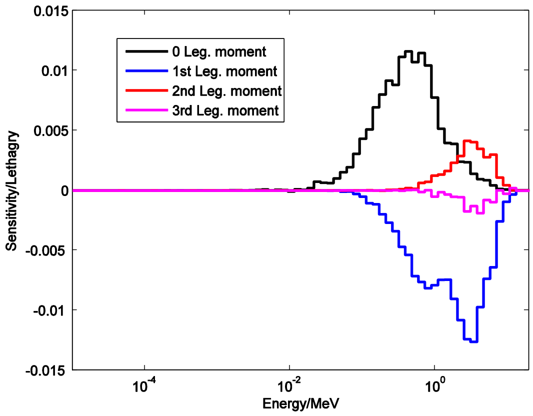

Fig.4 Flattop k_{eff} sensitivity to the first three Legendre moments of the ^{238}U elastic scattering distribution.

Sensitivities are also computed for the response R= F28/F25 which is defined as

$$R = \frac{\iiint \Sigma_f^{238U}(r,E)\Psi(r,E,\Omega)dEdrd\Omega}{\iiint \Sigma_f^{235U}(r,E)\Psi(r,E,\Omega)dEdrd\Omega}, \quad (13)$$

where Σ_f^{238U} and Σ_f^{235U} represent the fission cross section for ^{238}U and ^{235}U, respectively. The response function was calculated in a central sphere of 1-cm radius for both Jezebel and Flattop cases.

In Fig. 5, the Jezebel F28/F25 energy-resolved sensitivities to the first third Legendre moments of the ^{239}Pu elastic scattering angular distribution are shown.

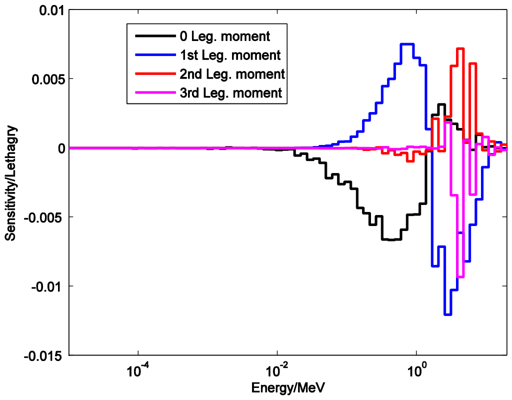

Fig.5 Jezebel R=F28/F25 sensitivity to the first three Legendre moments of the ^{239}Pu elastic scattering distribution.

In Fig. 6, the Flattop F28/F25 energy-resolved sensitivities to the first third Legendre moments of the ^{238}U elastic scattering angular distribution are shown.

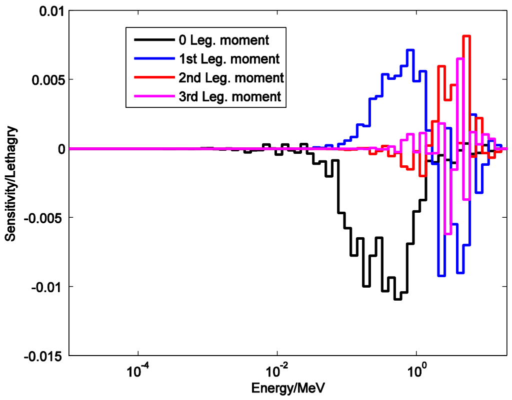

Fig.6 Flattop R=F28/F25 sensitivity to the first three Legendre moments of the ^{238}U elastic scattering distribution.

4 Conclusions

In this work, the capability of computing sensitivity coefficients with regard to Legendre scattering moments has been implemented in the continuous-energy Reactor Monte Carlo (RMC) code. The implementation is based on the collision history-based method as developed in the SERPENT2 code. The new capability of RMC has been verified by comparing with results from a deterministic code, ERANOS, and a Monte Carlo code, SERPENT2 through the Jezebel and Flattop test problems. Numerical results show that RMC, SERPENT2 and ERANOS reach a good agreement.

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