

## Preliminary Study of Generalized Sensitivity Analysis with Continuous-Energy Monte Carlo Code RMC

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### 1. Introduction

Recently, capabilities to compute eigenvalue sensitivity coefficients to nuclear data have been developed by several continuous-energy Monte Carlo codes, e. g., the Reactor Monte Carlo code RMC [1] developed by Tsinghua University, China. These capabilities should be extended to analyze a generalized set of response, such as power distributions and multi-group cross-sections. Therefore, several methods have been put forward to achieve this objective. These methods can be divided into three kinds. The first kind are direct perturbation based methods [2], which are time-consuming since multiple direct perturbation calculations are required to perform. The second kind are methods based on generalized perturbation theory (GPT), including the GEAR-MC method [3] implemented in continuous-energy TSUNAMI-3D and the collision history-based approach implemented in SERPENT [4]. The third kind are specific approaches, such as the differential operator sampling method [5]. However, the differential operator sampling method may be not accurate enough [3] since it ignores the impact of perturbations and cross-section uncertainties on the fission source.

### 2. Methodology

#### 2.1 Definition of Generalized Response Sensitivity Coefficients

The sensitivity coefficient of some generalized response,  $R$ , to some nuclear data  $x(r, E)$ , is defined as

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

where

$r$  = position and

$E$  = energy.

The generalized response function may have different types of expressions, for example, bilinear ratios involving adjoint flux. In this work, only linear ratios are investigated, which can be expressed as

$$R = \frac{\langle \sigma_1 \Psi \rangle}{\langle \sigma_2 \Psi \rangle} \quad (2)$$

where

$\langle \rangle$  = inner product over phase space,

$\Psi$  = flux and

$\sigma$  = cross-section.

The perturbation of generalized response,  $\delta R$ , caused by a small perturbation of cross-section,  $\delta x$ , can be expressed as

$$\delta R = \left\langle \frac{\partial R}{\partial x} \delta x + \frac{\partial R}{\partial \Psi} \frac{\partial \Psi}{\partial x} \delta x \right\rangle \quad (3)$$

Substituting Eq. 3 into Eq. 1, the generalized response sensitivity coefficients can be expressed as

$$S_{k,x(r,E)} = \left\langle \frac{x}{R} \frac{\partial R}{\partial x} \right\rangle + \left\langle \frac{x}{R} \frac{\partial R}{\partial \Psi} \frac{\partial \Psi}{\partial x} \right\rangle \quad (4)$$

The first term in Eq. 3 is called the direct effect term, which describes the impact of the perturbation of cross-section on the generalized response and can be computed by

$$\frac{\left\langle \frac{\partial \sigma_1}{\partial x} \Psi \right\rangle}{\langle \sigma_1 \Psi \rangle} - \frac{\left\langle \frac{\partial \sigma_2}{\partial x} \Psi \right\rangle}{\langle \sigma_2 \Psi \rangle} \quad (5)$$

The tally of the direct effect term in Monte Carlo simulations is straightforward and relative easy-implemented.

The second term in Eq. 3 is known as the indirect effect term, which describes the impact of the perturbations of cross-section on the flux and can be expressed as

$$\frac{\left\langle \frac{\partial \Psi}{\partial x} \sigma_1 \right\rangle}{\langle \sigma_1 \Psi \rangle} - \frac{\left\langle \frac{\partial \Psi}{\partial x} \sigma_2 \right\rangle}{\langle \sigma_2 \Psi \rangle} \quad (6)$$

Its tally is more complicated than the direct effect term and should use the generalized perturbation theory.

#### 2.2 Introduction of Generalized Perturbation Theory

The Boltzmann equation can be expressed in the form of

$$\left( A - \frac{1}{k} M \right) \Psi = 0 \quad (7)$$

where

$A$  = neutron loss operator,

$M$  = fission neutron production operator and

$k$  = effective multiplication factor.

And the adjoint equation of the Boltzmann equation is

$$\left( A^* - \frac{1}{k} M^* \right) \Psi^* = 0 \quad (8)$$

where

$\Psi^*$  = adjoint flux,

$A^*$  = adjoint neutron loss operator and

$M^*$  = adjoint fission neutron production operator.

With the adjoint equation, one can obtain perturbations in the effective multiplication factor,  $\delta k$ , in the form of

$$\delta k = \frac{\langle \Psi^* (\delta M \Psi - k \delta A) \Psi \rangle}{\langle \Psi^* \frac{1}{k} M \Psi \rangle} \quad (9)$$

Eq. 9 is the foundation to obtain sensitivity coefficients of effective multiplication factor,  $S_{k,x(r,E)}$

$$S_{k,x(r,E)} = \frac{\langle \Psi^* (\frac{1}{k} \delta M \Psi - \delta A) \Psi \rangle}{\langle \Psi^* \frac{1}{k} M \Psi \rangle} \quad (10)$$

In order to compute the indirect term of generalized response sensitivity coefficients, now introducing into the generalized adjoint equation, in the form of

$$(A^* - \frac{1}{k} M^*) \Gamma^* = S^* \quad (11)$$

where

$\Gamma^*$  = generalized adjoint flux and

$S^*$  = adjoint source for the generalized response.

The definition of  $S^*$  is

$$S^* = \frac{1}{R} \frac{\partial R}{\partial \Psi} = \frac{\sigma_1}{\langle \sigma_1 \Psi \rangle} - \frac{\sigma_2}{\langle \sigma_2 \Psi \rangle} \quad (12)$$

Therefore, one can readily obtain

$$\langle \Psi S^* \rangle = 0 \quad (13)$$

Now introducing perturbations in Eq. 7 and only reserving the first-order terms and then multiplying and taking the inner product over phase space, one can obtain

$$\langle \Gamma^* (kA - M) \delta \Psi \rangle = \langle \Gamma^* (\delta M - k \delta A) \Psi \rangle - \delta k \langle \Gamma^* A \Psi \rangle \quad (14)$$

Multiplying Eq. 11 by  $\delta \Psi$  and taking inner product over phase space, one can obtain

$$\langle \delta \Psi (A^* - \frac{1}{k} M^*) \Gamma^* \rangle = \langle \delta \Psi S^* \rangle \quad (15)$$

Combining Eqs. 13-15, one can obtain

$$\langle \frac{1}{R} \frac{\partial R}{\partial \Psi} \delta \Psi \rangle = \langle \Gamma^* (\frac{1}{k} \delta M - \delta A) \Psi \rangle - \frac{\delta k}{k} \langle \Gamma^* A \Psi \rangle \quad (16)$$

Multiplying Eq. 7 by  $\Gamma^*$ , one can obtain

$$\langle \Gamma^* A \Psi \rangle = \langle \Gamma^* \frac{1}{k} M \Psi \rangle \quad (17)$$

Substituting Eq. 9 and Eq. 17 into Eq. 16, one can obtain

$$\langle \frac{1}{R} \frac{\partial R}{\partial \Psi} \delta \Psi \rangle = \left\langle \Gamma^* - \frac{\langle \Gamma^* \frac{1}{k} M \Psi \rangle}{\langle \Psi^* \frac{1}{k} M \Psi \rangle} \Psi^*, (\frac{1}{k} \delta M - \delta A) \Psi \right\rangle \quad (18)$$

As well known, the solution of the Eq. 11 is the sum of a particular solution,  $\Gamma_p^*$ , and a homogeneous solution,  $\Psi^*$

$$\Gamma^* = \Gamma_p^* + c \Psi^* \quad (19)$$

where

$c$  = any constant.

If  $c$  is defined to be  $-\frac{\langle \Gamma_p^* \frac{1}{k} M \Psi \rangle}{\langle \Psi^* \frac{1}{k} M \Psi \rangle}$ , then one can obtain

$$\langle \Gamma^* \frac{1}{k} M \Psi \rangle = 0 \quad (20)$$

Therefore, the indirect effect term can be expressed as

$$S_{in} = \left\langle \Gamma^* x \left( \frac{1}{k} \frac{\delta M}{\partial x} - \frac{\delta A}{\partial x} \right) \Psi \right\rangle \quad (21)$$

Comparing Eq. 21 with Eq. 10, it can be observed that the calculation of the indirect effect term is similar to the eigenvalue sensitivity coefficients while the tally scores of reaction rates are weighted by  $\Gamma^*$  rather than  $\Psi^*$ .

### 2.3 How to compute generalized adjoint function

In this work, the GEAR-MC method [3], which has been implemented in SCALE, is used to compute the generalized adjoint function,  $\Gamma^*$ . The methodology of the GEAR-MC method is summarized here.

Considering  $I = \frac{1}{k} M \Psi$ , one can obtain

$$\langle \Gamma^* I \rangle = \langle \Gamma^* \frac{1}{k} M \Psi \rangle + \langle \Psi S^* \rangle \quad (22)$$

As can be seen, each term in Eq. 22 is zero. Now considering a single neutron source leaving from a collision at phase space  $\tau_s$ , then this source can be expressed as

$$I = I_s \delta(\tau - \tau_s) \quad (23)$$

where

$I_s$  = source strength.

Substituting Eq. 23 into Eq. 22, one can obtain

$$\Gamma^*(\tau_s) = \frac{1}{I_s} \left\langle \Psi(\tau_s \rightarrow r) \frac{1}{R} \frac{\partial R}{\partial \Psi} \right\rangle + \frac{1}{I_s} \left\langle \frac{1}{k} M \Psi(\tau_s \rightarrow r) \Gamma^*(r) \right\rangle \quad (24)$$

According to Eq. 24, the adjoint function at phase space is the sum of two components. The first component is known as the intra-generational component, which describes how much importance of this source neutron produces in the current generation until its death and can be computed by

$$\Gamma^s(\tau_s)_{intra} = \frac{1}{I_s} \left\langle \frac{\sigma_1 \Psi(\tau_s \rightarrow r) - \sigma_2 \Psi(\tau_s \rightarrow r)}{\langle \sigma_1 \Psi \rangle - \langle \sigma_2 \Psi \rangle} \right\rangle \quad (25)$$

The computing of the intra-generational component requires to store reaction rates of each collision until the death of the source neutron. The second component is known as the inter-generational component, which describes how much importance of this source neutron generates in the future generations and can be computed by tallying the cumulative score of  $\Psi(\tau_s \rightarrow r) \frac{1}{R} \frac{\partial R}{\partial \Psi}$  generated by the progeny of this source neutron.

### 3. Numerical Results

By applying the GEAR-MC method [3], a capability to compute generalized sensitivity coefficients is preliminarily developed in RMC. And the TSUNAMI-1D in the SCALE6.1 code package is used to verify this capability. It should be noted that TSUNAMI-1D is a one-dimensional sensitivity and uncertainty sequence based on a discrete ordinate transport code while the TSUNAMI-3D is a three-dimensional sequence based on a Monte Carlo transport code. However, the TSUNAMI-3D in SCALE6.1 does not have the generalized analysis capability. Therefore, due to the limitation of the geometry supported by TSUNAMI-1D in the SCALE6.1, a relative simple problem is used to make verifications. The selected problem is a sphere with a radius of 38.50 cm consisting of five isotopes, namely,  $^1\text{H}$ ,  $^{12}\text{C}$ ,  $^{19}\text{F}$ ,  $^{235}\text{U}$  and  $^{238}\text{U}$ . And only the response function of one group cross-section, in the form of  $\frac{\langle \sigma_1 \Psi \rangle}{\langle \Psi \rangle}$ , are investigated in this work.

A total of 16 different types of one-group cross-section are defined and their sensitivity coefficients to different types of nuclear data are shown in Tab. 1, where the difference is defined as the RMC result divided by the corresponding TSUNAMI-1D result and minus one. As can be seen, all differences are less than 10%, indicating RMC agrees with TSUNAMI-1D generally. It should be noted that TSUNAMI-1D requires to perform 16 adjoint transport calculations in order to solve the solutions of Eq. 11 for each response function while RMC calculates all the generalized sensitivity coefficients weighted by the generalized adjoint function directly in the forward transport calculation.

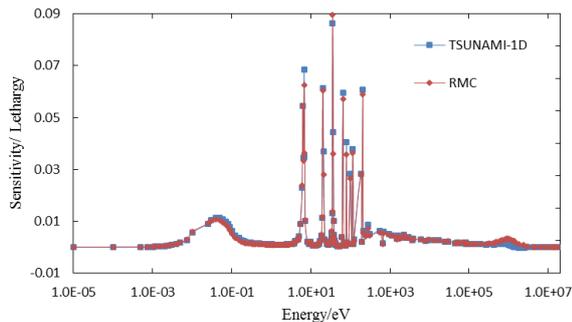


Fig. 1. Energy-Resolved Sensitivity Coefficients of  $^{238}\text{U}$  Inelastic Cross-Section to  $^{238}\text{U}$  Capture Cross-Section.

Some energy-resolved generalized sensitivity coefficients to some nuclear data are presented in Figs. 1-4. And the sensitivity profiles between RMC and TSUNAMI-1D agree roughly.

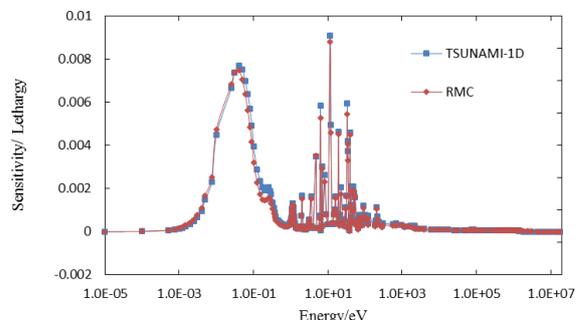


Fig. 2. Energy-Resolved Sensitivity Coefficients of  $^{238}\text{U}$  Fission Cross-Section to  $^{235}\text{U}$  Inelastic Cross-Section.

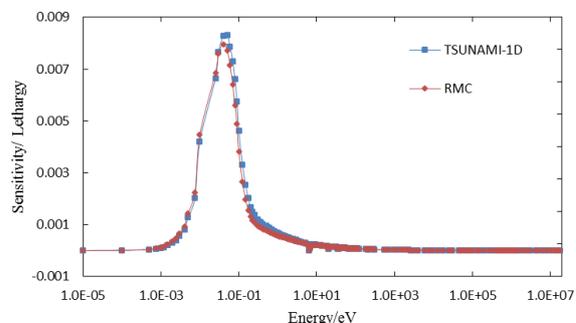


Fig. 3. Energy-Resolved Sensitivity Coefficients of  $^{235}\text{U}$  Inelastic Cross-Section to  $^1\text{H}$  Capture Cross-Section.

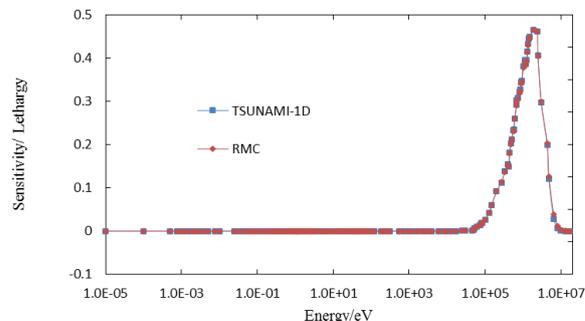


Fig. 4. Energy-Resolved Sensitivity Coefficients of  $^{235}\text{U}$  Inelastic Cross-Section to  $^{235}\text{U}$  Inelastic Cross-Section.

### 6. Conclusions

In this work, a capability of computing generalized response sensitivity coefficients to nuclear data has been preliminarily developed in RMC. In general, results computed by RMC agree with TSUNAMI-1D in SCALE6.1.

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Table I. Energy-Integrated Generalized Sensitivity Coefficients

Response Function		Nuclear Data		Code		Difference
Isotope	Reaction	Isotope	Reaction	TSUNAMI-1D	RMC	
<sup>1</sup> H	elastic	<sup>1</sup> H	elastic	1.30E+00	1.37E+00	5.65%
<sup>1</sup> H	capture	<sup>1</sup> H	capture	9.15E-01	1.01E+00	9.90%
<sup>12</sup> C	total	<sup>12</sup> C	elastic	1.01E+00	1.00E+00	-0.19%
<sup>12</sup> C	total	<sup>235</sup> U	inelastic	2.43E-04	2.29E-04	-6.05%
<sup>12</sup> C	elastic	<sup>12</sup> C	elastic	1.01E+00	1.01E+00	-0.19%
<sup>12</sup> C	elastic	<sup>235</sup> U	inelastic	2.44E-04	2.29E-04	-6.44%
<sup>12</sup> C	inelastic	<sup>1</sup> H	capture	2.14E-02	2.05E-02	-4.28%
<sup>12</sup> C	inelastic	<sup>235</sup> U	capture	2.58E-02	2.44E-02	-5.31%
<sup>12</sup> C	capture	<sup>12</sup> C	capture	1.00E+00	1.00E+00	0.05%
<sup>19</sup> F	total	<sup>19</sup> F	inelastic	1.07E-01	1.11E-01	3.90%
<sup>19</sup> F	total	<sup>19</sup> F	elastic	8.84E-01	9.01E-01	1.83%
<sup>19</sup> F	elastic	<sup>235</sup> U	inelastic	2.18E-04	2.28E-04	4.51%
<sup>19</sup> F	elastic	<sup>19</sup> F	elastic	9.94E-01	1.00E+00	0.60%
<sup>19</sup> F	inelastic	<sup>238</sup> U	capture	8.75E-02	8.80E-02	0.62%
<sup>19</sup> F	inelastic	<sup>1</sup> H	capture	2.13E-02	2.05E-02	-4.18%
<sup>19</sup> F	inelastic	<sup>235</sup> U	capture	2.56E-02	2.44E-02	-4.81%
<sup>19</sup> F	capture	<sup>19</sup> F	capture	9.99E-01	1.00E+00	0.21%
<sup>235</sup> U	elastic	<sup>235</sup> U	elastic	1.00E+00	1.00E+00	-0.01%
<sup>235</sup> U	inelastic	<sup>235</sup> U	inelastic	9.99E-01	1.00E+00	0.12%
<sup>235</sup> U	inelastic	<sup>19</sup> F	capture	6.54E-04	6.54E-04	0.06%
<sup>235</sup> U	inelastic	<sup>238</sup> U	capture	8.85E-02	8.81E-02	-0.48%
<sup>235</sup> U	inelastic	<sup>12</sup> C	capture	1.04E-04	1.02E-04	-2.30%
<sup>235</sup> U	inelastic	<sup>1</sup> H	capture	2.14E-02	2.05E-02	-4.23%
<sup>235</sup> U	inelastic	<sup>235</sup> U	capture	2.57E-02	2.44E-02	-4.96%
<sup>238</sup> U	total	<sup>238</sup> U	elastic	7.65E-01	7.74E-01	1.23%
<sup>238</sup> U	total	<sup>238</sup> U	inelastic	9.20E-02	8.35E-02	-9.32%
<sup>238</sup> U	elastic	<sup>238</sup> U	elastic	9.72E-01	9.89E-01	1.69%
<sup>238</sup> U	elastic	<sup>19</sup> F	inelastic	1.49E-02	1.42E-02	-4.70%
<sup>238</sup> U	inelastic	<sup>238</sup> U	capture	8.87E-02	8.81E-02	-0.63%
<sup>238</sup> U	inelastic	<sup>1</sup> H	capture	2.14E-02	2.05E-02	-4.24%
<sup>238</sup> U	inelastic	<sup>235</sup> U	capture	2.57E-02	2.44E-02	-4.97%
<sup>238</sup> U	fission	<sup>12</sup> C	capture	1.03E-04	1.02E-04	-1.11%
<sup>238</sup> U	fission	<sup>19</sup> F	capture	6.69E-04	6.54E-04	-2.15%
<sup>238</sup> U	fission	<sup>238</sup> U	capture	9.08E-02	8.81E-02	-2.93%
<sup>238</sup> U	fission	<sup>1</sup> H	capture	2.14E-02	2.05E-02	-4.31%
<sup>238</sup> U	fission	<sup>235</sup> U	capture	2.57E-02	2.44E-02	-5.22%