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CONTINUOUS-ENERGY MONTE CARLO METHODS FOR CALCULATING GENERALIZED RESPONSE SENSITIVITIES USING TSUNAMI-3D*

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ABSTRACT

This work introduces a new approach for calculating sensitivity coefficients for generalized neutronic responses to nuclear data uncertainties using continuous-energy Monte Carlo methods. The GEneralized Adjoint Responses in Monte Carlo (GEAR-MC) method has been developed to enable the calculation of generalized sensitivity coefficients for multiple responses in a single Monte Carlo calculation with no nuclear data perturbations or knowledge of nuclear covariance data. The theory behind the GEAR-MC method is presented here, and proof of principle is demonstrated by using the GEAR-MC method to calculate sensitivity coefficients for responses in several 3D, continuous-energy Monte Carlo applications.

Key Words: **TSUNAMI, Monte Carlo, GPT, continuous-energy, CLUTCH**

1. INTRODUCTION

Sensitivity coefficients describe the fractional change in a system response that is induced by changes to system parameters and nuclear data. Computational tools have been developed over the past decade that calculate sensitivity coefficients for the critical eigenvalue of three-dimensional (3D) systems using the Monte Carlo method, and the ability to model complex, real-world problems using these high-fidelity methods has resulted in the development of a suite of tools for quantifying the impact of cross-section uncertainties in criticality safety and reactor physics applications. The TSUNAMI (Tools for Sensitivity and UNcertainty Analysis Methodology Implementation) code suite within the SCALE code package has created a multitude of research and application opportunities in the field of sensitivity and uncertainty quantification, such as comparing computational models with experimental data to guide the adjustment of nuclear data parameters, assessing the similarity and sources of biases between different nuclear systems, designing effective nuclear criticality experiments, and many other criticality safety and reactor physics applications [1].

The current sensitivity and uncertainty analysis methodology in TSUNAMI-3D, the tool within the TSUNAMI suite for calculating sensitivity coefficients using 3D Monte Carlo methods, is limited to calculating eigenvalue sensitivity coefficients, and there is interest in extending this

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methodology to calculate sensitivity coefficients for a generalized set of neutronic responses, such as neutron fluxes, isotopic reaction rates, and power distributions. Eigenvalue sensitivity information is certainly useful for criticality safety applications, but uncertainty quantification for power distributions, the generation of multigroup cross sections, isotope production/destruction rates, and neutron fluence rates are especially useful for reactor design applications because these quantities often limit the operating power and lifetime of reactors. A more thorough understanding of how uncertainty in nuclear data impacts reactor design calculations would be useful for guiding regulatory limits and safety margins for these key reactor parameters.

Deterministic methods exist in SCALE for calculating generalized response sensitivity coefficients using Generalized Perturbation Theory (GPT), but the current methods are limited to one-dimensional (1D) and two-dimensional (2D) systems. Currently, SCALE cannot perform GPT calculations using high-fidelity, continuous-energy Monte Carlo techniques [1]. Alternatively, some methods have been developed by Abel-Khalik et al. for calculating generalized sensitivity coefficients in 3D, continuous-energy Monte Carlo applications, but these methods require performing multiple direct perturbation calculations and can require a large number of runs to calculate generalized sensitivity coefficients [2] [3]. Furthermore, these direct perturbation-based methods can produce poor sensitivity coefficient estimates if inaccurate nuclear covariance data is available because the data perturbations that are sampled are based on the nuclear covariance data.

The method described in this paper, referred to as the GEAR-MC method, enables the calculation of sensitivity and uncertainty information for generalized responses in 3D, continuous-energy Monte Carlo applications using a single Monte Carlo transport calculation with no data perturbations. This new method should substantially increase the applicability and ease of use of sensitivity analysis for a wide range of criticality safety, reactor physics, and other neutron transport applications. In this paper, the theory behind the GEAR-MC method is presented, and the method is used to calculate response sensitivities for several criticality safety and reactor physics applications. Reference response sensitivities are calculated for these applications using direct perturbation methods [1]. The test problems examined in this study were modeled using a 3D, continuous-energy Monte Carlo code, but also feature 1D spatial symmetry to allow for a comparison with sensitivity coefficients calculated using the TSUNAMI-1D code, an established tool for calculating generalized response sensitivities in 1D applications [1].

2. THEORY

Sensitivity coefficients describe the fractional change in a response, R, that is induced by changes to system parameters. The general response sensitivity coefficient for the parameter Σ_x is defined as

$$S_{R,\Sigma_x} = \frac{\delta R/R}{\delta \Sigma_x/\Sigma_x}. \quad (1)$$

Consider a response function R that is the ratio of two reaction rates integrated over some energy range such that

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

where Σ_1 and Σ_2 are nuclear cross sections. The reaction rates in Equation (2) can be isotope- or material-dependent reaction rates and can also represent flux responses by setting $\Sigma = 1$. The fractional change in R due to a perturbation $\delta\Sigma_x$ to the system parameter Σ_x is given by

$$\frac{\delta R}{R} = \left\langle \frac{1}{R}\frac{\partial R}{\partial \Sigma_x}\delta\Sigma_x + \frac{1}{R}\frac{\partial R}{\partial \phi}\frac{\partial \phi}{\partial \Sigma_x}\delta\Sigma_x \right\rangle. \tag{3}$$

The first term in Equation (3) is known as the Direct Effect term and describes how perturbations in Σ_x affect the response function of the response reaction rates. The second term, known as the Indirect Effect term, describes how perturbations throughout the system affect the neutron flux spectrum in the response region [4]. Calculating the sensitivity of the response to the Direct Effect term is relatively simple, and involves tallying the fraction of the total numerator and denominator responses that is generated for each energy, region, isotope, and material in the response region(s). For example, consider a response that is defined as the ratio of the energy-integrated fission rate to the energy-integrated capture rate in a uranium fuel pin. The Direct Effect sensitivity of this response to the thermal fission cross section is simply the fraction of the fission reaction rate in the pin that is caused by neutrons with thermal energies.

The Indirect Effect term in Equation (3) cannot be calculated as simply as the Direct Effect term, and this work describes an approach for calculating this term during a single, unperturbed Monte Carlo transport calculation. The neutron balance equation for an eigenvalue problem is given by

$$L\phi - \lambda P\phi = 0, \tag{4}$$

where L is the neutron loss operator and P is the fission neutron production operator. The change induced in the neutron balance equation in response to a first-order perturbation is given by

$$(L - \lambda P)\delta\phi = \delta\lambda P\phi + (\lambda\delta P - \delta L)\phi. \tag{5}$$

Consider now the generalized adjoint balance equation

$$(L^* - \lambda P^*)\Gamma^* = S^*, \tag{6}$$

where L^* is the adjoint loss term, S^* is a source of importance for the response that is defined such that $\langle \phi\, S^* \rangle = 0$, and Γ^* is the generalized importance function that provides the solution to this equation [4]. Multiplying Equations (5) and (6) by Γ^* and $\delta\phi$, respectively, and taking the inner product gives, respectively,

$$\langle \Gamma^* (L - \lambda P)\ \delta\phi \rangle = \ \delta\lambda \langle \Gamma^* P \phi \rangle + \langle \Gamma^*\ (\lambda \delta P - \delta L) \phi \rangle\ , \tag{7}$$

and

$$\langle \delta\phi\ (L^* - \lambda P^*)\ \Gamma^* \rangle = \langle \delta\phi\ S^* \rangle\ . \tag{8}$$

The source of adjoint importance in Equation (8) is defined to conveniently provide an expression for the Indirect Effect term [4]. Defining S^* as

$$S^* \equiv \frac{1}{R} \frac{\delta R}{\delta \phi} = \frac{\Sigma_1}{\langle \Sigma_1 \phi \rangle} - \frac{\Sigma_2}{\langle \Sigma_2 \phi \rangle}\, , \tag{9}$$

and applying the adjoint property allows Equations (7) and (8) to be combined and express the Indirect Effect term as

$$\langle \frac{1}{R} \frac{\delta R}{\delta \phi} \delta\phi \rangle = \ \langle \delta\lambda\, \Gamma^* P \phi \rangle + \langle \Gamma^*\ (\lambda \delta P - \delta L) \phi \rangle\ . \tag{10}$$

The $\langle \delta\lambda\, \Gamma^* P \phi \rangle$ term in Equation (10) is usually equal to zero because Γ^* is typically orthogonal to $P\phi$ [4]. The effect of this orthogonality can be interpreted in a more physical manner by realizing that perturbations to the eigenvalue of a system do not alter the steady-state neutron flux shape or spectrum of the system. As a result, the perturbations affect the response numerator and denominator terms equally. The $1/\partial \Sigma_x$ term is ignored in the above equation for ease of viewing.

The GEAR-MC methodology uses Equations (6) and (10) to calculate the generalized importance function Γ^* for neutrons during a single forward Monte Carlo simulation, thus enabling the calculation of sensitivity coefficients for generalized responses via generalized perturbation theory. The approach developed for calculating Γ^* is similar to the approach used by the CLUTCH (Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization) method for calculating eigenvalue sensitivity coefficients. Based on Williams' Contributon theory, the CLUTCH method was developed by Perfetti in 2012 to enable rapid and memory-efficient eigenvalue sensitivity coefficient calculations for continuous-energy Monte Carlo applications [5] [6] [7] [8].

Assuming that the fission production term, $\lambda P \phi$, in Equation (4) is the sole source of neutron production in a system, Q, multiplying Equations (4) and (6) by Γ^* and ϕ, respectively, and integrating over all phase space gives

$$\langle \Gamma^* L \phi \rangle = \langle \Gamma^* Q \rangle\ , \tag{11}$$

and

$$\langle \phi L^* \Gamma^* \rangle = \lambda \langle \phi P^* \Gamma^* \rangle + \langle \phi S^* \rangle \; . \tag{12}$$

Combining Equations (11) and (12) using the adjoint property gives

$$\langle \Gamma^* Q \rangle = \lambda \langle \Gamma^* P \phi \rangle + \langle \phi S^* \rangle \; . \tag{13}$$

The terms in Equation (13) are all equal to zero in inner product space, but Equation (13) can be used to extract information about the importance of events by considering the neutron source to be a single neutron traveling through the phase space τ_s, such as a neutron entering or leaving a collision at some point. This concept is used similarly in Williams' Contributon theory for calculating eigenvalue sensitivity coefficients, and assumes that

$$Q = Q_s \; \delta(\tau - \tau_s) \; , \tag{14}$$

where Q_s is the source strength for this neutron [5] [9]. Substituting Equation (14) into Equation (13) produces an expression for the generalized importance function at τ_s:

$$\begin{aligned} \Gamma^*(\tau_s) &= \frac{1}{Q_s} \langle S^*(r) \; \phi(\tau_s \rightarrow r) \rangle \; + \; \frac{\lambda}{Q_s} \langle \Gamma^*(r) \; P \; \phi(\tau_s \rightarrow r) \rangle \\ &= \frac{1}{Q_s} \langle \frac{1}{R} \frac{\delta R}{\delta \phi}(r) \; \phi(\tau_s \rightarrow r) \rangle \; + \; \frac{\lambda}{Q_s} \langle \Gamma^*(r) \; P \; \phi(\tau_s \rightarrow r) \rangle, \end{aligned} \tag{15}$$

where $\phi(\tau_s \rightarrow r)$ is the neutron flux created at r by the neutron originating at τ_s. The two terms on the right-hand side of Equations (13) and (15) represent the intragenerational and intergenerational effects of an event on the importance of a particle, respectively. The intragenerational effect term describes how much importance the neutron in phase space τ_s generates in the response region(s) during its lifetime, while the intergenerational effect term describes how many fission neutrons this neutron creates and how much importance these fission neutrons will generate in future generations. The intragenerational term can be determined by tallying the amount of flux generated in the response region(s) and weighted by $S^*(r)$ from Equation (9) from the time the particle enters phase space τ_s until its death; thus, the intragenerational term is given by

$$\langle S^*(r) \; \phi(\tau_s \rightarrow r) \rangle = \frac{\Sigma_1 \phi(\tau_s \rightarrow r)}{\langle \Sigma_1 \phi \rangle} - \frac{\Sigma_2 \phi(\tau_s \rightarrow r)}{\langle \Sigma_2 \phi \rangle} \; . \tag{16}$$

The approach for calculating the intragenerational importance term in Equation (16) is similar to the approach used by the CLUTCH method during eigenvalue sensitivity coefficient calculations, and requires storing tracklength information for each collision a particle enters and determining the importance of that collision after the particle dies [6]. It should be noted that the presence of both positive and negative terms in Equation (16) allows a single event to generate either a positive or negative importance. The intergenerational contribution to the importance function can be calculated by tallying the cumulative score of $\phi(\tau_s \rightarrow r)$ weighted by $S^*(r)$ that is generated by the particle's daughter fission neutrons, or "progeny," over some number of generations. This approach is used similarly by the Iterated Fission Probability (IFP) approach for calculating the importance of events during eigenvalue sensitivity calculations, except that the IFP method tallies the importance only one time once the daughter neutrons have established an asymptotic population in the system [5] [10]. The GEAR-MC method estimates the intergenerational importance by summing the importance created by each ith generation of fission neutrons, $\Gamma_i^* F_i$, where $\Gamma_i^* = \langle S^*(r)\ \phi(F_i \rightarrow r)\rangle$, over some number of generations:

$$\lambda\langle \Gamma^*(r)\ P\ \phi(\tau_s \rightarrow r)\rangle = \Gamma_1^* F_1 + \Gamma_2^* F_2 + \Gamma_3^* F_3 + \ldots + 0\,. \tag{17}$$

As previously discussed for the $\delta\lambda$ term in Equation (10), the $\langle \Gamma^* P\phi\rangle$ term is typically constrained to equal zero, causing the $\Gamma_i^* F_i$ terms to approach zero as i approaches infinity; therefore, the intergenerational importance term is obtained by taking the sum of the $\Gamma_i^* F_i$ terms as they asymptotically approach zero.

3. PROOF OF PRINCIPLE

The GEAR-MC methodology was implemented in the KENO Monte Carlo code within the continuous-energy TSUNAMI sequence of the SCALE code system and used to calculate generalized response sensitivities for several responses in models of several systems using continuous-energy Monte Carlo transport calculations. The applications selected for this study deliberately feature 1D spatial symmetry so that response sensitivities could also be calculated using the SCALE TSUNAMI-1D tool and compared with GEAR-MC sensitivities. Direct perturbation continuous-energy KENO calculations were used to generate reference sensitivity coefficients and evaluate the accuracy of the TSUNAMI-1D and GEAR-MC methods [1].

Three critical systems were examined in this study: HEU-MET-FAST-001 (Godiva) [11], PU-MET-FAST-006 (Flattop) [11], and an infinitely-reflected 2.7%-enriched PWR fuel pin (Fuel Pin) [12]. Several response ratio and spectral index sensitivities were examined for each system, as described in Table 1. The first letter of the spectral indices in Table 1 describes the reaction being examined (C is capture and F is fission), and the following number represents the nuclide being examined (25 is U-235, 28 is U-238, and 37 is Np-237). F-ALL represents the total fission rate in all regions and isotopes in the system. For example, the Fuel Pin response "C28 / F-ALL" describes the ratio of the capture reaction rate in U-238 to the fission rate in the entire fuel pin. The responses examined in this study include both integral responses and activation foil responses.

Table 1. Response ratios examined.

Experiment	Response Ratio	Response Equation	Response Region	Response Energy Range
Godiva	C25 / F25	$\frac{\langle \Sigma_{cap}^{U-235}\phi\rangle}{\langle \Sigma_{fis}^{U-235}\phi\rangle}$	$\frac{Fuel\ Region}{Fuel\ Region}$	$\frac{All\ Energies}{All\ Energies}$
	F28 / F25	$\frac{\langle \Sigma_{fis}^{U-238}\phi\rangle}{\langle \Sigma_{fis}^{U-235}\phi\rangle}$	$\frac{Fuel\ Region}{Fuel\ Region}$	$\frac{All\ Energies}{All\ Energies}$

Flattop	F28 / F25	$\frac{\langle \Sigma_{fis}^{U-238} \phi \rangle}{\langle \Sigma_{fis}^{U-235} \phi \rangle}$	$\frac{Foil\ Activity}{Foil\ Activity}$	$\frac{All\ Energies}{All\ Energies}$
	F37 / F25	$\frac{\langle \Sigma_{fis}^{Np-237} \phi \rangle}{\langle \Sigma_{fis}^{U-235} \phi \rangle}$	$\frac{Foil\ Activity}{Foil\ Activity}$	$\frac{All\ Energies}{All\ Energies}$
Fuel Pin	C28 / F-ALL	$\frac{\langle \Sigma_{cap}^{U-238} \phi \rangle}{\langle \Sigma_{fis}^{Fuel} \phi \rangle}$	$\frac{Fuel\ Region}{Fuel\ Region}$	$\frac{All\ Energies}{All\ Energies}$
	F28 / F25	$\frac{\langle \Sigma_{fis}^{U-238} \phi \rangle}{\langle \Sigma_{fis}^{U-235} \phi \rangle}$	$\frac{Fuel\ Region}{Fuel\ Region}$	$\frac{All\ Energies}{All\ Energies}$

3.1. Godiva Results

The Godiva responses examined in this study consist of ratios of integral reaction rates in the Godiva critical assembly. The TSUNAMI-1D Godiva simulations used an S_{16} discrete ordinates quadrature set and a 238-group energy structure, and the GEAR-MC calculations used 3D, continuous-energy models of the Godiva system. The reference direct perturbation sensitivities and the calculated GEAR-MC and TSUNAMI-1D (T1D) sensitivities are given below for the most significant nuclides in the Godiva system. The difference between the calculated and reference sensitivities in terms of the number of effective standard deviations (σ_{eff}) is shown in parentheses in Table 2. The sensitivity coefficient uncertainties used to calculate σ_{eff} for the TSUNAMI-1D sensitivity coefficient comparison are equal to the uncertainty in the direct perturbation sensitivity coefficients because the TSUNAMI-1D calculations use deterministic transport methods. The GEAR-MC and TSUNAMI-1D methods both produced total nuclide sensitivities that agreed well with the direct perturbation sensitivities, and none of the calculated total nuclide sensitivities produced a statistically significant (more than two standard deviation) disagreement with the direct perturbation sensitivities.

Table 2. Godiva integral response nuclide sensitivity coefficients.

Experiment	Response	Isotope	Direct Perturbation	GEAR-MC	T1D
Godiva	C25 / F25	U-235	0.1658 ± 0.0103	0.1501 ± 0.0002 (-1.53 σ_{eff})	0.1610 (-0.47 σ_{eff})
		U-238	0.0211 ± 0.0012	0.0205 ± 0.0001 (-0.46 σ_{eff})	0.0211 (-0.02 σ_{eff})
	F28 / F25	U-235	-1.3200 ± 0.0768	-1.2333 ± 0.0002 (1.13 σ_{eff})	-1.2443 (0.99 σ_{eff})
		U-238	1.0235 ± 0.0598	0.9680 ± 0.0001 (-0.93 σ_{eff})	0.9675 (-0.02 σ_{eff})

Figures 1 and 2 show the energy-dependent sensitivity profiles for the C25 / F25 response to various U-235 and U-238 reactions, respectively. The C25 / F25 sensitivity to U-235 is dominated by the fission and capture reaction components, and there is a positive-to-negative inflection in the U-235 total nuclide sensitivity around 1 MeV. The GEAR-MC sensitivity coefficients accurately capture this inflection point, and there is little visible difference between the GEAR-MC and TSUNAMI-1D sensitivity coefficients for this or any other sensitivity profile in the figure.

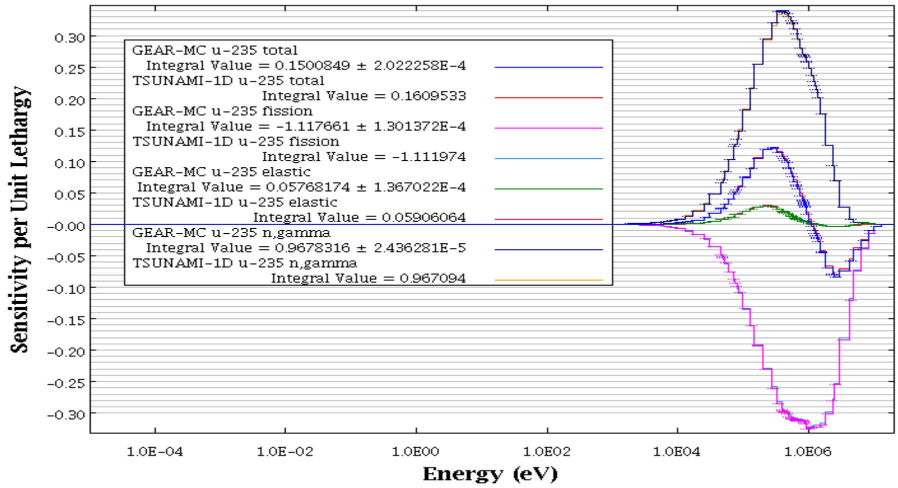

Figure 1. Godiva C25 / F25 U-235 sensitivity coefficients.

Figure 2 shows the Godiva C25 / F25 sensitivity to various U-238 reactions. These sensitivity coefficients contain no Direct Effect component because U-238 reactions are not in the numerator or denominator of the C25 / F25 response ratio; thus, these sensitivity profiles describe only how U-238 affects the flux spectrum in the activation foils, that is, the Indirect Effect term. The U-238 total nuclide sensitivity is dominated by the elastic scattering component until about 500 keV, at where inelastic, (*n,n'*), scattering reaction becomes more important. Some small differences between the GEAR-MC and TSUNAMI-1D sensitivities are visible, but in general the two codes again produced energy-dependent sensitivity coefficients that agreed very well. As with the U-235 response sensitivities from Figure 1, there is almost no visible difference between the GEAR-MC and TSUNAMI-1D sensitivity profiles in Figure 2.

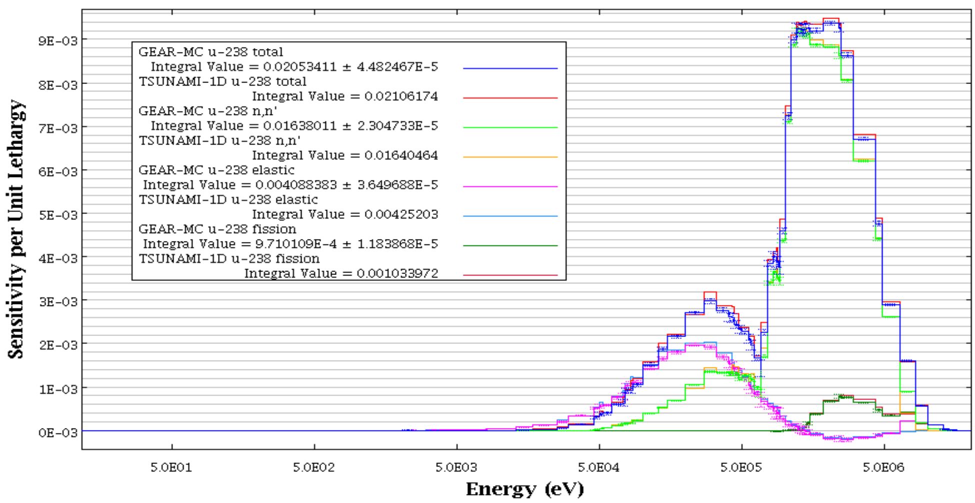

Figure 2. Godiva C25 / F25 U-238 sensitivity coefficients.

3.2. Flattop Results

The Flattop experiment consists of a sphere of plutonium-gadolinium alloy that is reflected by a region of depleted uranium [11]. Unlike the responses examined for the Godiva and Fuel Pin systems, the Flattop responses examined in this study were not integral responses but reaction rate ratios for irradiation foils at the center of the Flattop experiment. Table 3 compares the reference and calculated total nuclide sensitivity coefficients for the most important nuclides for the Flattop foil responses. U-235 sensitivities are not included in this table because U-235 was not present in this system except for in the foil response region and in small quantities in the depleted uranium reflector. The effect of the U-235 in the reflector on the flux spectrum in the foil response region is very small, and the calculated U-235 sensitivities are almost entirely dominated by the Direct Effect component from the U-235 in the irradiation foils, which causes the U-235 nuclide sensitivities to be approximately equal to negative one. Benchmarking such a predictable sensitivity coefficient does not provide useful insight on the accuracy of the GEAR-MC and TSUNAMI-1D sensitivity methods, and thus the Flattop U-235 sensitivities were not examined in this analysis.

The TSUNAMI-1D Flattop simulations in this study used an S_{32} discrete ordinates quadrature set. As shown in Table 3, the calculated U-238 nuclide sensitivities agree well with the direct perturbation sensitivities, but the TSUNAMI-1D Pu-239 nuclide sensitivities show significant disagreement compared to the direct perturbation sensitivities for both responses. The GEAR-MC Pu-239 sensitivities both agree well with the direct perturbation sensitivities, suggesting that high-fidelity, continuous-energy Monte Carlo methods may offer an improvement in sensitivity coefficient accuracy for generalized responses, even for relatively simple 1D systems.

Table 3. Flattop foil response nuclide sensitivity coefficients.

Exp.	Response	Isotope	Direct Perturbation	GEAR-MC	T1D
Flattop	F28 / F25	U-238	0.8006 ± 0.0533	0.7954 ± 0.0018 (-0.10 σ_{eff})	0.8024 (0.03 σ_{eff})
		Pu-239	0.0528 ± 0.0043	0.0561 ± 0.0012 (0.73 σ_{eff})	0.0657 (2.99 σ_{eff})
	F37 / F25	U-238	-0.1540 ± 0.0102	-0.1608 ± 0.0016 (-0.66 σ_{eff})	-0.1551 (-0.11 σ_{eff})
		Pu-239	0.0543 ± 0.0048	0.0489 ± 0.0010 (-1.10 σ_{eff})	0.0736 (3.99 σ_{eff})

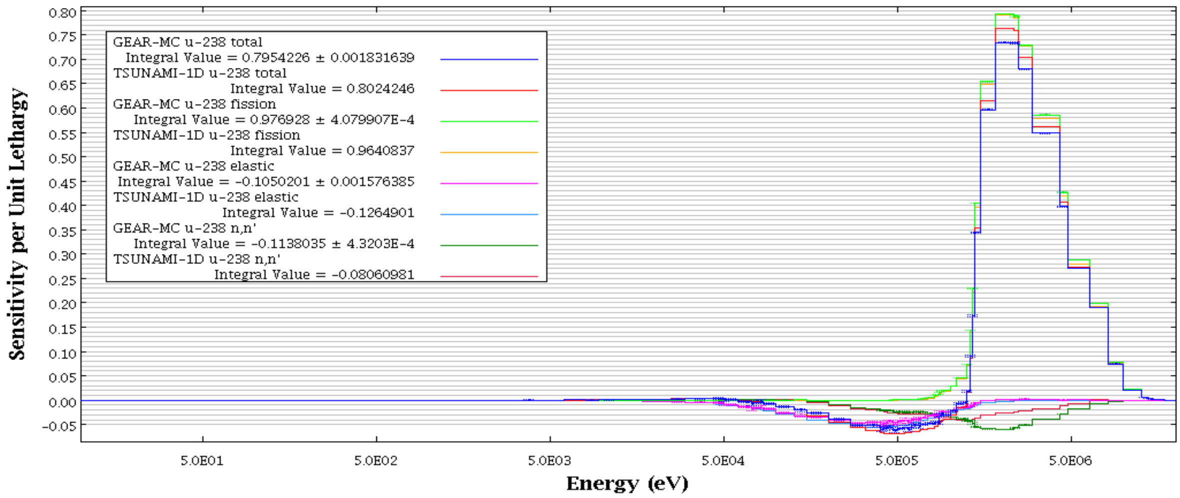

Figure 3. Flattop F28 / F25 U-238 sensitivity coefficients.

Figures 3 and 4 show the energy-dependent sensitivities for the Flattop F28 / F25 response to various U-238 and Pu-239 reactions, respectively. Some disagreement is visible in the U-238 inelastic scattering sensitivities above about 1 MeV, and this disagreement propagates to induce some small disagreement in the total U-238 sensitivities in this same energy range; similar disagreement is visible in the Pu-239 sensitivities in Figure 4 in this same energy range. While the U-238 sensitivities disagreed principally for the inelastic scattering reaction, the Pu-239 sensitivities show noticeable disagreement for the elastic, inelastic, and, most notably, the fission reactions. Such disagreement causes the TSUNAMI-1D energy-integrated F28 / F25 Pu-239 sensitivity coefficients in Table 3 to differ significantly from the GEAR-MC sensitivities. The TSUNAMI-1D Pu-239 sensitivity coefficients exhibited statistically significant disagreement with the direct perturbation sensitivities, indicating that the high-fidelity, continuous-energy Monte Carlo methods used in the GEAR-MC calculations may offer an improvement in sensitivity coefficient accuracy.

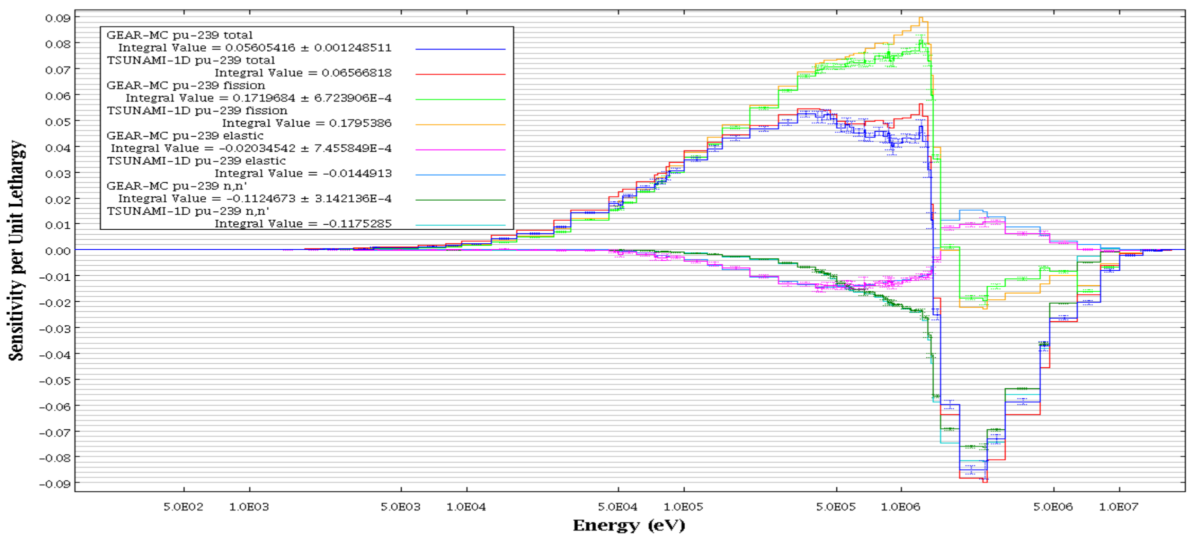

Figure 4. Flattop F28 / F25 Pu-239 sensitivity coefficients.

3.3. Fuel Pin Results

The Fuel Pin system describes a typical, infinitely-reflected, 2.7%-enriched PWR fuel pin, and the responses examined for this system were the ratio of the U-238 capture rate to the fission rate in all nuclides (C28 / F-ALL), and the ratio of the U-238 and U-235 fission reaction rates (F28 / F25). Table 4 compares the reference and calculated total nuclide sensitivity coefficients for the most important nuclides for the Fuel Pin responses.

Table 4. Fuel pin integral response nuclide sensitivity coefficients.

Exp.	Response	Isotope	Direct Perturbation	GEAR-MC	T1D
Fuel Pin	C28 / F-ALL	H-1	-0.4204 ± 0.0323	-0.4413 ± 0.0010 (-0.65 σ_{eff})	-0.4930 (-2.25 σ_{eff})
		U-235	-0.4557 ± 0.0308	-0.4764 ± 0.0002 (-0.67 σ_{eff})	-0.4670 (-0.37 σ_{eff})
		U-238	0.7690 ± 0.0733	0.7970 ± 0.0004 (0.38 σ_{eff})	0.7977 (0.39 σ_{eff})
	F28 / F25	H-1	-0.5463 ± 0.0112	-0.5511 ± 0.0018 (-0.42 σ_{eff})	-0.5581 (-1.05 σ_{eff})
		U-235	-0.1962 ± 0.0038	-0.1871 ± 0.0004 (2.37 σ_{eff})	-0.2127 (-4.28 σ_{eff})
		U-238	0.8727 ± 0.0232	0.8728 ± 0.0007 (0.00 σ_{eff})	0.9037 (1.34 σ_{eff})

As shown in Table 4, the GEAR-MC and TSUNAMI-1D methods produced response sensitivity coefficients that generally agreed well with the direct perturbation sensitivities, although the TSUNAMI-1D C28 / F-ALL H-1 sensitivities exhibited a statistically significant disagreement. As shown in Figure 5, which compares the GEAR-MC and TSUNAMI-1D energy-dependent sensitivity profiles for H-1, the GEAR-MC and TSUNAMI-1D sensitivity profiles are nearly identical for all energies except for those corresponding to the peaks of large capture resonances. This disagreement may be due to approximations in the TSUNAMI-1D treatment for sensitivity coefficients near resonance absorption energies. Similar behavior has been observed previously in eigenvalue sensitivity calculations, and has been attributed to approximations in the calculation of implicit sensitivity coefficients, which describe how nuclear data uncertainties affect the generation of self-shielded multigroup cross sections [8]. The GEAR-MC calculations do not need to account for implicit effects because GEAR-MC uses continuous-energy cross sections, which could be responsible for the observed improvement in sensitivity coefficient accuracy. The F28 / F25 U-235 sensitivity calculated by TSUNAMI-1D disagreed with the direct perturbation sensitivity by more than four standard deviations, indicating a statistically significant difference. It is unclear whether this disagreement indicates a weakness in the sensitivity methods or if the direct perturbation sensitivity coefficients include some second-order sensitivity effects.

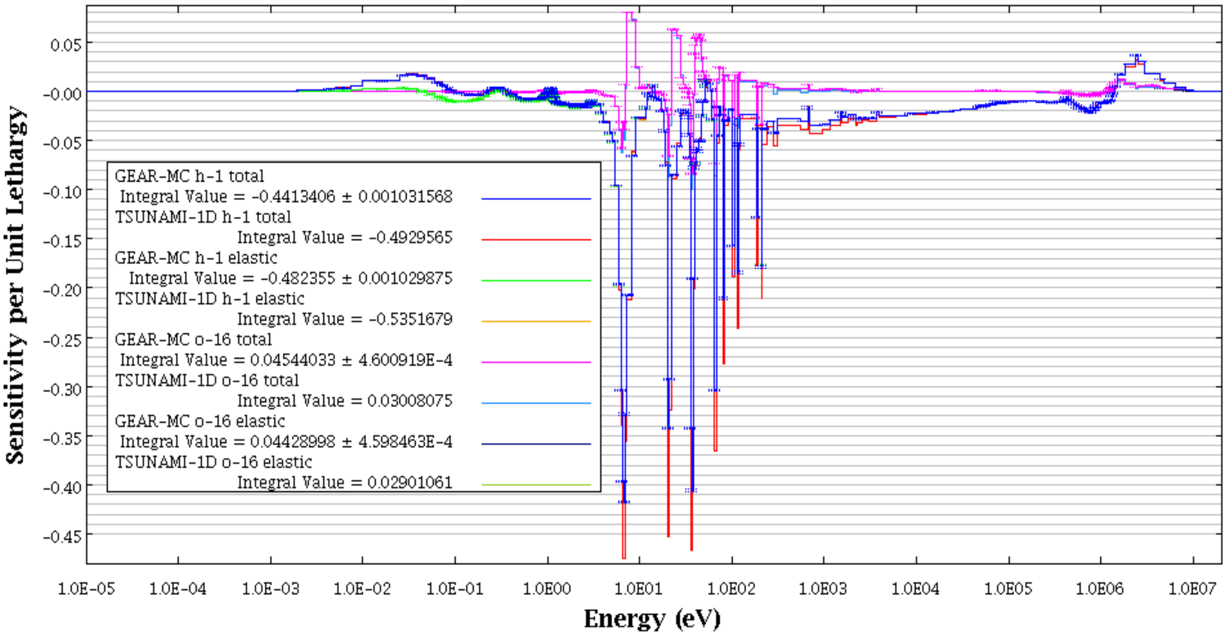

Figure 5. Fuel Pin C28 / F-ALL H-1 sensitivity coefficients.

4. INTERGENERATIONAL EFFECTS

4.1 Intragenerational VS Intergenerational Effects

The GEAR-MC method has been shown to calculate generalized response sensitivity coefficients that are at least as accurate than those produced by TSUNAMI-1D, but it remains to be determined if the problems examined in this study were difficult enough to demonstrate proof of principle. If the response sensitivities are dominated by intragenerational, rather than intergenerational, effects, then existing Monte Carlo tools that ignore the impact of perturbations and cross-section uncertainties on the fission source of systems, such as Differential Operator or fixed-source sensitivity methods, can easily calculate generalized response sensitivities [13].

The accuracy of the GEAR-MC treatment of intergenerational effects and the applicability of these test cases was quantified by examining the fractional contribution of the intergenerational effect to the previously examined total nuclide sensitivities for the responses in each system. As shown in Table 5, the Godiva experiment saw some intergenerational effects, but the Flattop total nuclide sensitivities were dominated by intergenerational effects. In particular, the intergenerational effects for the Godiva Pu-239 sensitivities were especially significant, sometimes outweighing the intragenerational effect terms. The GEAR-MC Pu-239 sensitivity coefficients for these responses agree well with the direct perturbation sensitivity coefficients, indicating that GEAR-MC is correctly calculating the intergenerational effect terms for these responses; in fact, the GEAR-MC sensitivity coefficients for these nuclides and responses showed better agreement with direct perturbation sensitivities than the TSUNAMI-1D sensitivity coefficients, indicating a possible improvement in generalized response sensitivity coefficient accuracy offered by combining the GEAR-MC method for calculating intergenerational effects with high-fidelity continuous-energy Monte Carlo methods. The fuel pin response sensitivities saw almost no intergenerational effects, which was expected because perturbations and data uncertainties do not greatly perturb the shape of the fission source in the infinitely-reflected system.

Table 5. Fractional contribution of intergenerational effects to GEAR-MC response sensitivities

Experiment	Response	Isotope	Intergenerational Contribution
Godiva	C25 / F25	U-235	4.8%
		U-238	0.9%
	F28 / F25	U-235	0.6%
		U-238	0.0%
Flattop	F28 / F25	U-238	1.7%
		Pu-239	70.3%
	F37 / F25	U-238	2.8%
		Pu-239	27.9%
Fuel Pin	C28 / F-ALL	H-1	0.0%
		U-235	0.0%
		U-238	0.0%
	F28 / F25	H-1	0.2%
		U-235	0.2%
		U-238	0.0%

4.2 Convergence of Intergenerational Importance Estimates

Because $\langle \Gamma^* P\phi \rangle$ must equal zero, the importance of each *i*th generation of progeny in Equations (15) and (17) approaches zero as *i* approaches infinity and the progeny of a fission event disperse through the system. From a practical standpoint, the GEAR-MC method tallies the intergenerational effect term by tallying the response that is generated as $\langle \Gamma^* P\phi \rangle$ approaches zero over some finite number of asymptotic generations, and GEAR-MC calculations must tally these terms for a sufficiently large number of asymptotic generations to accurately predict the intergenerational importance effects.

Previous work performing eigenvalue sensitivity calculations has shown that the number of latent generations, the equivalent of asymptotic generations for eigenvalue sensitivity coefficient calculations, that are required to reach an asymptotic population for IFP eigenvalue sensitivity calculations is between two and ten for most systems, but it is not known how many asymptotic generations are necessary for calculating generalized response sensitivities [6] [10]. The required number of asymptotic generations for accurately capturing intergenerational importance effects was quantified for the responses in this study by examining the average importance of neutrons in fission chains, relative to the different system responses, as a function of the number of generations since the fission chain was created. The behavior of these average importances is plotted in Figure 6.

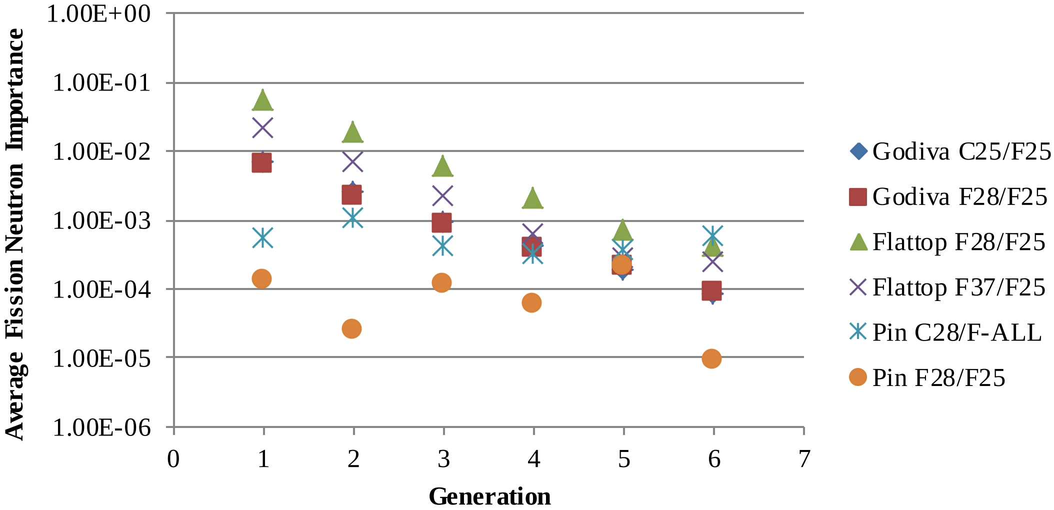

Figure 6. Average importance of fission neutrons in the *i*th generation of a fission chain (log scale).

Based on Figure 6, it can be concluded that the six asymptotic generations used in this study allowed for sufficient convergence of the intergenerational effect term, and the intergenerational importance terms appear to be close to zero even after four or five generations. Interestingly, the log-scale plots in Figure 6 indicate that the intergenerational effect terms continue to decrease in size after the fifth generation, and they appear to do so exponentially.

5. CONCLUSIONS

This work has introduced the GEAR-MC method, a new approach for calculating generalized response sensitivities in continuous-energy Monte Carlo applications, and has demonstrated proof of principle for the method. The GEAR-MC method produced response sensitivity coefficients that agree well with reference direct perturbation sensitivity coefficients for most responses and systems examined, and in some instances produced sensitivity coefficient estimates that were more accurate than those produced by the TSUNAMI-1D code. Analysis of the behavior of the intergenerational importance estimates indicates that about five asymptotic generations are required to accurately calculate the intergenerational effect term.

Future work includes improving the efficiency of the GEAR-MC method, developing a production version of the tool, and applying this first-of-its-kind capability to perform sensitivity and uncertainty analysis for various criticality safety, reactor physics, and radiation shielding applications.

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