Performance Enhancements to the SCALE TSUNAMI-3D Generalized Response Sensitivity Capability

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INTRODUCTION

The sensitivity and uncertainty analysis tools of the SCALE nuclear modeling and simulation code system have been developed over the last decade and have proven indispensable for numerous application and design studies for nuclear criticality safety and reactor physics [1]. Recent advancements in SCALE TSUNAMI (Tools for Sensitivity and UNcertainty Analysis Methodology Implementation) methods have enabled sensitivity analysis in continuous-energy Monte Carlo calculations for neutron reaction rate and flux tallies [2] [3]. This work documents recent advancements in the TSUNAMI-3D generalized response sensitivity methodology that have resulted in significantly enhanced computational performance for these analysis tools.

METHODOLOGY

The GEneralized Adjoint Response in Monte Carlo method (GEAR-MC) was developed by Perfetti in 2013 to enable sensitivity coefficient calculations for neutronic response ratios in continuous-energy Monte Carlo calculations. Similar to continuous-energy TSUNAMI sensitivity calculations, the GEAR-MC method calculates the sensitivity of neutronic response ratios to all of the materials and nuclides in a computational model during a single, unperturbed KENO transport calculation and does so by storing and analyzing information about each neutron history. The GEAR-MC method calculates generalized response sensitivity coefficients by solving the generalized adjoint transport equation, defined as [2] [3]

$$(L^* - \lambda P^*)\Gamma^* = S^* \,, \tag{1}$$

where L^* and P^* are the adjoint neutron loss and production operators, respectively, Γ^* is the generalized adjoint function, and S^* is the generalized adjoint source, which is defined for the response ratio R as

$$S^* = \frac{1}{R}\frac{\partial R}{\partial \phi} \,, \tag{2}$$

where ϕ is the neutron flux in the response region.

The GEAR-MC sensitivity method determines the importance of an event during a particle's lifetime by storing information about each collision and tracklength during that lifetime and examining this information post-mortem. For example, a collision that scatters a neutron into a highly fissile region would be considered important in an eigenvalue sensitivity calculation, whereas a collision that causes a neutron to leak from the system would not be important. This approach must account for the impact of the production of neutrons from future fission events on the importance of neutrons in the current generation. The generalized response importance for a neutron source of strength Q_s traveling in phasespace τ_s is given by

$$\Gamma^*(\tau_s) = \frac{1}{Q_s}\langle \frac{1}{R}\frac{\partial R}{\partial \phi}(r)\,\phi(\tau_s \to r)\rangle + \frac{\lambda}{Q_s}\langle \Gamma^*(r)P(r)\phi(\tau_s \to r)\rangle. \tag{3}$$

The first term on the right-hand side of Eq. 3 describes the intragenerational importance, or the importance generated by a neutron from the time it leaves the phasespace τ_s until its death, and the second term describes the intergenerational importance, or the importance that is generated by daughter fission neutrons of the original particle in phasespace τ_s.

Previously the GEAR-MC method calculated the intragenerational importance using the CLUTCH (Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization) method and the intergenerational importance using an adaptation of the IFP (Iterated Fission Probability) method, which was originally developed for eigenvalue sensitivity coefficient calculations [4] [5]. The IFP method sometimes produces large computational memory footprints and long simulation runtimes for sensitivity calculations in some (usually complex) systems, and this work has improved the efficiency of the GEAR-MC by replacing its use of the IFP method with a purely CLUTCH-based methodology.

Previous intergenerational term calculations using the IFP method would store reaction rates for each particle that generated a fission chain and weight these tallies by the importance that is generated by the daughter neutrons, or progeny, of the fission chain for some number of generations. The value of the intergenerational term for neutrons in a fission chain approaches zero as the progeny become more removed from the event that initiated the fission chain; therefore, this approach tallies the integral of these contributions as they approached zero. The IFP method can produce a significant memory footprint because the method stores reactions that are energy, material, nuclide, and reaction dependent and must do so for a number of generations for every particle that is simulated. The memory footprint for the tallies that the IFP method stores can be on the order of 10's or 100's of GB for complex systems with a large number of unique materials or simulations that require use of a large number of particle histories in each generation.

The IFP method has seen use recently, albeit in a slightly different form, for eigenvalue sensitivity calculations. The CLUTCH sensitivity method was developed by Perfetti in 2012 to enable eigenvalue sensitivity calculations that maintained the accuracy offered by the IFP method yet avoided its large memory footprints and long runtimes [6]. The CLUTCH method achieved this by using a weighting function, denoted $F^*(r)$, that described the average importance generated by fission neutrons at a location r within a spatial mesh. Whenever a neutron creates a fission event at r, rather than wait for the end of the fission chain to determine the importance of the fission event, the CLUTCH method obtains a tally by weighting the score of that fission event by the value of $F^*(r)$. This approach retains the accuracy of the IFP method because it uses the IFP method to calculate $F^*(r)$ during the inactive histories, yet avoids generating a large memory footprint because $F^*(r)$ is only a function of r and has no energy, material, nuclide, or reaction dependence. After the inactive generations end, the CLUTCH method normalizes the scores of $F^*(r)$ in each spatial mesh interval by the number of fission neutrons born in that interval (which has the added effect of allowing $F^*(r)$ tallies to begin before the fission source has converged) [7]. In this work this approach for calculating $F^*(r)$ has been extended to give the value of $\Gamma^*(r)$ in Eq. 3, thereby allowing GEAR-MC calculations to be performed using only the CLUTCH method.

RESULTS

The accuracy of the methodology described above was used to calculate generalized response sensitivities for several responses and several systems using continuous-energy KENO Monte Carlo simulations. The results of these calculations are used to compare the new GEAR-MC methodology (GEAR-MC – CLUTCH only) with the original GEAR-MC methodology (GEAR-MC with IFP). All of the systems examined in this study were 3D models of 1D systems, which allowed for a comparison with sensitivities calculated using the TSUNAMI-1D method in SCALE [1]. Reference sensitivities were generated using direct perturbation continuous-energy KENO calculations.

Three critical systems were examined in this study: HEU-MET-FAST-001 (Godiva) [8], PU-MET-FAST-006 (Flattop) [8], and a typical 2.7%-enriched PWR fuel pin (Fuel Pin). Several response ratio and spectral index sensitivities were examined for each system, as described in Table I. The first letter of the spectral indices in Table I 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, 37 is Np-237, etc.). The response examined for the Fuel Pin was the thermal fission cross section, or the ratio of the thermal (<0.625 eV) fission rate in all fuel isotopes to the thermal flux generated in the fuel pin. The responses examined for the Fuel Pin and Godiva cases are integral responses measured in the fuel region of each problem, and the Flattop responses are reaction rates in irradiation foils positioned at the center of Flattop.

TABLE I. Response Ratios Examined

Experiment	Response Ratio	Response Equation
Godiva	C25 / F25	$\frac{\langle \Sigma_{cap}^{U-235} \phi \rangle}{\langle \Sigma_{fis}^{U-235} \phi \rangle}$
	F28 / F25	$\frac{\langle \Sigma_{fis}^{U-238} \phi \rangle}{\langle \Sigma_{fis}^{U-235} \phi \rangle}$
Flattop	F28 / F25	$\frac{\langle \Sigma_{fis}^{U-238} \phi \rangle}{\langle \Sigma_{fis}^{U-235} \phi \rangle}$
	F37 / F25	$\frac{\langle \Sigma_{fis}^{Np-237} \phi \rangle}{\langle \Sigma_{fis}^{U-235} \phi \rangle}$
Fuel Pin	Thermal Fission Cross Section	$\frac{\langle \Sigma_{fis}^{Fuel} \phi \rangle_{therm}}{\langle \phi \rangle_{therm}}$

Table II compares the total sensitivity coefficients for several of the most important nuclides in the Godiva system and shows the difference between the calculated total sensitivities and the reference direct perturbation (DP) sensitivities in parenthesis below the sensitivity values. The TSUNAMI-1D (T1D) sensitivities in Table II do not have uncertainty estimates because TSUNAMI-1D calculates them deterministically. Table II indicates that each of the sensitivity methods produced sensitivity coefficients that agreed well with the reference calculations and with each other. The agreement is emphasized further in Figure 1, where almost no disagreement is visible for the U-238 energy-dependent sensitivity profiles for the C25/F25 response.

TABLE II. Godiva Integral Response Nuclide Sensitivity Coefficients

Response	Isotope	Direct Pert.	GEAR-MC with IFP	GEAR-MC CLUTCH only	T1D
C25 / F25	U-235	0.1658 ± 0.0103	0.1501 ± 0.0002 (-1.53 σ)	0.1585 ± 0.00005 (-0.71 σ)	0.1610 (-0.47 σ)
	U-238	0.0211 ± 0.0012	0.0205 ± 0.00004 (-0.46 σ)	0.0207 ± 0.00001 (-0.31 σ)	0.0211 (-0.02 σ)
F28 / F25	U-235	-1.3200 ± 0.0768	-1.2333 ± 0.0002 (1.13 σ)	-1.2419 ± 0.0001 (1.02 σ)	-1.2443 (-0.99 σ)
	U-238	1.0235 ± 0.0598	0.9680 ± 0.00006 (-0.93 σ)	0.9678 ± 0.00004 (-0.93 σ)	0.9675 (-0.94 σ)

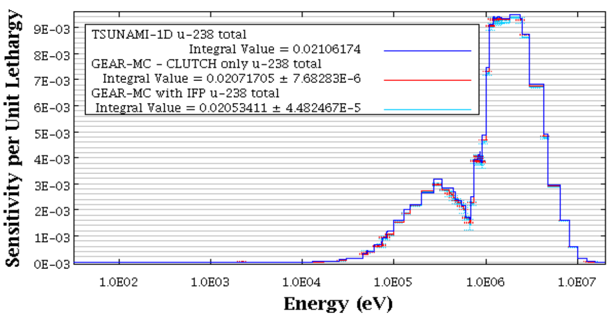

Fig. 1. Godiva energy-dependent C25/F25 response sensitivity to the U-238 total cross section.

Table III compares the total sensitivity coefficients for several nuclides in the Flattop system. Several important nuclides (U-235 and Np-237) were not included in this table because these nuclides are not present in the system in significant quantities except for in the foil response region. This causes the sensitivity of the responses to these nuclides to be equal to ±1.0 (depending whether the nuclide is included in the response numerator or denominator). These nuclides were omitted from Table III because analyzing such predictable sensitivity coefficients does not contribute to the understanding of the sensitivity method accuracy.

TABLE III. Flattop Foil Response Nuclide Sensitivity Coefficients

Response	Isotope	Direct Pert.	GEAR-MC with IFP	GEAR-MC CLUTCH only	T1D
F28 / F25	U-238	0.8006 ± 0.0533	0.7954 ± 0.0018 (-0.10 σ)	0.7771 ± 0.0040 (-0.44 σ)	0.8024 (0.03 σ)
	Pu-239	0.0528 ± 0.0043	0.0561 ± 0.0012 (0.73 σ)	0.0225 ± 0.0015 (-6.63 σ)	0.0657 (2.99 σ)
F37 / F25	U-238	-0.1540 ± 0.0102	-0.1608 ± 0.0016 (-0.66 σ)	-0.1700 ± 0.0040 (-1.46 σ)	-0.1551 (-0.11 σ)
	Pu-239	0.0543 ± 0.0048	0.0489 ± 0.0010 (-1.10 σ)	0.0384 ± 0.0014 (-3.17 σ)	0.0736 (3.99 σ)

Table III indicates that the GEAR-MC with IFP approach produced accurate irradiation foil sensitivity estimates and that the TSUNAMI-1D and GEAR-MC – CLUTCH only methods struggled to produce accurate estimates. Figure 2 shows the energy-dependent sensitivity profiles for the sensitivity of the F28/F25 response to the Pu-239 nuclide, one of the responses where the TSUNAMI-1D and GEAR-MC – CLUTCH only methods encountered the most disagreement with the reference sensitivities. Despite the large differences reported in Table III, the three sensitivity methods produced sensitivity profiles that appear very similar, but the positive-to-negative inflection in the sensitivity profiles makes slight differences in the profiles more pronounced when integrating sensitivity profiles over energy. The CLUTCH method has encountered some difficulty in the past when calculating eigenvalue sensitivity coefficients in the Flattop system, and it is possible that the number of fission events used to populate $\Gamma^*(r)$ tallies in Flattop's thick depleted uranium reflector region was not sufficient to produce accurate sensitivity estimates.

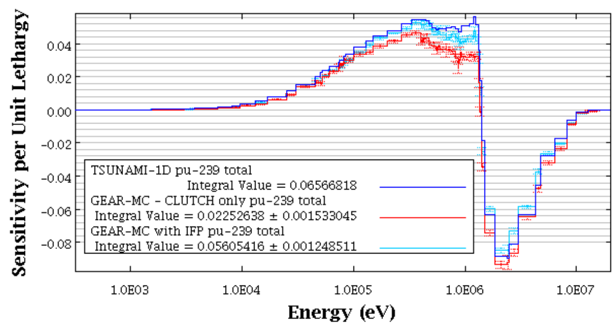

Fig. 2. Flattop energy-dependent F28/F25 response sensitivity to the Pu-239 total cross section.

Table IV compares the total sensitivity coefficients for the nuclides in the Fuel Pin system. Both GEAR-MC methods produced sensitivity estimates that agreed well with the reference sensitivities, and the TSUNAMI-1D approach had difficulty producing accurate sensitivity estimates.

TABLE IV. Fuel Pin Integral Response Nuclide Sensitivity Coefficients

Isotope	Direct Pert.	GEAR-MC with IFP	GEAR-MC CLUTCH only	T1D
H-1	0.1984 ± 0.0064	0.1978 ± 0.0055 (-0.07 σ)	0.2048 ± 0.0053 (0.77 σ)	0.1865 (-1.88 σ)
O-16	0.0054 ± 0.0003	0.0051 ± 0.0016 (-0.17 σ)	0.0061 ± 0.0011 (0.61 σ)	0.0045 (-2.61 σ)
U-235	0.7419 ± 0.0235	0.7474 ± 0.0005 (0.24 σ)	0.7479 ± 0.0003 (0.26 σ)	0.8219 (3.40 σ)
U-238	-0.0394 ± 0.0013	-0.0392 ± 0.0013 (0.16 σ)	-0.0385 ± 0.0009 (0.64 σ)	-0.0250 (11.42 σ)

Figure 3 shows the estimates of the sensitivity of the Fuel Pin thermal fission cross section to the H-1 nuclide. The three sensitivity methods produced similar sensitivity profiles, but the sensitivities calculated using the GEAR-MC with IFP approach were contaminated by a large amount of statistical noise, which is surprising because the two GEAR-MC with IFP and CLUTCH-only calculations simulated the same number of active particle histories. The CLUTCH method has been observed to produce sensitivity estimates with a lower amount of statistical uncertainty than the IFP method, and these new results speak to the potential efficiency enhancements offered by the use of the CLUTCH method [6] [9].

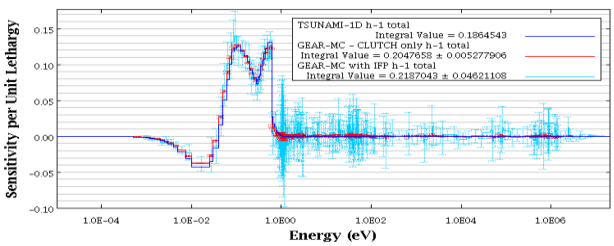

Fig. 3. Fuel Pin energy-dependent thermal cross section response sensitivity to the H-1 total cross section.

PERFORMANCE COMPARISON

Lastly the GEAR-MC methods were evaluated in terms of computational memory usage and computational efficiency to quantify what performance enhancements are possible through the use of a CLUTCH-only approach. Table V shows the memory footprint created by each GEAR-MC approach (minus the memory usage required by a non-sensitivity, eigenvalue-only simulation). These results indicate that moving away from an IFP-based approach for calculating the intergenerational importance results in a substantial (greater than 99.5%) reduction in the memory footprint for these systems.

TABLE V. Memory Usage over Eigenvalue-Only Calculations

Model	GEAR-MC with IFP	GEAR-MC CLUTCH only	Memory Reduction
Godiva	581 MB	2.8 MB	99.52%
Flattop	1,082 MB	5.2 MB	99.52%
Fuel Pin	6,358 MB	3.2 MB	99.95%

The computational efficiency of the GEAR-MC sensitivity methods was estimated by calculating Figures of Merit, a commonly used metric evaluating the efficiency of Monte Carlo calculations, for the nuclide sensitivity coefficients presented in Tables II through IV. Shown in Table VI, the “Average Speedup” offered by the CLUTCH-only approach was then determined by calculating the average ratio of the Figures of Merit for these nuclide sensitivities. These Average Speedups suggest that a CLUTCH-only approach can accelerate the Godiva and Fuel Pin sensitivity tally convergence by an order of magnitude or more, but the CLUTCH-only Flattop sensitivity calculations were actually less efficient than those using the IFP method. In these cases the CLUTCH calculations had shorter runtimes than the IFP calculations but produced lower Figures of Merit because the sensitivity tallies had larger uncertainties. As discussed previously, the CLUTCH Flattop simulations may not have obtained a sufficiently converged $\Gamma^*(r)$ function in the depleted uranium reflector before beginning active sensitivity tallies, and the residual uncertainty in this weighting function could be inflating the uncertainty of these sensitivity estimates, thereby lowering their Figures of Merit.

TABLE VI. Sensitivity Method Efficiency Comparison

Model	Average Runtime (hours)		Average Speedup
	IFP	CLUTCH	
Godiva	328.2	165.3	26.0
Flattop	261.1	197.1	0.52
Fuel Pin	191.4	44.1	10.25

CONCLUSIONS

GEAR-MC, a novel approach for calculating sensitivity coefficients for generalized responses in continuous-energy Monte Carlo applications, has been developed and implemented in the KENO Monte Carlo code. Preliminary sensitivity calculations indicate that a modification of the GEAR-MC method that only uses the CLUTCH sensitivity methodology has the potential to retain the accuracy offered by the original IFP-based approach. Performance metrics indicate that moving to a CLUTCH only methodology can reduce the memory footprint of these calculations by more than 99% and may accelerate sensitivity tally convergence.

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