SCALE 6.2 CONTINUOUS-ENERGY TSUNAMI-3D CAPABILITIES

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ABSTRACT

The TSUNAMI (Tools for Sensitivity and UNcertainty Analysis Methodology Implementation) capabilities within the SCALE code system make use of sensitivity coefficients for an extensive number of criticality safety applications, such as quantifying the data-induced uncertainty in the eigenvalue of critical systems, assessing the neutronic similarity between different systems, quantifying computational biases, and guiding nuclear data adjustment studies. The need to model geometrically complex systems with improved ease of use and fidelity and the desire to extend TSUNAMI analysis to advanced applications have motivated the development of a SCALE 6.2 module for calculating sensitivity coefficients using three-dimensional (3D) continuous-energy (CE) Monte Carlo methods: CE TSUNAMI-3D.

This paper provides an overview of the theory, implementation, and capabilities of the CE TSUNAMI-3D sensitivity analysis methods. CE TSUNAMI contains two methods for calculating sensitivity coefficients in eigenvalue sensitivity applications: (1) the Iterated Fission Probability (IFP) method and (2) the Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Track length importance CHaracterization (CLUTCH) method. This work also presents the GEneralized Adjoint Response in Monte Carlo method (GEAR-MC), a first-of-its-kind approach for calculating adjoint-weighted, generalized response sensitivity coefficients—such as flux responses or reaction rate ratios—in CE Monte Carlo applications. The accuracy and efficiency of the CE TSUNAMI-3D eigenvalue sensitivity methods are assessed from a user perspective in a companion publication, and the accuracy and features of the CE TSUNAMI-3D GEAR-MC methods are detailed in this paper.

KEYWORDS
TSUNAMI, sensitivity analysis, eigenvalue, Generalized Perturbation Theory, SCALE 6.2

1. INTRODUCTION

The TSUNAMI (Tools for Sensitivity and UNcertainty Analysis Methodology Implementation) capabilities within the SCALE code system make use of sensitivity coefficients for an extensive number of criticality safety applications, such as quantifying the data-induced uncertainty in the eigenvalue of critical systems, assessing the neutronic similarity between different systems, quantifying computational

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biases, and guiding nuclear data adjustment studies [1]. The need to model geometrically complex systems with improved ease of use and fidelity and the desire to extend TSUNAMI analysis to advanced applications have motivated the development of methodologies for calculating sensitivity coefficients using three-dimensional (3D) continuous-energy (CE) Monte Carlo methods [2]. In SCALE 6.2, CE TSUNAMI-3D offers two distinct approaches for performing eigenvalue sensitivity coefficient calculations: the Iterated Fission Probability (IFP) method, and the Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Track length importance CHaracterization (CLUTCH) method. This work also presents a first-of-its-kind approach for calculating adjoint-weighted, generalized response sensitivity coefficients in CE Monte Carlo applications: the GEneralized Adjoint Response in Monte Carlo (GEAR-MC) method. This paper provides an overview of the capabilities of the CE TSUNAMI-3D sensitivity analysis methods, with an emphasis on the accuracy, performance, and functionality of the GEAR-MC method.

2. CE TSUNAMI-3D SENSITIVITY ANALYSIS METHODS

The TSUNAMI capabilities in the version 6.1 release of SCALE allowed for the calculation of eigenvalue sensitivity coefficients in 1D, 2D, and 3D problems using the multigroup physics approximation [1]. In the SCALE 6.2 release, TSUNAMI has been improved to allow for eigenvalue sensitivity coefficient calculations using the CE KENO Monte Carlo code in 3D applications [3]. This new CE TSUNAMI-3D sequence also includes the novel ability to calculate sensitivity coefficients for reaction rate ratios using the GEAR-MC method [4], a class of analysis that was previously available only to the TSUNAMI-1D and TSUNAMI-2D sequences using multigroup physics.

These various sensitivity coefficient calculation modes can be activated in CE TSUNAMI-3D using the '`cet=`' option, and are described in Table I below.

Table I. CE TSUNAMI-3D sensitivity calculation modes

`cet=`	Sensitivity Method	Method Description
0	None	Does not perform sensitivity coefficient calculations.
1	CLUTCH	Performs k_{eff} sensitivity coefficient calculations using the CLUTCH method.
2	IFP	Performs k_{eff} sensitivity coefficient calculations using the IFP method.
3	None	Does not perform sensitivity coefficient calculations; used for debugging.
4	GEAR-MC with $F^*(r)$	Performs reaction rate response sensitivity calculations using the GEAR-MC method; uses an $F^*(r)$ mesh in lieu of the IFP method.
5	GEAR-MC	Performs reaction rate response sensitivity calculations using the GEAR-MC method.

In this paper, the theory behind each of these sensitivity algorithms is discussed briefly, and the implementation and functionality of these capabilities is described.

2.1. IFP k_{eff} Sensitivity Calculations

The IFP method is enabled by inputting the parameter '`cet=2.`' The IFP method obtains adjoint-weighted reaction rate tallies based on the notion that the importance of an event to the eigenvalue calculation can be determined by counting the population of particles in the system during a future generation that are descendants, or "progeny" of the particle that caused the original event [5][6]. *Asymptotic population* is the population of particles used to infer the importance of the initial event, and the term *latent generations* is used to describe the number of generations between the time of the original event and the time that the asymptotic population is tallied. This approach is illustrated in Figure 1 below [6].

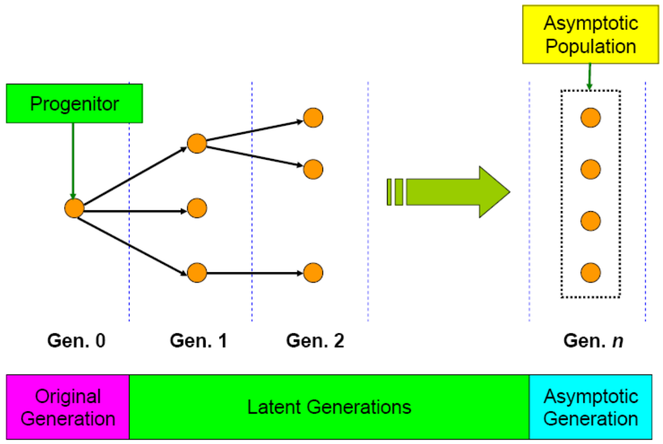

Figure 1. The IFP Approach for Determining the Importance of Events [6].

The IFP method allows for calculation of these adjoint-weighted reaction rates (which are needed to determine eigenvalue sensitivity coefficients) in a single calculation, which is typically more desirable than the original two-calculation approach used in the multigroup implementation of TSUNAMI-3D. The IFP method produces very accurate sensitivity coefficient estimates because its only fundamental assumption is that the asymptotic population is representative of the true importance of the original neutron [6] [3]. Increasing this number of latent generations typically increases the accuracy of the asymptotic population; most simulations can obtain accurate sensitivity estimates using 2–10 latent generations, and 20 has been shown to be a very conservative number of latent generations [6]. In CE TSUNAMI-3D, the number of latent generations can be selected using the '`cfp=`' parameter.

2.2. CLUTCH k_{eff} Sensitivity Calculations

Unfortunately, the memory footprint of the IFP method scales linearly with the number of particle histories used in each generation, and complex models with a large number of materials can produce large memory footprints. Therefore, the Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance Characterization (CLUTCH) method was developed in CE TSUNAMI-3D to decrease the memory footprint and increase the efficiency of sensitivity calculations [2]. The CLUTCH method is enabled by inputting the parameter '`cet=1.`'

The CLUTCH method calculates the importance of events by examining how many fission neutrons are created from the time the event occurs until the particle's death. This approach is similar to that used by other eigenvalue sensitivity methods, such as the Differential Operator method [7], but CLUTCH results in more accurate sensitivity tallies due to its improved treatment of multigenerational importance effects. The CLUTCH method improves on accuracy by calculating and storing a weighting function on a spatial mesh—$F^*(r)$—that describes the expected importance generated by a fission neutron emitted at position r. Approaches for calculating $F^*(r)$ are described in detail in References [2] [8], but essentially, CLUTCH calculates this function during inactive (or skipped) generations using a more memory-efficient form of the IFP algorithm. This improved algorithm allows CLUTCH to operate with a significantly lower memory footprint than that of the IFP method. The memory footprint is also less than the traditional multigroup TSUNAMI-3D approach. These improvements are described below in Table II [3]. The memory footprints presented in this table were obtained by subtracting the memory footprints produced by CE KENO calculations for the models from the memory footprints that were produced by

CE TSUNAMI-3D. A memory footprint is not reported for the NAC-UMC case in Table II because a multigroup TSUNAMI model was not available for this system at the time of this work.

Table II. Improvements in computational memory footprint offered by CLUTCH [3]

Model	**Multigroup TSUNAMI (MB)**	**IFP (MB)**	**CLUTCH (MB)**
Godiva	135	26	0.1
MIX-COMP-THERM-004-001	13,785	10,643	63
NAC-UMS	-----	21,201	3,416

Like the IFP k_{eff} calculation, the IFP calculation that estimates $F^*(r)$ must use a set number of latent generations, which can be chosen by the user using the '`cfp=`' parameter. As in the IFP method, 20 is typically a conservative number of latent generations to ensure accurate $F^*(r)$ and CLUTCH sensitivity calculations. Selecting '`cfp=-1`' will set all $F^*(r)$ values to one, an assumption that ignores the multigenerational importance effects; although this setting often produces inaccurate sensitivity estimates, it is often useful for estimating the runtime and memory footprint of a CLUTCH sensitivity calculation. The spatial mesh that is used for $F^*(r)$ can be selected by specifying a KENO "`geometryGrid`" and passing the ID of this grid to CLUTCH using the '`cgd=`' parameter [1]. The degree of spatial resolution for the $F^*(r)$ mesh and the degree of convergence for the mesh quantities are ongoing research topics, but initial studies have indicated that a 1–2 cm $F^*(r)$ mesh that simulates around 50–100 inactive particle histories per mesh interval will result in accurate eigenvalue sensitivity estimates [2] [8].

3. GEAR-MC REACTION RATE RATIO SENSITIVITY CALCULATIONS

The CE TSUNAMI-3D module within the SCALE 6.2 release includes a first-of-its-kind capability for calculating the sensitivity of reaction rate ratios using Generalized Perturbation Theory (GPT) [9]. This approach, dubbed the GEneralized Adjoint Responses in Monte Carlo (GEAR-MC) Method, uses the CLUTCH and IFP sensitivity algorithms together to estimate the GPT importance for reaction rate ratios, as described in greater detail in Reference [4]. GPT-based sensitivity analysis has the potential to extend the insights offered by eigenvalue sensitivity analysis in the area of criticality safety to a broad spectrum of nuclear engineering applications, including (1) assessing the nuclear data-induced uncertainty in fuel fission rates in reactors, (2) improving heavy actinide production by shifting neutron fluxes to energy regimes with favorable capture-to-fission ratios, or (3) guiding integral experiment design for measuring difficult cross sections. This section describes the functionality of the GEAR-MC method and discusses several recent improvements to the GEAR-MC sensitivity algorithms.

As in eigenvalue sensitivity coefficient analysis, generalized response 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

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

In GPT sensitivity analysis, the response function R is the ratio of two reaction rates integrated over some region of phase space such that

$$R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}, \quad (2)$$

where Σ_1 and Σ_2 are nuclear cross sections. The reaction rates in Eq. 2 can be isotope- or material-dependent reaction rates and can also represent neutron flux responses by setting $\Sigma = 1$. The GEAR-MC method currently supports calculating sensitivity coefficients for responses comprised of fission rates, captures, total interaction rates, and flux tallies, but future versions are expected to support a more comprehensive set of reaction rate responses. Currently users can specify the reaction rates for Eq. 2 using entries in the KENO parameter block [1]. Work is under way (and is expected to be completed in time for the SCALE 6.2 release) to simplify this response input format to allow users to enter responses using the more convenient “Definitions” and “SystemResponses” blocks within SCALE. These are used to enter GPT responses by the TSUNAMI-1D/2D GPT calculation modes [1].

Users can enable the GEAR-MC method setting ‘`cet=5`’ in the KENO parameter block. Because GEAR-MC uses the CLUTCH method in combination with the IFP method, users must provide GEAR-MC with a number of latent generations to use for sensitivity calculations. As with the IFP method, this number of latent generations is set using the ‘`cfp`’ parameter. Extensive studies have not been performed to produce a recommended ‘`cfp`’ value for GEAR-MC calculations, but preliminary studies have indicated that GEAR-MC requires slightly more latent generations than for IFP-based eigenvalue sensitivity calculations [8].

3.1. Accuracy of GEAR-MC Sensitivity Coefficients

The GEAR-MC sensitivity algorithms have demonstrated the potential to produce reaction rate response ratio sensitivity coefficients that meet, and sometimes exceed, the accuracy of those produced using the multigroup TSUNAMI-1D. Table III shows several energy-integrated sensitivity coefficients for irradiation foil fission rate ratios in a model of the Flattop irradiation experiment; these sensitivity coefficients describe the sensitivity of several reaction rate ratios to the isotopic composition of the Flattop experiment [4] [10]. These GEAR-MC calculations were performed using ‘`cfp=8`’ latent generations. The multigroup TSUNAMI-1D and CE TSUNAMI-3D GEAR-MC methods produced sensitivity coefficient estimates that typically agreed well with each other, but several of the GEAR-MC sensitivity coefficients showed markedly improved agreement with the reference direct perturbation sensitivity coefficients than those produced by TSUNAMI-1D. This disagreement is perhaps more noticeable in the energy-dependent sensitivity coefficients shown in Fig. 2, which disagree noticeably for neutron energies of around 1-2 MeV.

Table III. Flattop irradiation foil response sensitivity coefficients [4]

Exp.	Response	Isotope	Direct Perturbation	GEAR-MC	TSUNAMI-1D
Flattop	^{238}U Fission Rate / ^{235}U Fission Rate	^{238}U	0.8006 ± 0.0533	0.7954 ± 0.0018 (-0.10 σ_{eff})	0.8024 (0.03 σ_{eff})
		^{239}Pu	0.0528 ± 0.0043	0.0561 ± 0.0012 (0.73 σ_{eff})	0.0657 (2.99 σ_{eff})
	^{237}Np Fission Rate / ^{235}U Fission Rate	^{238}U	-0.1540 ± 0.0102	-0.1608 ± 0.0016 (-0.66 σ_{eff})	-0.1551 (-0.11 σ_{eff})
		^{239}Pu	0.0543 ± 0.0048	0.0489 ± 0.0010 (-1.10 σ_{eff})	0.0736 (3.99 σ_{eff})

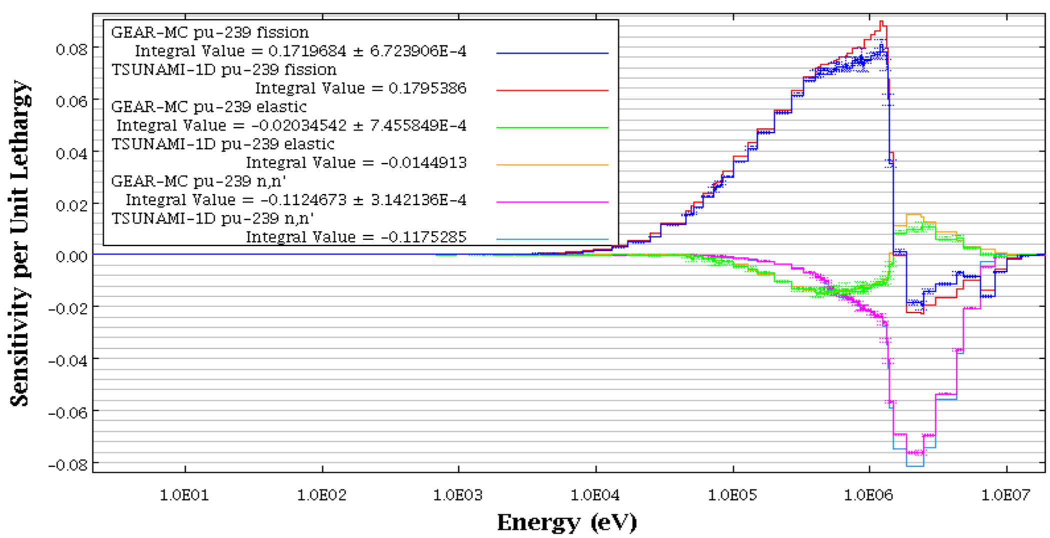

Figure 2. Sensitivity of the Flattop ^{238}U / ^{235}U Foil Fission Rate to ^{239}Pu reactions [4].

3.2. GEAR-MC Performance Improvements

The initial GEAR-MC implementation only allowed for the calculation of sensitivity coefficients for one response per simulation [4]. The current GEAR-MC algorithm has since been improved to allow for the calculation of sensitivity coefficients for multiple responses during a single Monte Carlo simulation. This single-simulation approach offers an improvement in scalability over the traditional TSUNAMI-1D/2D multigroup GPT implementations, which require (N+2) transport equation solutions for a problem, where N is the number of generalized responses of interest [1].

The IFP calculations within GEAR-MC are responsible for the majority of the computational memory footprint produced by the method. The IFP method requires a significant amount of memory overhead to store the reaction rates tallies needed to estimate the asymptotic importance for any sensitivity coefficient response, and producing multiple asymptotic importance estimates was not expected to greatly increase the memory footprint of the IFP algorithms. Table IV shows the memory footprint produced by GEAR-MC for the applications from Ref. 11 and also from a model of irradiation targets for producing ^{252}Cf in the Oak Ridge National Laboratory's High Flux Isotope Reactor (HFIR). Using the IFP method to produce multiple asymptotic importance estimates within a single GEAR-MC calculation has been found to result in a relatively minor—approximately 1% per response—increase in the memory footprint of the simulation. This result is promising because it suggests that the GEAR-MC algorithm will scale well for future analyses that require a large number of response sensitivity calculations, such as determining the uncertainty in pin powers within a model of a reactor, or determining the sensitivity of the isotopic content of irradiated material to the initial composition of that material.

Table IV. Computational memory footprint for the multi-response GEAR-MC algorithm

Model	Original Algorithm	Improved Algorithm
Godiva	523 MB	523 MB (+0% for 2 responses)
Flattop	1,052 MB	1,061 MB (+0.7% for 3 responses)
Fuel Pin	6,289 MB	6,292 MB (+0% for 2 responses)
HFIR	42,959 MB	44,512 MB (+3.6% for 5 responses)

3.3. GEAR-MC Memory Reduction using Importance Weighting Functions

Because of its use of the IFP algorithms, the GEAR-MC method sometimes produces large memory footprints for systems with a large number of materials, models that require a large number of latent generations to properly estimate the asymptotic importance of events, or problems that require the simulation of a large number of particle histories within each generation to mitigate undersampling biases. These potentially large memory footprints have motivated the development of an alternate implementation of the GEAR-MC method that does not use IFP algorithms for sensitivity coefficient calculations. Instead of using IFP algorithms to directly calculate sensitivity coefficients, this alternate GEAR-MC approach uses a more memory-efficient form of the IFP algorithm to calculate an $F^*(r)$ weighting function, which describes the average importance generated by a fission neutron born at r. This approach is used in a similar way by the CLUTCH method when calculating eigenvalue sensitivity coefficients [8], but here the $F^*(r)$ mesh describes the average generalized response importance created by a fission neutron born at r rather than the average eigenvalue importance [11]. Avoiding the direct use of IFP algorithms by using an $F^*(r)$ mesh was found to substantially reduce the memory footprint of the GEAR-MC method, as described in Table V.

Table V. Memory footprint of the GEAR-MC Method with and without IFP-based algorithms [11]

Model	GEAR-MC with IFP (MB)	GEAR-MC without IFP (MB)	Memory Reduction
Godiva	581	2.8	99.52%
Flattop	1,082	5.2	99.52%
Fuel Pin	6,358	3.2	99.95%
HFIR	42,959	20.1	99.95%

This GEAR-MC calculation mode is activated by entering ‘`cet=5`’ in the KENO parameter block and assigning ‘`cfp`’ and ‘`cgd`’ for the $F^*(r)$ mesh, as would be done for a CLUTCH calculation. Unfortunately, the previously discussed work to enable multiple generalized response sensitivity calculations within a single GEAR-MC simulation has not yet been extended to this $F^*(r)$-based GEAR-MC approach. This $F^*(r)$-based GEAR-MC approach is not expected to scale as well as the original GEAR-MC algorithm for multiple-response systems because each additional response will require storing an additional $F^*(r)$ mesh, which may create a significant memory footprint for models of physically large systems. The $F^*(r)$-based GEAR-MC algorithm is expected to see an increase in its memory footprint of ~100% for each additional generalized response, rather than the ~1% increase observed for the original GEAR-MC algorithm. On the other hand, the $F^*(r)$-based approach begins with a lower overall memory footprint than the original algorithm, so it remains to be determined which approach will demonstrate superior scaling for difficult, multi-response applications.

4. CONCLUSIONS

This paper describes the improvements to the TSUNAMI sensitivity analysis algorithms to be included in the SCALE 6.2 release. SCALE 6.2 will include the new CE TSUNAMI-3D module, which allows for sensitivity coefficient calculations to be performed using SCALE’s 3D, CE Monte Carlo methods. CE TSUNAMI-3D contains two algorithms for performing eigenvalue sensitivity coefficient calculations, the IFP and CLUTCH methods, and a first-of-its-kind approach for performing sensitivity analysis for reaction rate ratio responses, the GEAR-MC method, which was developed by combining the IFP and CLUTCH algorithms. This paper summarizes the improvements to the GEAR-MC sensitivity analysis algorithm that will be available in the SCALE 6.2 release, including the capability to calculate generalized sensitivity coefficients for multiple responses within a single simulation, as well as the ability to reduce the computational memory footprint of the GEAR-MC method by integrating an $F^*(r)$ importance-weighting mesh.

5. ACKNOWLEDGEMENTS

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