PHYSOR 2012 – Advances in Reactor Physics – Linking Research, Industry, and Education
Knoxville, Tennessee, USA, April 15-20, 2012, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2012)

DEVELOPMENT OF CONTINUOUS-ENERGY EIGENVALUE SENSITIVITY COEFFICIENT CALCULATION METHODS IN THE SHIFT MONTE CARLO CODE*

Christopher Perfetti and William Martin
University of Michigan
Department of Nuclear Engineering and Radiological Sciences
2355 Bonisteel Boulevard
Ann Arbor, MI 48109-2104, USA
cperfett@umich.edu; wrm@umich.edu

Bradley Rearden and Mark Williams
Oak Ridge National Laboratory
Reactor and Nuclear Systems Division
P.O. Box 2008, Bldg. 5700
Oak Ridge, TN 37831-6170, USA
reardenb@ornl.gov; williamsml@ornl.gov

ABSTRACT

Three methods for calculating continuous-energy eigenvalue sensitivity coefficients were developed and implemented into the Shift Monte Carlo code within the SCALE code package. The methods were used for two small-scale test problems and were evaluated in terms of speed, accuracy, efficiency, and memory requirements. A promising new method for calculating eigenvalue sensitivity coefficients, known as the CLUTCH method, was developed and produced accurate sensitivity coefficients with figures of merit that were several orders of magnitude larger than those from existing methods.

Key Words: Eigenvalue sensitivity coefficients, TSUNAMI, Monte Carlo, SCALE, Shift, CLUTCH, continuous-energy.

1. INTRODUCTION

The need to model more complex problems with increased accuracy has motivated extension of SCALE's current multigroup eigenvalue sensitivity coefficient estimation methodologies into the continuous-energy regime. SCALE's TSUNAMI-3D (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation) code currently calculates sensitivity coefficients by running both a forward and adjoint Monte Carlo calculation, and tallying the forward and adjoint fluxes as a function of space, energy, and angle on a mesh [1]. This methodology faces challenges when performing continuous-energy calculations because an inadequately-resolved mesh can result in inaccurate results, and also because of the inherent difficulty in transposing a continuous-energy scattering matrix for continuous-energy, adjoint Monte Carlo calculations.

*This manuscript has been authored by UT-Battelle LLC under Contract No. DE-AC05-00OR22725 with the US Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes.

This paper details efforts to develop sensitivity coefficient methodologies that are well-suited for continuous-energy calculations and to implement these methods into the Shift code within the SCALE code package. All of the methods detailed in this paper calculate eigenvalue sensitivity coefficients during a single forward Monte Carlo simulation without the use of a flux mesh. Although these methods are developed for continuous-energy calculations, all results presented in this study were obtained for multigroup calculations because Shift's continuous-energy capability is still under development. The methods discussed in this paper include the Eigenvalue Contributon Method developed by Williams, and two new methods: the CLUTCH Method and a hybrid Contributon-Iterated Fission Probability Method [2, 3, 4]. These methods were implemented into Shift, used to calculate sensitivity coefficients for several sample problems, and then evaluated in terms of speed, accuracy, efficiency, and memory requirements.

2. METHODOLOGY THEORY

2.1. Contributon Method

The Contributon Method determines the importance of a neutron by simulating secondary particles at the site of each collision [2]. After allowing these secondary particles to undergo random walks and terminate, the importance of the initial collision is determined by tallying how many fission neutrons were created by each daughter particle. This process is described graphically in Fig. 1. The Contributon Method requires a very small amount of memory to calculate sensitivity coefficients because it determines the importance of a collision before allowing the initiating particle to continue onto its next collision. However, the Contributon Method causes a large increase in the problem runtime because the number of secondary particles that are simulated is typically much larger than the number of primary neutrons that are simulated.

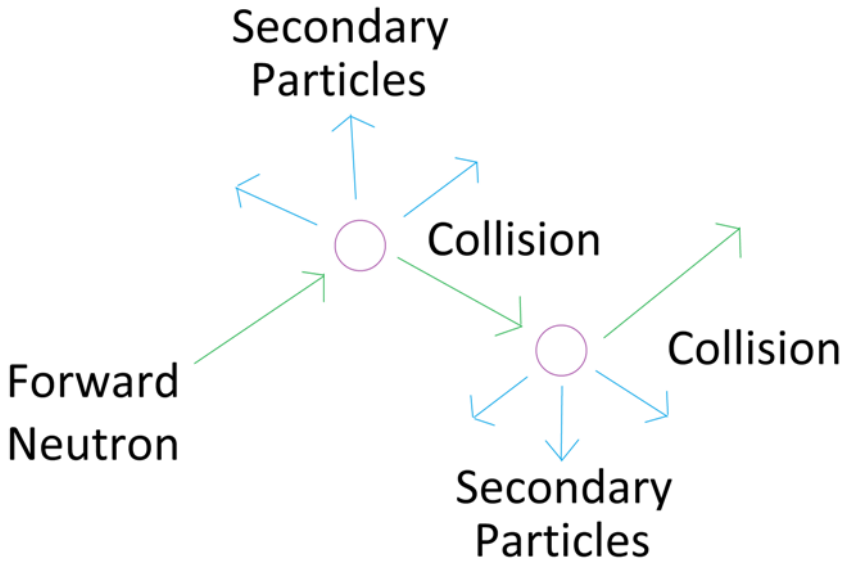

Figure 1. Illustration of the Contributon process.

The underlying theory behind the Contributon Method will now be described [2]. Consider a neutron source Q that is equal to the fission source of a system:

$$Q = \lambda F \phi. \tag{1}$$

Multiplying this source by the adjoint flux and integrating over phase space gives

$$\langle \phi^* Q \rangle = \lambda \langle \phi^* F \phi \rangle. \tag{2}$$

Consider now a neutron emitted in phase space τ_s such that $Q = Q_s\, \delta(\tau - \tau_s)$. This source definition reduces Eq.(2) and allows the importance of the neutron in phase space τ_s to be calculated by

$$\phi^*(\tau_s) = \frac{\lambda}{Q_s} \int_V G(\tau_s \to r) F^*(r)\, dr, \tag{3}$$

where the transfer function $G(\tau_s \to r)$ is equal to the expected number of fission neutrons generated in all energies and directions at r due to a source neutron emitted at phase space τ_s and is given by

$$G(\tau_s \to r) = \frac{1}{Q_s(\tau_s)} \int_E \int_\Omega \nu \Sigma_f(r, E) \phi(\, r, E, \Omega \mid Q(\tau_s)\,) d\Omega dE, \tag{4}$$

and $\phi(\, r, E, \Omega \mid Q(\tau_s)\,)$ is the flux created in phase space (r, E, Ω) given the source $Q(\tau_s)$. The weighting function $F^*(r)$ is defined to be equal to the expected importance generated by a fission neutron emitted at r and is given by

$$F^*(r) = \int_E \int_\Omega \frac{\chi(r, E)}{4\pi}\, \phi^*(r, E, \Omega) d\Omega dE. \tag{5}$$

The Contributon Method determines the importance of a particle at a collision by simulating secondary particles at the site of the collision and tallying $G(\tau_s \to r)$, weighted by $F^*(r)$, for each secondary particle. Because the forward and adjoint flux terms in the first-order perturbation equation contain three different sets of energy and angular phase spaces, three distinct secondary particles must be simulated at the site of every collision to tally all sensitivity coefficients [3]. A neutron may undergo 10's to 100's of collisions during its lifetime, meaning that the Contributon Method can increase the runtime of a problem by as much as a factor of 300. Although this runtime increase seems large, it may not be prohibitive for performing

sensitivity coefficient calculations, especially when large-scale computing clusters are available. Performing sensitivity coefficient calculations with the conventional TSUNAMI Methodology can require a significant number of man-hours because the researcher must ensure that the flux mesh is sufficiently resolved to give accurate sensitivity coefficients. In many cases, it is more efficient to perform a single Contributon calculation with a large computing cluster than to spend the man-hours investigating and fine-tuning a problem using the conventional TSUNAMI method.

2.2. CLUTCH Method

A new method for sensitivity coefficient calculation has been derived based on Contributon Theory. This method, known as the **C**ontributon-**L**inked eigenvalue sensitivity/**U**ncertainty estimation via **T**racklength importance **CH**aracterization, or CLUTCH Method, preserves the Contributon Method's mesh-free, memory-efficient means for calculating adjoint-weighted tallies, and circumvents the need to simulate any secondary particles by instead analyzing the random walks of forward neutrons. Instead of simulating a secondary particle at every collision, the CLUTCH method tallies $G(\tau_s \rightarrow r)$ by looking forward in time to see how many fission neutrons are produced from the time of the collision until the particle's death. For example, the importance of a scattering collision is determined by tallying the importance that is generated by the neutron that emerges from the collision up until its death. Because this process can only be done a posteriori (after the particle dies), the method requires information, such as reaction rates, and the neutron's energy at every collision, to be stored for each track in a particle's history. Although storing this data requires significantly more memory than is used by the Contributon Method, the amount of memory required is not prohibitive for large-scale sensitivity coefficient calculations, and is typically on the order of megabytes or gigabytes. Additional details about the Modified Contributon Method can be found in Reference 3.

The Contributon and CLUTCH methods both use the $F^*(r)$ function to weight $G(\tau_s \rightarrow r)$ tallies when calculating the importance of a neutron, and thus require that the $F^*(r)$ function is determined before active tallying begins. Calculation of the $F^*(r)$ function is paramount to these methods and is discussed in detail in Reference 5.

2.3. Contributon-IFP Hybrid Method

Another new method for sensitivity coefficient calculation has been developed by combining the Iterated Fission Probability (IFP) methodology with the Contributon notion of simulating secondary particles. The IFP Method obtains adjoint-weighted tallies using the definition that the importance of a neutron in an eigenvalue calculation can be determined by counting the population of neutrons in some future generation that are progeny of the original neutron. Thus whenever a neutron in an IFP calculation creates a fission point, the calculation stores reaction rates for that particle for some number of latent generations (typically for 20 generations), and then calculates an "asymptotic" population of fission neutrons created in the system that are descendants of the original, "progenitor" neutron. This asymptotic population measures the importance of the original particle and is used to weight the reaction rate tallies that were stored for the progenitor neutron [6]. This process is illustrated in Fig. 2 [7].

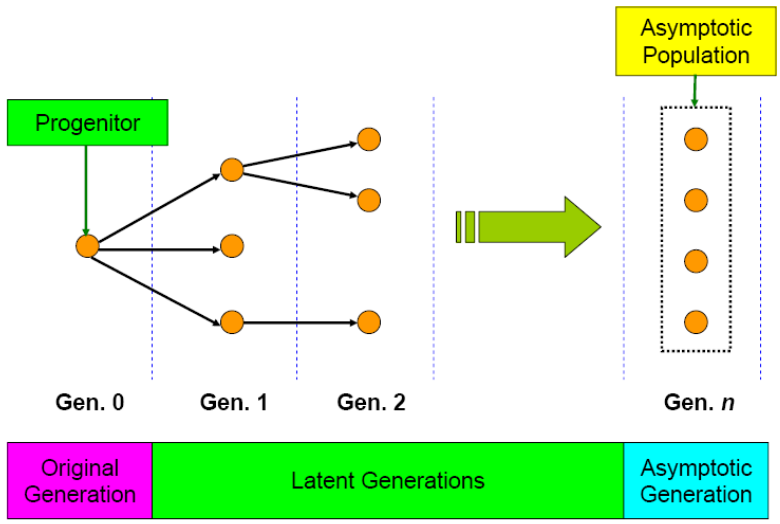

Figure 2. Illustration of the Iterated Fission Probability process [7].

The IFP Method must store reaction rates for all materials of interest and for every particle that is simulated for approximately 20 generations, and thus can require on the order of 10's to 1000's of gigabytes of memory for very detailed problems [3]. These potentially large memory requirements have motivated the development of the Contributon-IFP Hybrid Method, which avoids these large memory requirements through the use of secondary particles. Instead of storing reaction rates for 20 generations when a particle causes a fission event, the Contributon-IFP Hybrid Method simulates 20 generations of secondary particles and obtains an estimate of the original particle's asymptotic population (and thus importance) before that particle is allowed to continue its random walk [4].

Unlike the Contributon and CLUTCH methods, the Contributon-IFP Hybrid Method does not require calculation of the $F^*(r)$ weighting function, and the method's only basic assumption is that the asymptotic population of a progenitor neutron is reached after 20 latent generations. The number of latent generations used by this method can be specified in the Shift input file, but the use of 20 latent generations has been previously shown to be sufficiently accurate [6]. Although the Contributon-IFP Hybrid Method is free from any concerns about $F^*(r)$ mesh resolution or convergence, the method suffers from the same runtime issues as the Contributon Method because simulating 20 generations of secondary particles after every fission can theoretically increase the runtime of a critical (k = 1) problem by a factor of 20. Furthermore, the Contributon-IFP Hybrid Method is generally less efficient than the Contributon and Modified Contributon Methods because it combines the runtime increase of simulating secondary particles with the inherently inefficient IFP methodology. If a particle in an IFP simulation fails to cause a fission event during its lifetime, then all of the progenitor fission chains containing that particle are lost and the importance returned by those tallies is zero. In contrast, the Contributon and CLUTCH methods generate sensitivity coefficient tallies for every collision. Therefore,

whenever a generation of secondary particles in a Contributon-IFP Hybrid simulation results in no new fission points, the initiating fission event for that fission chain receives an importance tally of zero and the time spent simulating secondary particles in that sequence of secondary particles is wasted.

3. RESULTS

The above methods were implemented into the Shift Monte Carlo code within the Denovo framework of the SCALE code package and used to calculate eigenvalue sensitivity coefficients for two simple test problems: an infinitely-reflected light water reactor (LWR) fuel pin and the Godiva device. Because the Shift continuous-energy physics package is still under development, the sensitivity coefficient Monte Carlo calculations were performed using the multigroup approximation. Neutron cross sections for these energy groups were obtained using 2-D models of the corresponding systems in the TRITON code [1]. Reference sensitivity coefficients were obtained for the two systems through direct perturbations of neutron cross sections.

3.1. Fuel Pin Sensitivity Coefficient Results

After simulating 3.5 million active neutron histories, eigenvalue sensitivity coefficients were obtained for the fuel and moderator regions of the LWR fuel pin model. A seven-group energy structure was used for these calculations and is given in Table I; this energy group structure was chosen such that energy groups could represent the fast fission region, the fast energy region, slowing-down energies, and energies containing various U-235 thermal fission resonances. Fission neutron emission energy, or $\chi(E)$, sensitivity coefficients are given for only the first three energy groups of the LWR fuel pin model because $\chi(E)$ equals zero for groups four through seven. A sufficiently-resolved $F^*(r)$ mesh was used for the Contributon and Modified Contributon methodologies; the development of this mesh is described in depth in Reference 5. Tables II and III give the sensitivity coefficients calculated using each method for the fuel and moderator regions, respectively. Tables IV and V give the difference in standard deviations between the reference sensitivity coefficients and the calculated sensitivity coefficients for the fuel and moderator regions, respectively; the differences are presented in terms of standard deviations instead of percent differences because analyzing percent differences for very small sensitivity coefficients results in deceptively-large percent differences.

Table I. LWR fuel pin model neutron energy group structure

Group Number	Energy Range
1	>1.0 MeV
2	500 keV–1.0 MeV
3	3.0 eV–500 keV
4	0.625 eV–3.0 eV
5	0.1 eV–0.625 eV
6	0.02 eV–0.1 eV
7	< 0.02 eV

Table II. Fuel region sensitivity coefficients for the LWR fuel pin model

Sensitivity	Reference	CLUTCH	Contributon	Hybrid-Contributon
$\boldsymbol{\Sigma_{cap_1}}$	-0.00832	-0.00271	-0.00271	-0.00272
$\boldsymbol{\Sigma_{cap_2}}$	-0.00317	-0.00286	-0.00285	-0.00286
$\boldsymbol{\Sigma_{cap_3}}$	-0.17918	-0.17936	-0.17894	-0.17929
$\boldsymbol{\Sigma_{cap_4}}$	-0.00564	-0.00862	-0.00865	-0.00862
$\boldsymbol{\Sigma_{cap_5}}$	-0.06563	-0.07006	-0.06943	-0.06999
$\boldsymbol{\Sigma_{cap_6}}$	-0.10161	-0.10207	-0.10187	-0.10215
$\boldsymbol{\Sigma_{cap_7}}$	-0.03306	-0.03661	-0.03759	-0.03647
$\boldsymbol{\Sigma_{s_1}}$	-0.00069	-0.00632	-0.00583	-0.00659
$\boldsymbol{\Sigma_{s_2}}$	-0.00545	0.00027	-0.00009	0.00070
$\boldsymbol{\Sigma_{s_3}}$	0.00323	-0.00046	0.00203	0.00191
$\boldsymbol{\Sigma_{s_4}}$	-0.00343	-0.00013	-0.00005	0.00012
$\boldsymbol{\Sigma_{s_5}}$	-0.00178	0.00022	0.00066	-0.00002
$\boldsymbol{\Sigma_{s_6}}$	-0.00634	-0.00017	-0.00092	-0.00221
$\boldsymbol{\Sigma_{s_7}}$	0.00185	-0.00075	-0.00066	-0.00116
$\boldsymbol{\Sigma_{f_1}}$	0.02799	0.02874	0.02896	0.02850
$\boldsymbol{\Sigma_{f_2}}$	-0.00046	0.00079	0.00075	0.00066
$\boldsymbol{\Sigma_{f_3}}$	0.02311	0.02849	0.02840	0.02867
$\boldsymbol{\Sigma_{f_4}}$	0.01142	0.00620	0.00643	0.00633
$\boldsymbol{\Sigma_{f_5}}$	0.08930	0.09006	0.08916	0.09070
$\boldsymbol{\Sigma_{f_6}}$	0.14078	0.14529	0.14401	0.14442
$\boldsymbol{\Sigma_{f_7}}$	0.04954	0.04934	0.05057	0.04994
$\boldsymbol{\bar{\nu}_1}$	0.06175	0.05624	0.05643	0.05604
$\boldsymbol{\bar{\nu}_2}$	0.00201	0.00161	0.00157	0.00148
$\boldsymbol{\bar{\nu}_3}$	0.06861	0.06111	0.06094	0.06128
$\boldsymbol{\bar{\nu}_4}$	0.01570	0.01824	0.01852	0.01837
$\boldsymbol{\bar{\nu}_5}$	0.26867	0.26706	0.26457	0.26752
$\boldsymbol{\bar{\nu}_6}$	0.43511	0.43997	0.43812	0.43933
$\boldsymbol{\bar{\nu}_7}$	0.15054	0.15576	0.15985	0.15597
$\boldsymbol{\chi(E_1)}$	0.03323	0.02865	0.02886	0.03016
$\boldsymbol{\chi(E_2)}$	-0.00584	-0.00534	-0.00567	-0.00556
$\boldsymbol{\chi(E_3)}$	-0.00611	-0.00493	-0.00469	-0.00524

Table III. Moderator region sensitivity coefficients for the LWR fuel pin model

Sensitivity	Reference	CLUTCH	Contributon	Hybrid-Contributon
Σ_{cap_1}	0.00428	-0.00188	-0.00188	-0.00188
Σ_{cap_2}	-0.00201	0.00000	0.00000	0.00000
Σ_{cap_3}	-0.00673	-0.00222	-0.00222	-0.00222
Σ_{cap_4}	-0.00308	-0.00327	-0.00327	-0.00327
Σ_{cap_5}	-0.02606	-0.02735	-0.02724	-0.02735
Σ_{cap_6}	-0.05082	-0.04455	-0.04423	-0.04458
Σ_{cap_7}	-0.01974	-0.01747	-0.01727	-0.01741
Σ_{s_1}	-0.01180	-0.01684	-0.01784	-0.01705
Σ_{s_2}	0.00312	0.00221	0.00242	0.00324
Σ_{s_3}	0.14975	0.14641	0.15362	0.14607
Σ_{s_4}	0.00926	0.00473	0.00475	0.00515
Σ_{s_5}	0.00205	0.00581	0.00652	0.00687
Σ_{s_6}	-0.00670	-0.00332	-0.00450	-0.01453
Σ_{s_7}	-0.01023	-0.00082	-0.00044	-0.00178

Table IV. Difference in standard deviations between the calculated and reference fuel region sensitivity coefficients for the LWR fuel pin model

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
Σ_{cap_1}	-1.498	-1.499	-1.497
Σ_{cap_2}	-0.081	-0.084	-0.082
Σ_{cap_3}	0.047	-0.066	0.027
Σ_{cap_4}	0.795	0.803	0.794
Σ_{cap_5}	0.803	0.688	0.782
Σ_{cap_6}	0.123	0.070	0.138
Σ_{cap_7}	0.945	1.207	0.904
Σ_{s_1}	1.461	1.328	1.382
Σ_{s_2}	-1.029	-0.963	-1.082
Σ_{s_3}	0.864	0.277	0.192

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
Σ_{s_4}	-0.875	-0.894	-0.922
Σ_{s_5}	-0.520	-0.641	-0.416
Σ_{s_6}	-1.105	-0.975	-0.712
Σ_{s_7}	0.692	0.670	0.796
Σ_{f_1}	-0.200	-0.259	-0.138
Σ_{f_2}	-0.333	-0.321	-0.299
Σ_{f_3}	-1.436	-1.413	-1.479
Σ_{f_4}	1.391	1.330	1.354
Σ_{f_5}	-0.200	0.037	-0.364
Σ_{f_6}	-1.191	-0.850	-0.925
Σ_{f_7}	0.054	-0.274	-0.105
$\bar{\nu}_1$	1.468	1.418	1.516
$\bar{\nu}_2$	0.105	0.118	0.140
$\bar{\nu}_3$	1.998	2.045	1.947
$\bar{\nu}_4$	-0.680	-0.753	-0.713
$\bar{\nu}_5$	0.426	1.090	0.297
$\bar{\nu}_6$	-1.280	-0.796	-1.062
$\bar{\nu}_7$	-1.387	-2.477	-1.427
$\chi(E_1)$	1.156	1.131	0.660
$\chi(E_2)$	-0.134	-0.044	-0.072
$\chi(E_3)$	-0.313	-0.380	-0.229

Table V. Difference in standard deviations between the calculated and reference moderator region sensitivity coefficients for the LWR fuel pin model

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
Σ_{cap_1}	-1.498	-1.499	-1.497
Σ_{cap_2}	-0.081	-0.084	-0.082
Σ_{cap_3}	0.047	-0.066	0.030
Σ_{cap_4}	0.795	0.803	0.794
Σ_{cap_5}	0.803	0.688	0.789
Σ_{cap_6}	0.123	0.070	0.143

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
Σ_{cap_7}	0.945	1.207	0.909
Σ_{s_1}	-1.427	-1.340	-1.207
Σ_{s_2}	0.655	0.213	0.216
Σ_{s_3}	-0.316	-0.315	-0.122
Σ_{s_4}	-0.481	-0.591	-0.304
Σ_{s_5}	-0.746	-0.752	-0.229
Σ_{s_6}	0.229	0.258	0.127
Σ_{s_7}	-0.140	-0.200	-0.055

In general, the calculated sensitivity coefficients agreed very well with the reference sensitivity coefficients. It is expected that about 68% of the sensitivity coefficients will fall within one standard deviation of the reference sensitivities. In the calculations we observe that 69% of the CLUTCH sensitivity coefficients, 71% of the Contributon sensitivity coefficients, and 76% of the Contributon-IFP Hybrid sensitivity coefficients were within one standard deviation of the expected values. Although not shown, the uncertainty for the reference sensitivity coefficients was generally several orders of magnitude larger than the calculated sensitivity uncertainties because using direct perturbation methods for obtaining sensitivities that are on the order of 1% is very difficult. Furthermore, obtaining sensitivity coefficients using direct perturbation techniques is somewhat of an art, and the uncertainty for the reference sensitivities does not incorporate any systematic uncertainty that is introduced by human error. The fact that the calculated sensitivity coefficients generally differ from the reference sensitivities by about the same amount across the different methodologies suggests that the three methods are converging to the same sensitivity coefficients.

Table VI gives the different case runtimes, and Tables VI and VII present sensitivity figures of merit for each of the methodologies [8]. The runtime for the case with no sensitivity coefficient calculations was 39.33 minutes; hence, the CLUTCH method increased the problem runtime by about 6.3%. The Contributon and Contributon-IFP Hybrid method runtimes were significantly longer due to their need to simulate a large number of secondary particles; this dramatic difference in runtime is reflected in the figures of merit, and the CLUTCH method gave much larger figures of merit than the other methods. Although they differ dramatically in figures of merit, the uncertainty for the CLUTCH and Contributon sensitivity coefficients was very similar in magnitude; this was expected because the two methods are theoretically equivalent. The Contributon uncertainties were slightly smaller than the CLUTCH uncertainties because each Contributon collision independently obtains an importance estimate by simulating a secondary particle, whereas the CLUTCH importance estimates are correlated across the collisions seen in a particle's lifetime.

The CLUTCH sensitivity coefficients were calculated with figures of merit that were approximately two orders of magnitude higher than the corresponding Contributon-IFP Hybrid sensitivities. The Hybrid method figures of merit suffer both from the use of secondary particles and also from the inherent inefficiency of the IFP approach. Because the IFP method requires a "fission chain" of a particle's progeny to survive for 20 generations before creating a tally, any neutrons that leak from the system or are absorbed without creating a new fission point result in an importance tally of zero for the tallies contained in the fission chain; in contrast, the Contributon and CLUTCH method are guaranteed to produce importance tallies for every particle track and collision.

Table VI. Figures of merit for the LWR fuel pin model fuel region sensitivities

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
Runtime (minutes)	41.82	2459.90	902.98
$\boldsymbol{\Sigma_{cap_1}}$	$2.8\ 10^{7}$	$4.4\ 10^{5}$	$2.1\ 10^{4}$
$\boldsymbol{\Sigma_{cap_2}}$	$1.9\ 10^{7}$	$2.4\ 10^{5}$	$1.7\ 10^{4}$
$\boldsymbol{\Sigma_{cap_3}}$	$9.7\ 10^{3}$	$1.7\ 10^{2}$	$5.0\ 10^{0}$
$\boldsymbol{\Sigma_{cap_4}}$	$2.1\ 10^{6}$	$2.3\ 10^{4}$	$1.9\ 10^{3}$
$\boldsymbol{\Sigma_{cap_5}}$	$4.6\ 10^{4}$	$1.0\ 10^{3}$	$3.2\ 10^{1}$
$\boldsymbol{\Sigma_{cap_6}}$	$2.1\ 10^{4}$	$5.4\ 10^{2}$	$1.5\ 10^{1}$
$\boldsymbol{\Sigma_{cap_7}}$	$9.3\ 10^{4}$	$1.9\ 10^{3}$	$9.9\ 10^{1}$
$\boldsymbol{\Sigma_{s_1}}$	$5.0\ 10^{2}$	$7.3\ 10^{0}$	$4.4\ 10^{0}$
$\boldsymbol{\Sigma_{s_2}}$	$1.0\ 10^{3}$	$1.4\ 10^{1}$	$1.0\ 10^{1}$
$\boldsymbol{\Sigma_{s_3}}$	$9.4\ 10^{1}$	$1.4\ 10^{0}$	$6.0\ 10^{-1}$
$\boldsymbol{\Sigma_{s_4}}$	$2.5\ 10^{3}$	$3.4\ 10^{1}$	$2.4\ 10^{1}$
$\boldsymbol{\Sigma_{s_5}}$	$5.7\ 10^{2}$	$1.5\ 10^{1}$	$4.7\ 10^{0}$
$\boldsymbol{\Sigma_{s_6}}$	$7.0\ 10^{2}$	$2.5\ 10^{1}$	$6.0\ 10^{0}$
$\boldsymbol{\Sigma_{s_7}}$	$7.1\ 10^{3}$	$2.6\ 10^{2}$	$7.1\ 10^{1}$
$\boldsymbol{\Sigma_{f_1}}$	$1.5\ 10^{4}$	$6.9\ 10^{2}$	$1.8\ 10^{2}$
$\boldsymbol{\Sigma_{f_2}}$	$5.8\ 10^{5}$	$5.0\ 10^{5}$	$8.3\ 10^{3}$
$\boldsymbol{\Sigma_{f_3}}$	$1.4\ 10^{4}$	$1.2\ 10^{3}$	$1.6\ 10^{2}$
$\boldsymbol{\Sigma_{f_4}}$	$5.0\ 10^{4}$	$2.8\ 10^{3}$	$6.1\ 10^{2}$
$\boldsymbol{\Sigma_{f_5}}$	$2.8\ 10^{3}$	$5.0\ 10^{1}$	$2.7\ 10^{1}$
$\boldsymbol{\Sigma_{f_6}}$	$1.6\ 10^{3}$	$2.2\ 10^{1}$	$1.4\ 10^{1}$
$\boldsymbol{\Sigma_{f_7}}$	$4.5\ 10^{3}$	$6.3\ 10^{1}$	$4.7\ 10^{1}$
$\boldsymbol{\bar{\nu}_1}$	$1.2\ 10^{4}$	$1.0\ 10^{3}$	$1.5\ 10^{2}$

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
$\bar{\nu}_2$	$5.6\ 10^5$	$8.2\ 10^5$	$8.0\ 10^3$
$\bar{\nu}_3$	$1.1\ 10^4$	$1.5\ 10^3$	$1.3\ 10^2$
$\bar{\nu}_4$	$4.4\ 10^4$	$5.0\ 10^3$	$5.3\ 10^2$
$\bar{\nu}_5$	$2.0\ 10^3$	$6.8\ 10^1$	$2.1\ 10^1$
$\bar{\nu}_6$	$1.1\ 10^3$	$2.9\ 10^1$	$1.1\ 10^1$
$\bar{\nu}_7$	$3.8\ 10^3$	$1.1\ 10^2$	$4.2\ 10^1$
$\chi(E_1)$	$2.4\ 10^2$	$7.5\ 10^0$	$2.4\ 10^0$
$\chi(E_2)$	$2.7\ 10^3$	$9.1\ 10^1$	$2.8\ 10^1$
$\chi(E_3)$	$4.3\ 10^3$	$1.6\ 10^2$	$4.6\ 10^1$

Table VII. Figures of merit for the LWR fuel pin model moderator region sensitivities

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
Σ_{cap_1}	$2.8\ 10^7$	$4.4\ 10^5$	$2.1\ 10^4$
Σ_{cap_2}	$1.9\ 10^7$	$2.4\ 10^5$	$1.7\ 10^4$
Σ_{cap_3}	$9.7\ 10^3$	$1.7\ 10^2$	$5.0\ 10^0$
Σ_{cap_4}	$2.1\ 10^6$	$2.3\ 10^4$	$1.9\ 10^3$
Σ_{cap_5}	$4.6\ 10^4$	$1.0\ 10^3$	$3.2\ 10^1$
Σ_{cap_6}	$2.1\ 10^4$	$5.4\ 10^2$	$1.5\ 10^1$
Σ_{cap_7}	$9.3\ 10^4$	$1.9\ 10^3$	$9.9\ 10^1$
Σ_{s_1}	$5.7\ 10^7$	$1.2\ 10^6$	$4.3\ 10^4$
Σ_{s_2}	$9.4\ 10^{12}$	$2.2\ 10^{11}$	$8.1\ 10^9$
Σ_{s_3}	$6.6\ 10^7$	$1.3\ 10^6$	$3.3\ 10^4$
Σ_{s_4}	$2.1\ 10^7$	$4.7\ 10^5$	$1.4\ 10^4$
Σ_{s_5}	$3.4\ 10^5$	$8.1\ 10^3$	$2.1\ 10^2$
Σ_{s_6}	$1.2\ 10^5$	$2.9\ 10^3$	$7.8\ 10^1$
Σ_{s_7}	$6.1\ 10^5$	$1.5\ 10^4$	$4.8\ 10^2$

3.1. Godiva Sensitivity Coefficient Results

After simulating 50 million active neutron histories, eigenvalue sensitivity coefficients were obtained for the Godiva model using each method. Our results for the Contributon and Contributon-IFP Hybrid cases are preliminary because we were only able to simulate 13.5 million and 10 million neutron histories, respectively. A sufficiently resolved $F^*(r)$ mesh was used for the Contributon and Modified Contributon methodologies; development of this mesh is described in Reference 5. Table IX gives the sensitivity coefficients that were calculated using each method, and Table X gives the difference in standard deviations between the reference and calculated sensitivity coefficients. A six-group energy structure was used for these calculations and is given in Table VIII; this energy group structure was chosen to divide the fission neutron emission energy spectrum approximately evenly across several groups and to allow for a non-fast energy group below 100 keV.

Table VIII. Godiva model neutron energy group structure

Group Number	Energy Range
1	>3.0 MeV
2	1.5 MeV–3.0 MeV
3	1.0 MeV–1.5 MeV
4	500 keV–1.0 MeV
5	100 keV–500 keV
6	<100 keV

Table IX. Sensitivity coefficients for the Godiva model

Sensitivity	Reference	CLUTCH	Contributon	Hybrid-Contributon
$\boldsymbol{\Sigma_{cap_1}}$	-0.0001	-0.0011	-0.0011	-0.0011
$\boldsymbol{\Sigma_{cap_2}}$	-0.0050	-0.0036	-0.0036	-0.0036
$\boldsymbol{\Sigma_{cap_3}}$	-0.0050	-0.0040	-0.0040	-0.0041
$\boldsymbol{\Sigma_{cap_4}}$	-0.0071	-0.0083	-0.0084	-0.0084
$\boldsymbol{\Sigma_{cap_5}}$	-0.0210	-0.0213	-0.0213	-0.0216
$\boldsymbol{\Sigma_{cap_6}}$	-0.0037	-0.0063	-0.0063	-0.0063
$\boldsymbol{\Sigma_{s_1}}$	0.0382	0.0369	0.0358	0.0334
$\boldsymbol{\Sigma_{s_2}}$	0.0402	0.0386	0.0375	0.0371
$\boldsymbol{\Sigma_{s_3}}$	0.0318	0.0327	0.0321	0.0321
$\boldsymbol{\Sigma_{s_4}}$	0.0545	0.0550	0.0537	0.0533

Sensitivity	Reference	CLUTCH	Contributon	Hybrid-Contributon
Σ_{s_5}	0.0665	0.0655	0.0640	0.0606
Σ_{s_6}	0.0062	0.0070	0.0067	0.0060
Σ_{f_1}	0.1339	0.1330	0.1328	0.1331
Σ_{f_2}	0.1163	0.1175	0.1172	0.1176
Σ_{f_3}	0.0824	0.0831	0.0829	0.0822
Σ_{f_4}	0.1191	0.1182	0.1181	0.1161
Σ_{f_5}	0.1514	0.1520	0.1519	0.1507
Σ_{f_6}	0.0193	0.0203	0.0204	0.0209
$\bar{\nu}_1$	0.2074	0.2072	0.2072	0.2080
$\bar{\nu}_2$	0.1847	0.1849	0.1847	0.1851
$\bar{\nu}_3$	0.1277	0.1282	0.1282	0.1281
$\bar{\nu}_4$	0.1860	0.1837	0.1839	0.1824
$\bar{\nu}_5$	0.2573	0.2562	0.2560	0.2562
$\bar{\nu}_6$	0.0408	0.0399	0.0399	0.0403
$\chi(E_1)$	0.0317	0.0326	0.0325	0.0320
$\chi(E_2)$	-0.0002	-0.0012	-0.0006	-0.0026
$\chi(E_3)$	-0.0122	-0.0120	-0.0118	-0.0108
$\chi(E_4)$	-0.0162	-0.0155	-0.0156	-0.0147
$\chi(E_5)$	-0.0008	-0.0001	-0.0006	-0.0004
$\chi(E_6)$	0.0023	0.0015	0.0015	0.0015

Table X. Difference in standard deviations between the calculated and reference sensitivity coefficients for the Godiva model

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
Σ_{cap_1}	0.967	0.970	0.977
Σ_{cap_2}	-1.283	-1.272	-1.277
Σ_{cap_3}	-0.905	-0.889	-0.838
Σ_{cap_4}	1.147	1.185	1.245
Σ_{cap_5}	0.304	0.293	0.538
Σ_{cap_6}	2.286	2.285	2.242
Σ_{s_1}	1.197	1.859	1.438
Σ_{s_2}	1.384	2.037	1.066

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
$\boldsymbol{\Sigma_{s_3}}$	-0.851	-0.233	-0.109
$\boldsymbol{\Sigma_{s_4}}$	-0.533	0.611	0.300
$\boldsymbol{\Sigma_{s_5}}$	0.840	1.574	0.939
$\boldsymbol{\Sigma_{s_6}}$	-0.693	-0.372	0.090
$\boldsymbol{\Sigma_{f_1}}$	0.846	0.956	0.479
$\boldsymbol{\Sigma_{f_2}}$	-1.117	-0.749	-0.817
$\boldsymbol{\Sigma_{f_3}}$	-0.627	-0.496	0.117
$\boldsymbol{\Sigma_{f_4}}$	0.763	0.843	1.857
$\boldsymbol{\Sigma_{f_5}}$	-0.574	-0.412	0.405
$\boldsymbol{\Sigma_{f_6}}$	-0.850	-0.896	-1.171
$\boldsymbol{\bar{\nu}_1}$	0.210	0.183	-0.337
$\boldsymbol{\bar{\nu}_2}$	-0.149	-0.017	-0.231
$\boldsymbol{\bar{\nu}_3}$	-0.531	-0.583	-0.315
$\boldsymbol{\bar{\nu}_4}$	2.153	1.900	2.209
$\boldsymbol{\bar{\nu}_5}$	0.937	1.061	0.591
$\boldsymbol{\bar{\nu}_6}$	0.625	0.585	0.356
$\boldsymbol{\chi(E_1)}$	-0.905	-0.714	-0.138
$\boldsymbol{\chi(E_2)}$	0.947	0.377	1.119
$\boldsymbol{\chi(E_3)}$	-0.178	-0.389	-0.833
$\boldsymbol{\chi(E_4)}$	-0.694	-0.604	-0.984
$\boldsymbol{\chi(E_5)}$	-0.650	-0.162	-0.272
$\boldsymbol{\chi(E_6)}$	0.726	0.745	0.658

As was observed for the LWR fuel pin case, the calculated sensitivity coefficients in Table IX agreed very well with the reference sensitivity coefficients. 76% of the CLUTCH sensitivity coefficients, 73% of the Contributon sensitivity coefficients, and 70% of the Contributon-IFP Hybrid sensitivity coefficients in Table X were within one standard deviation of the expected reference values. However, an unexpected number of sensitivity coefficients were more than two standard deviations from the reference coefficients. Again, the uncertainty for the reference sensitivity coefficients was generally several orders of magnitude larger than the calculated sensitivity coefficient uncertainties, and imperfect measurement of the reference sensitivity coefficients may have caused these greater-than-two standard deviation differences.

Table XI gives the case runtimes and sensitivity figures of merit for each of the methodologies. The runtime for the case with no sensitivity coefficient calculations was 22.96 minutes, and it should be noted that about half of the CLUTCH method runtime was used for generating the $F^*(r)$ mesh during inactive generations. Using a predetermined $F^*(r)$ mesh or generating the

mesh using Denovo before the active generations begin could significantly decrease the runtime of the CLUTCH method for this model. The Contributon and Contributon-IFP Hybrid method runtimes were significantly longer than the CLUTCH runtime, even though they only ran 27% and 20% as many particles as the CLUTCH method, respectively. The CLUTCH method gave figures of merit that were dramatically larger than the figures of merit from the Contributon and Contributon-IFP Hybrid methods, and it appears that the high-leakage nature of this system significantly lowered the efficiency of the Contributon and Contributon-IFP Hybrid methods; this impact was greatest for the Contributon-IFP Hybrid Method, which requires neutrons in a secondary-particle fission chain to survive for at least 20 generations to give a non-zero importance tally.

Table XI. Figures of merit for the Godiva sensitivities

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
Runtime (minutes)	52.45	504.30	892.15
$\boldsymbol{\Sigma_{cap_1}}$	$9.0\ 10^{2}$	$9.3\ 10^{0}$	$3.7\ 10^{-1}$
$\boldsymbol{\Sigma_{cap_2}}$	$8.8\ 10^{2}$	$9.1\ 10^{0}$	$3.4\ 10^{-1}$
$\boldsymbol{\Sigma_{cap_3}}$	$6.8\ 10^{2}$	$7.4\ 10^{0}$	$2.6\ 10^{-1}$
$\boldsymbol{\Sigma_{cap_4}}$	$8.7\ 10^{2}$	$9.6\ 10^{0}$	$3.1\ 10^{-1}$
$\boldsymbol{\Sigma_{cap_5}}$	$9.0\ 10^{2}$	$1.1\ 10^{1}$	$3.2\ 10^{-1}$
$\boldsymbol{\Sigma_{cap_6}}$	$1.7\ 10^{2}$	$2.7\ 10^{0}$	$6.8\ 10^{-2}$
$\boldsymbol{\Sigma_{s_1}}$	$6.4\ 10^{0}$	$7.4\ 10^{-2}$	$2.0\ 10^{-3}$
$\boldsymbol{\Sigma_{s_2}}$	$1.1\ 10^{1}$	$1.3\ 10^{-1}$	$4.0\ 10^{-3}$
$\boldsymbol{\Sigma_{s_3}}$	$1.1\ 10^{1}$	$1.4\ 10^{-1}$	$4.0\ 10^{-3}$
$\boldsymbol{\Sigma_{s_4}}$	$1.3\ 10^{1}$	$1.8\ 10^{-1}$	$4.0\ 10^{-3}$
$\boldsymbol{\Sigma_{s_5}}$	$6.1\ 10^{0}$	$1.0\ 10^{-1}$	$2.0\ 10^{-3}$
$\boldsymbol{\Sigma_{s_6}}$	$3.3\ 10^{-1}$	$6.0\ 10^{-3}$	$1.0\ 10^{-4}$
$\boldsymbol{\Sigma_{f_1}}$	$5.2\ 10^{2}$	$4.6\ 10^{0}$	$2.1\ 10^{-1}$
$\boldsymbol{\Sigma_{f_2}}$	$4.7\ 10^{2}$	$4.4\ 10^{0}$	$1.9\ 10^{-1}$
$\boldsymbol{\Sigma_{f_3}}$	$3.5\ 10^{2}$	$3.6\ 10^{0}$	$1.4\ 10^{-1}$
$\boldsymbol{\Sigma_{f_4}}$	$4.7\ 10^{2}$	$4.8\ 10^{0}$	$1.8\ 10^{-1}$
$\boldsymbol{\Sigma_{f_5}}$	$5.2\ 10^{2}$	$4.7\ 10^{0}$	$2.0\ 10^{-1}$
$\boldsymbol{\Sigma_{f_6}}$	$6.3\ 10^{1}$	$6.4\ 10^{-1}$	$2.9\ 10^{-2}$
$\boldsymbol{\bar{\nu}_1}$	$1.1\ 10^{3}$	$1.2\ 10^{1}$	$4.5\ 10^{-1}$
$\boldsymbol{\bar{\nu}_2}$	$1.0\ 10^{3}$	$1.1\ 10^{1}$	$4.1\ 10^{-1}$
$\boldsymbol{\bar{\nu}_3}$	$7.7\ 10^{2}$	$9.2\ 10^{0}$	$3.2\ 10^{-1}$

Sensitivity	CLUTCH	Contributon	Hybrid-Contributon
$\bar{\nu}_4$	$1.0\ 10^{3}$	$1.2\ 10^{1}$	$4.1\ 10^{-1}$
$\bar{\nu}_5$	$1.3\ 10^{3}$	$1.4\ 10^{1}$	$5.2\ 10^{-1}$
$\bar{\nu}_6$	$2.9\ 10^{2}$	$3.1\ 10^{0}$	$1.3\ 10^{-1}$
$\chi(E_1)$	$2.6\ 10^{4}$	$1.6\ 10^{2}$	$4.3\ 10^{0}$
$\chi(E_2)$	$3.3\ 10^{4}$	$2.1\ 10^{2}$	$5.6\ 10^{0}$
$\chi(E_3)$	$6.7\ 10^{4}$	$6.0\ 10^{2}$	$1.3\ 10^{1}$
$\chi(E_4)$	$7.0\ 10^{4}$	$6.3\ 10^{2}$	$1.4\ 10^{1}$
$\chi(E_5)$	$9.4\ 10^{4}$	$1.0\ 10^{3}$	$2.2\ 10^{1}$
$\chi(E_6)$	$8.0\ 10^{5}$	$2.0\ 10^{4}$	$3.2\ 10^{2}$

4. CONCLUSIONS

This study introduced the CLUTCH methodology for performing eigenvalue sensitivity coefficient calculations; the method was shown to accurately calculate coefficients with a figure of merit that was several orders of magnitude larger than that of alternative methods. As development on the Shift physics and geometry packages continues, these Contributon-based eigenvalue sensitivity coefficient methods tests will be expanded to model more-complex systems, such as light water reactors, shielded spent nuclear fuel assemblies, high-temperature gas-cooled reactors, and fast reactors. Also, these Contributon-based sensitivity coefficient methods will be compared to additional existing methods, including the Differential Operator and Iterated Fission Probability Methods. Sensitivity coefficient calculation methods will also be expanded so that the coefficients can be calculated as a function of isotope, energy, and region within a system.

ACKNOWLEDGMENTS

This research was performed using funding received from the DOE Office of Nuclear Energy's Nuclear Energy University Programs. The U.S. Department of Energy Nuclear Criticality Safety Program sponsored the preparation of this paper.

REFERENCES

1. *SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, ORNL/TM-2005/39, Version 6.1, Oak Ridge National Laboratory, Oak Ridge, Tennessee (June 2011). Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785.
2. M. L. Williams, *Equations for Contributon Eigenvalue Solution*. Unpublished document (2007).
3. C. M. Perfetti, *Methods for Continuous-Energy Eigenvalue Sensitivity Coefficient Calculation*, doctoral dissertation, University of Michigan (2012).
4. Private Communication with Dr. Forrest B. Brown, Hollywood, Florida, June 2011.

5. C. M. Perfetti, W. R. Martin, B. T. Rearden, M. L. Williams, "Determining Importance Weighting Functions for Contributon Theory Eigenvalue Sensitivity Coefficient Methodologies," *Proceedings of PHYSOR 2012*, Knoxville, Tennessee, April 15–20, 2012.
6. B. C. Kiedrowski, F. B. Brown, P. P. H. Wilson, "Adjoint-Weighted Tallies for *k*-Eigenvalue Calculations with Continuous-Energy Monte Carlo," *Nuclear Science and Engineering*, **168**, pp.226–241 (2011).
7. B. C. Kiedrowski, *Adjoint Weighting for Continuous-Energy Monte Carlo Radiation Transport*, doctoral dissertation, University of Wisconsin (2009).
8. E. E. Lewis, W. F. Miller, Jr., *Computational Methods of Neutron Transport*, American Nuclear Society, La Grange Park, Illinois, USA (1993).