Advanced Methods for Eigenvalue Sensitivity Coefficient Calculations[1]

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INTRODUCTION

Since the release of the Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) code in SCALE [1], the use of sensitivity and uncertainty techniques for criticality safety applications has greatly increased. Some methodologies for estimating sensitivity coefficients are difficult to implement in continuous-energy because they require multiple highly-converged transport calculations or inversion of scattering kernels. This study investigates five methods, including two new methods, that avoid both difficulties and therefore show great promise for estimating sensitivity coefficients using continuous-energy Monte Carlo.

The five methods were implemented in the Shift Monte Carlo code within the Denovo framework of the SCALE code package. The methods were applied to three test problems and evaluated in terms of accuracy and computational efficiency. Because the Shift continuous-energy physics package is still under development, the test problems used a multigroup cross-section energy structure.

METHODS FOR EIGENVALUE SENSITIVITY COEFFICIENT CALCULATION

This study investigates three previously-published Monte Carlo methods for generating sensitivity coefficients: the Differential Operator method, the Iterated Fission Probability (IFP) method, and the Contributon method; and two newly developed methods: the CLUTCH (**C**ontributon-**L**inked eigenvalue sensitivity/**U**ncertainty estimation via **T**racklength importance **CH**aracterization) method and the Contributon-IFP Hybrid method. These methods estimate the sensitivity coefficients for an eigenvalue problem using first-order perturbation theory, which involves weighting the reaction-rate tally of interest by the importance of the reaction to the eigenvalue.

The Differential Operator method calculates the importance of neutrons at collisions by weighting the differential probability that the collision occurs by the total number of fission neutrons produced from the time of the collision to the end of the neutron's lifetime [2]. Unlike the other methodologies, the Differential Operator methodology estimates sensitivity coefficients without using adjoint-weighted tallies; it can therefore produce inaccurate sensitivity coefficient estimates for systems in which the adjoint source (F^*) is not constant or cross-section perturbations significantly affect the fundamental mode.

The IFP method calculates the importance for a reaction of interest by waiting several generations after a neutron undergoes the reaction and then tallying the "asymptotic population" of the neutron's progeny [2]. While it provides a very accurate and generally efficient means for calculating sensitivity coefficients, the IFP method can require a large amount of memory for sensitivity coefficient calculations in complex systems.

The Contributon method calculates the importance of neutrons entering a collision by simulating secondary particles at the site of the collision and tallying the importance generated by these secondary particles [3] [4]. Although the Contributon method can produce accurate estimates of eigenvalue sensitivity coefficients, the method's use of secondary particles can dramatically increase problem runtime and lower the calculation efficiency.

The CLUTCH method calculates sensitivity coefficients using the same methodology as the Contributon method, but it avoids simulating secondary particles to calculate the importance of an event by instead examining the future importance created by the neutron leaving the event [5]. The CLUTCH and Differential Operator methods are similar, but the CLUTCH method calculates the importance of a neutron by weighting the number of fission neutrons produced after the neutron leaves the collision by an adjoint function that describes the average importance generated by these fission neutrons [6]. The CLUTCH and Differential Operator methods tend to be more efficient for sensitivity coefficient calculations than the IFP method because they score non-zero tallies for essentially every collision seen by a particle, while the IFP method requires that particles emerging from a collision produce several generations of progeny if non-zero sensitivities are to be recorded for that collision.

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The Contributon-IFP Hybrid method is based on the IFP methodology, but reduces memory requirements by simulating multiple generations of secondary particles to determine the asymptotic population of neutrons created by a neutron entering a fission event [7]. Although this allows the IFP methodology to be applied to complex systems with fewer memory limitations, the method's use of secondary particles reduces the efficiency of its sensitivity coefficient calculations.

RESULTS

The sensitivity coefficient calculation methodologies were used to calculate the eigenvalue sensitivity coefficients for three 3-D test cases: an infinitely reflected LWR fuel pin, the Godiva assembly, and the MIX-COMP-THERM-001 Case 4 (MCT-001) model [8]. The Godiva and infinitely reflected fuel pin cases are fairly well-known test problems, the MCT-001 model describes a criticality safety accident scenario where an assembly of reprocessed fast reactor fuel in a steel shipping cask is partially submerged in water, as shown in Fig. 1.

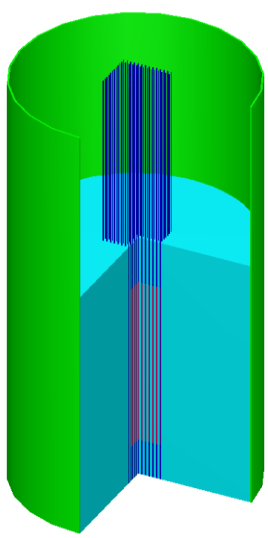

Fig. 1. KENO-3D image of the MCT-001 model; reprocessed fast reactor fuel (red) in a fuel assembly (dark blue) sits partially submerged in water (light blue) inside of a steel cask (green).

To assess a Monte Carlo methodology's computational efficiency, the commonly used figure of merit (FOM) is defined

$$FOM \equiv \frac{1}{R^2 T}, \qquad (1)$$

where T is the Monte Carlo simulation time and R is the relative uncertainty for the Monte Carlo tally of interest [9].

The generation of the weighting function for the Contributon and CLUTCH methods is described in Ref. 6. All models used 44-group cross sections; reference sensitivity coefficients were obtained through the direct perturbation of these cross sections.

Infinitely Reflected Fuel Pin Model

The infinitely reflected fuel pin model describes an infinite lattice of 2.7%-enriched PWR fuel pins and was chosen for this study to test the accuracy and efficiency of the methods for thermal applications with small amounts of neutron leakage [8].

Figures 2 and 3 give energy-integrated sensitivity coefficients and FOM, respectively, for several reactions of interest in the infinitely reflected fuel pin model. One-sigma error bars are given in Fig. 2 to represent the uncertainty associated with each sensitivity coefficient, but some error bars are indiscernibly small.

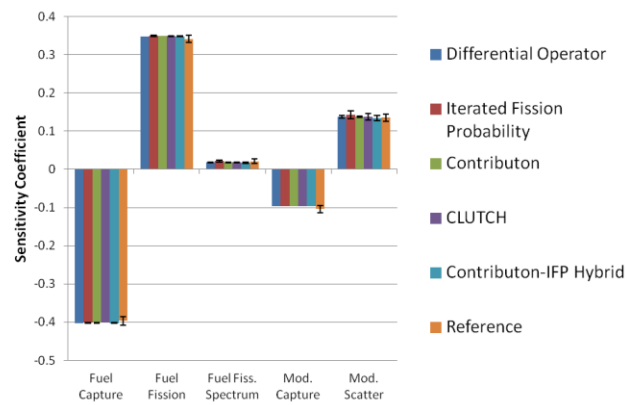

Fig. 2. Sensitivity coefficients for the LWR fuel pin model produced by the sensitivity coefficient methods.

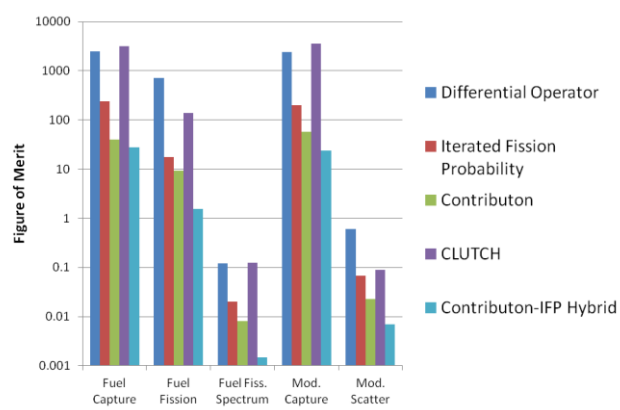

Fig. 3. Figures of merit for the LWR fuel pin model produced by the sensitivity coefficient methods.

As shown in Fig. 2, all of the sensitivity methodologies agree well with the reference sensitivity coefficients. All of the sensitivities were within one standard deviation of the reference values, and in most cases the results agree very well among the methodologies.

The FOM for the methods (Fig. 3) span several orders of magnitude and demonstrate the Differential Operator and CLUTCH methodologies' efficiency. As expected, the IFP methodology was somewhat less efficient due to its requirement that particles emerging from a collision survive for several generations if non-zero sensitivities are to be recorded for that collision, and the Contributon and Contributon-IFP Hybrid calculations were even less efficient because of their use of secondary particle histories.

Godiva Model

The Godiva model describes a sphere of highly-enriched uranium and was chosen for this study to test the performance of the methods for highly-enriched, high-leakage systems.

Figures 4 and 5 give the sensitivity coefficients and FOM, respectively, for the Godiva model. Most of the methods calculated sensitivity coefficients within one standard deviation of the reference coefficients, but the Differential Operator and Contributon-IFP Hybrid results significantly differed from the reference fuel scattering sensitivity coefficients.

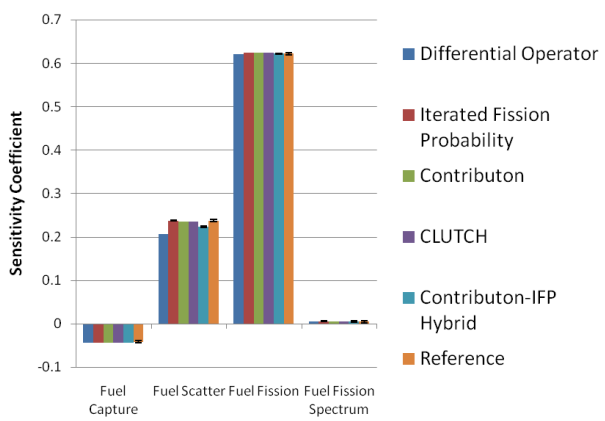

Fig. 4. Sensitivity coefficients for the Godiva model produced by the sensitivity coefficient methods.

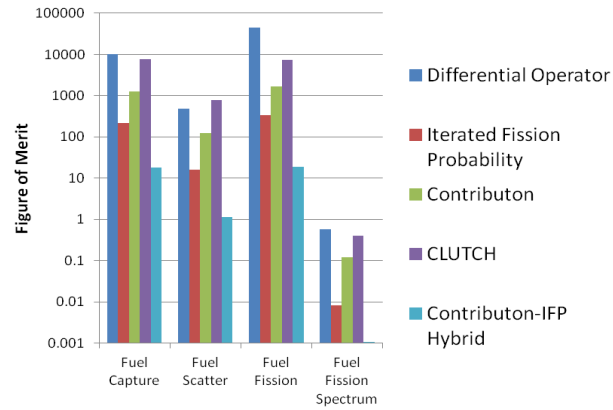

Fig. 5. Figures of merit for the Godiva model produced by the sensitivity coefficient methods.

As shown in Fig. 5, the Differential Operator and CLUTCH methods most efficiently estimated sensitivity coefficients for the Godiva model. The Contributon FOM was nearly comparable with the Differential Operator or CLUTCH FOM due to the nature of the Godiva model: neutron lifetimes are very short, and neutrons typically undergo few collisions in the system during those histories. These two factors reduced the amount of time the Contributon method spent simulating secondary particles and increased its efficiency for the Godiva model. Because the IFP and Contributon-IFP Hybrid methods skip several generations before recording tallies, the high-leakage nature of Godiva causes them to produce lower FOM for the system.

MCT-001 Model

The MCT-001 model was selected for this study to test the performance of the methods for a real-world system where both neutron leakage and thermalization affect the eigenvalue calculation. Once again the different sensitivity coefficients (Fig. 6) generally agree well with the reference sensitivities and only the Differential Operator and Contributon-IFP Hybrid results show significant disagreement. The FOM plot (Fig. 7) shows that the Differential Operator and CLUTCH methods once again performed well and that the Contributon method produced low FOM. The Contributon methodology is particularly inefficient for this model due to moderation in the thick water region surrounding the fuel region; each collision incurs the performance penalty of simulating secondary neutron histories. This penalty for highly-scattering materials was so great that using the Contributon method increased the MCT-001 problem run time 400-fold compared to simulations with no sensitivity calculations. Since the Contributon-IFP Hybrid methodology only simulates secondary particles at fission sites, it only increased the simulation time roughly 20-fold.

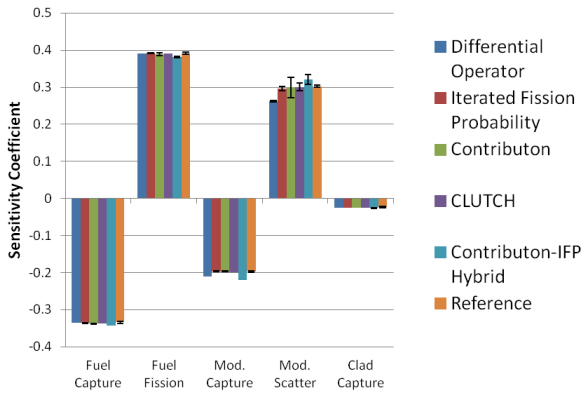

Fig. 6. Sensitivity coefficients for the MCT-001 model produced by the sensitivity coefficient methods.

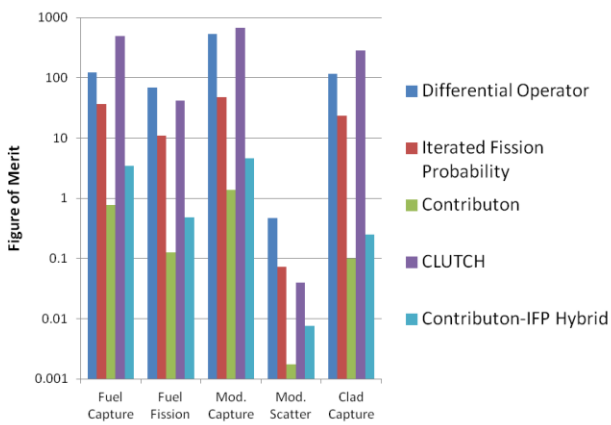

Fig. 7. Figures of merit for MCT-001 model produced by the sensitivity coefficient methods.

CONCLUSIONS

Five methodologies for calculating eigenvalue sensitivity coefficients were implemented in the Monte Carlo code Shift and applied to three test problems.

Only the Differential Operator and Contributon-IFP methodologies yielded significantly inaccurate results. The Differential Operator methodology is only accurate when F^* is constant and the fundamental mode does not change significantly in response to cross-section perturbations; those conditions are not met in the Godiva and MCT-001 models. The cause for the disagreement in the Contributon-IFP Hybrid results is less clear.

The Differential Operator and CLUTCH methods provided the most efficient estimates of sensitivity coefficients. Because the IFP and Contributon-IFP Hybrid methods skip several generations before recording tallies, those methods are particularly inefficient in high-leakage problems like Godiva. Conversely, the Contributon methodology is reasonably efficient for the Godiva model, though it is typically much less efficient than the Differential Operator or CLUTCH methodologies.

The newly developed CLUTCH method has shown the potential to accurately calculate eigenvalue sensitivity coefficients and produces FOM that are about an order of magnitude larger than those from the IFP method. Studies are underway to investigate using the CLUTCH method for continuous-energy applications.

ACKNOWLEDGEMENTS

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