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SCALE Sensitivity Calculations Using Contributon Theory*

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The SCALE TSUNAMI-3D sensitivity and uncertainty analysis sequence computes the sensitivity of k_{eff} to each constituent multigroup cross section using adjoint techniques with the KENO Monte Carlo codes. A new technique to simultaneously obtain the product of the forward and adjoint angular flux moments within a single Monte Carlo calculation has been developed and implemented in the SCALE TSUNAMI-3D analysis sequence. A new concept in Monte Carlo theory has been developed for this work, an eigenvalue contributon estimator, which is an extension of previously developed fixed-source contributon estimators. A *contributon* is a particle for which the forward solution is accumulated, and its importance to the response, which is equivalent to the adjoint solution, is simultaneously accumulated. Thus, the contributon is a particle coupled with its contribution to the response, in this case k_{eff}. As implemented in SCALE, the contributon provides the importance of a particle exiting at any energy or direction for each location, energy and direction at which the forward flux solution is sampled.

Although currently implemented for eigenvalue calculations in multigroup mode in KENO, this technique is directly applicable to continuous-energy calculations for many other responses such as fixed-source sensitivity analysis and quantification of reactor kinetics parameters. This paper provides the physical bases of eigenvalue contributon theory, provides details of implementation into TSUNAMI-3D, and provides results of sample calculations.

KEYWORDS: eigenvalue sensitivity, uncertainty, Monte Carlo, contributon, adjoint, SCALE, KENO, TSUNAMI

I. Introduction

Since the release of the **T**ools for **S**ensitivity and **Un**certainty **A**nalysis **M**ethodology **I**mplementation (TSUNAMI) codes in SCALE, the use of sensitivity and uncertainty analysis techniques for criticality safety applications has greatly increased within the user community.[1)] In general, sensitivity and uncertainty analysis is transitioning from a technique used only by specialists to a practical tool in routine use. Along with the desire to use the tool more routinely comes the need to improve the solution methodology to more easily address complex problems and extend the current multigroup approach to continuous-energy calculations. This paper reviews the current solution methodology of the Monte Carlo eigenvalue sensitivity analysis sequence TSUNAMI-3D and describes the development and presents preliminary results of an alternative approach.

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II. TSUNAMI-3D

The TSUNAMI-3D analysis sequence, based on the KENO Monte Carlo codes, computes the sensitivity of k_{eff} to each constituent multigroup cross-section data component used in the criticality analysis.[2)] TSUNAMI-3D performs forward and adjoint criticality calculations that tally the angular moments of the neutron flux solution. The flux solution must have adequate spatial resolution to minimize the variation of the angular moments across any given interval.[3)] To reduce the user intervention required to obtain spatially resolved flux solutions, a mesh flux accumulator has been implemented into KENO. Individual mesh accumulators are established for each region defined in the model. Any flux accumulated in a given region is stored within a specific mesh interval accumulator based on the position of the tally within the outermost or "global" unit of the model.

In the sensitivity calculation, the products of the forward and adjoint flux solutions are obtained for each mesh interval and then summed for all mesh intervals for a given Legendre order, ℓ, for a given region as

$$P^{\ell}_{g,g',z} = \sum_{j\in \ell}\left(\sum_{m\in z}\phi_{j,g,m}\phi^{\dagger}_{j,g',m}\right), \qquad (1)$$

where

$\phi_{j,g,m}$ = forward flux for energy group g, mesh interval m, and spherical harmonics component j,

$\phi^{\dagger}_{j,g',m}$ = adjoint flux for energy group g', mesh interval m, and spherical harmonics component j,

ℓ = Legendre order, and

z = material region or zone of computational model.

Once the forward–adjoint products are computed for each region and Legendre order, the sensitivity coefficients can be computed from an algebraic expression of the cross-section data, material densities, and region volumes.

In the production version of TSUNAMI-3D, the multigroup adjoint solution often requires extensive sampling to obtain adequate source convergence and acceptable statistics. Additionally, the user must choose appropriate intervals for the mesh flux accumulator to adequately resolve the spatial variation of the angular flux moments. When large systems are adequately spatially resolved, several gigabytes of computer memory can be required to store the angular flux moments for each energy group, material region, and mesh interval for both the forward and adjoint solutions. Furthermore, traditional adjoint techniques are difficult to implement in continuous-energy Monte Carlo calculations, and no production Monte Carlo code offers a continuous-energy adjoint option.

III. Eigenvalue Contributon Approach

To reduce the need for user input and the large amounts of computer memory required by the current TSUNAMI-3D methodology and explore techniques suitable for continuous-energy implementation, the eigenvalue contributon estimator, which simultaneously computes the product of the forward and adjoint angular flux moments, has been implemented into the TSUNAMI-3D analysis sequence.[4] The eigenvalue contributon estimator is an extension of previously developed fixed-source contributon estimators.[5] A *contributon* is a particle for which the forward solution is accumulated, and its importance to the response, which is equivalent to the adjoint solution, is simultaneously accumulated. Thus, the contributon is a particle coupled with its contribution to the response. For criticality problems, the response of interest is the largest eigenvalue, k_{eff}. Contributon particles are created at the site of every forward particle collision, and their histories are simulated within the forward KENO calculation. The contributon provides equivalent information to forward–adjoint product for each location and energy at which the forward flux solution is sampled and spatial refinement of the forward–adjoint product is inherent to contributon the methodology, thus eliminating the need for meshing. Because the contributon is simply a different accumulator for forward particles, it can be directly implemented in continuous-energy calculations. Additionally, the contributon can be extended to responses other than k_{eff}, such as reactivity coefficients and kinetics parameters.[6]

IV. Contributon Theoretical Development

A method for generating the product of the forward and adjoint fluxes, integrated over each computational region, as a function of the forward group and the adjoint group and the Legendre order has been developed. In this technique, only a forward-mode Monte Carlo calculation is conducted. The adjoint solution is derived from additional importance sampling in the forward mode. In this technique, the forward flux is computed with a track-length estimator, where the group-wise j^{th} term of the spherical harmonics expansion of the flux moments within a single region for a single generation of particles is calculated as

$$\varphi_{j,g,z} = \frac{\sum_{k=1}^{K} \sum_{\substack{t \\ g_t = g \\ z_t = z}} W_{k_t} l_{k_t,g,\hat{\Omega},z} R_j\left(\hat{\Omega}\right)}{V_z \sum_{k=1}^{K} W_{k_0}} , \qquad (2)$$

where

$l_{k_t,g,\hat{\Omega},z}$ = distance traversed by track t of particle k in energy group g and direction $\hat{\Omega}$ while within region z,

W_{k_t} = weight of particle k during track length t,

$R_j\left(\hat{\Omega}\right)$ = j^{th} term of real-valued spherical harmonics function for direction $\hat{\Omega}$,

V_z = volume of region z,

W_{k_0} = initial weight of particle k, and

K = total number of particles in the generation.

In Eq. (2), the scalar flux is simply the 0th moment, where $j = 0$ and $R_j\left(\hat{\Omega}\right) = 1.0$.

The importance function is computed by individually tallying the k_{eff} estimator for a series of secondary particles for each track length of the forward solution. Thus, for a single track length of a forward solution, a single particle estimator of the importance of a particle, s, started at the same position as the forward track length, but energy group g' and direction $\hat{\Omega}'$, is accumulated as

$$\varphi_{j,g',\hat{\Omega}',z} = \sum_t W_{s_t} \frac{\nu\Sigma_{f,g'_t,z_t}}{\Sigma_{T,g'_t,z_t}} R_j\left(\hat{\Omega}'\right) \quad , \tag{3}$$

where

W_{s_t} = weight of secondary particle s during track length t,

$\nu\Sigma_{f,g'_t,z_t}$ = neutron production macroscopic cross section in energy group g_t of region z_t,

Σ_{T,g'_t,z_t} = total macroscopic cross section in energy group g_t of region z_t,

$R_j\left(\hat{\Omega}'\right)$ = j^{th} term of real-valued spherical harmonics function for direction $\hat{\Omega}'$,

g_t = energy group of track length t of secondary particle s, and

z_t = material region of track length t of secondary particle s.

Unlike the forward flux accumulator, this importance accumulator assigns the accumulated values to initial position, energy, and direction of the secondary particle.

The product of the forward and adjoint flux moments for Legendre order ℓ for region z, forward group g, and adjoint group g' is accumulated as

$$P^{\ell}_{g,g',z} = \sum_{\substack{j \\ j\in\ell}} \phi_{j,g,z}\phi_{j,g',z} \quad . \tag{4}$$

The general procedure to accumulate $P^{\ell}_{g,g',z}$ is to perform normal tracking in the forward mode, conduct importance sampling by starting additional secondary particles, and accumulate the Legendre moments for the product of the forward and adjoint solutions at each tally site. Thus, substituting Eqs. (2) and (3) into Eq. (4), the eigenvalue contributon estimator becomes

$$P^{\ell}_{g,g',z} = \frac{\sum_{k=1}^{K}\sum_{\substack{j \\ j\in\ell}}\sum_{\substack{t \\ g_t=g \\ z_t=z}}\left(W_{k_t} l_{k_t,\hat{\Omega},z} R_j\left(\hat{\Omega}\right)\sum_{\hat{\Omega}'}\sum_{t'} W_{s_{t'},z_{t'}} \frac{\nu\Sigma_{f,g'_{t'},z'_t}}{\Sigma_{T,g'_{t'},z'_t}} R_j\left(\hat{\Omega}'\right)\right)}{V_z \sum_{k=1}^{K} W_{k_0}} \quad . \tag{5}$$

V. Results

The contributon methodology outlined above was implemented into the TSUNAMI-3D computational sequence. Two test problems were selected and simulated in TSUNAMI-3D using the contributon methodology and were compared with reference results obtained using the conventional forward–adjoint TSUNAMI methodology. The test problems were critical experiments selected from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* and are identified as follows.[7)]

1. HEU-MET-FAST-001 – The Godiva highly enriched uranium bare sphere.
2. MIX-COMP-THERM-001 Case 4 – A model of a reprocessed fast reactor fuel assembly in a shipping cask in an accident scenario where water partially fills the cask. This model will be referred to as MCT-001 below.

The test calculations were performed with the SCALE 44-group ENDB/B-V cross section data with appropriate resonance self-shielding and implicit sensitivity coefficient generation.

P_0 and P_1 forward–adjoint flux product matrices for the Godiva test problem were computed with the traditional TSUNAMI-3D methodology and the contributon accumulator of TSUNAMI-3D and are shown in **Figure 1** and **Figure 2**, respectively. It can be observed that the shapes of the matrices from each methodology are nearly equivalent, as are the relative magnitudes between P_0 and P_1. The values of the contributon matrices differ between the two calculations because of differences in flux normalizations between XSDRNPM used with TSUNAMI-1D and KENO used with TSUNAMI-3D.

Sensitivity coefficient results for the Godiva test problem from conventional TSUNAMI-3D and the contributon accumulator of TSUNAMI-3D contributon accumulator are shown in **Figure 3** and **Figure 4** for ^{235}U and ^{238}U, respectively. Good agreement is observed for the corresponding curves between the two methodologies, except for scattering, which has a higher uncertainty.

For the MCT-001 test problem, P_0 and P_1 forward–adjoint flux product matrices computed with conventional TSUNAMI-3D and the contributon accumulator of TSUNAMI-3D are shown in **Figures 5** and **6**, respectively. It can be observed that the shapes of the matrices from each methodology are nearly equivalent, as are the relative magnitudes between P_0 and P_1.

Sensitivity coefficient results for the MCT-001 test problem from conventional TSUNAMI-3D and the TSUNAMI-3D contributon accumulator are shown in **Figure 7**. Good agreement is observed for the corresponding curves between the two methodologies, except for scattering, which has larger associated uncertainties.

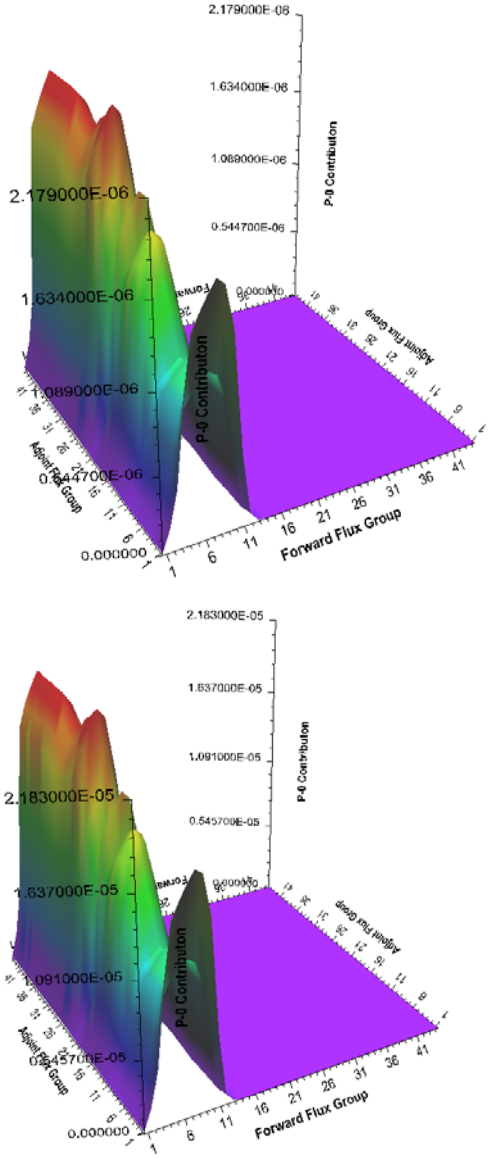

Fig. 1 Forward–adjoint P_0 flux product matrices for forward energy group "Group" and adjoint energy group "Group-Prime" from conventional TSUNAMI-3D (top) and the TSUNAMI-3D contributon accumulator (bottom) for the Godiva test problem.

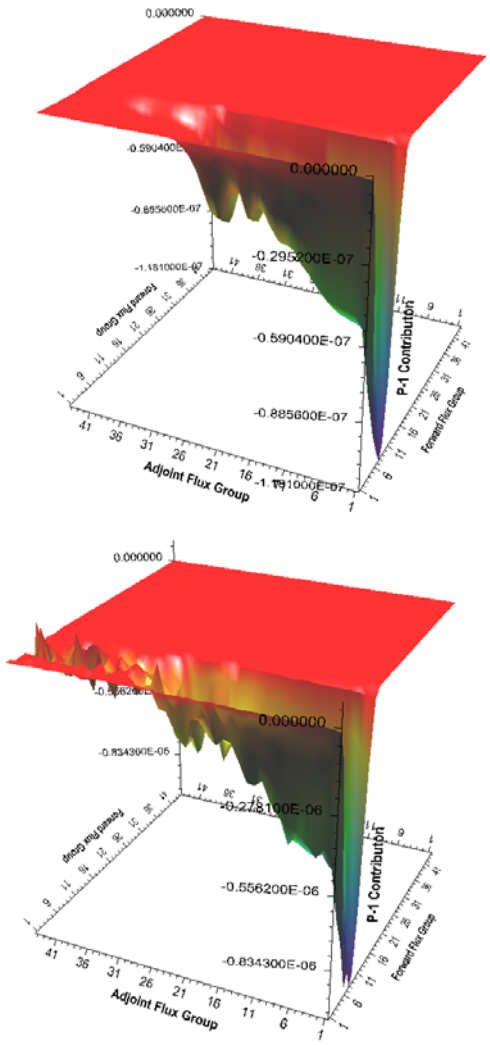

Fig. 2 Forward–adjoint P_1 flux product matrices for forward energy group "Group" and adjoint energy group "Group-Prime" from conventional TSUNAMI-3D (top) and the TSUNAMI-3D contributon accumulator (bottom) for the Godiva test problem.

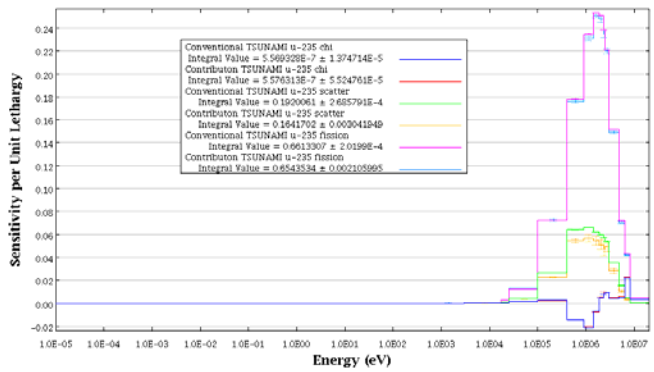

Fig. 3 Energy-dependent sensitivity data for ^{235}U for Godiva test problem from conventional TSUNAMI-3D and the TSUNAMI-3D contributon accumulator.

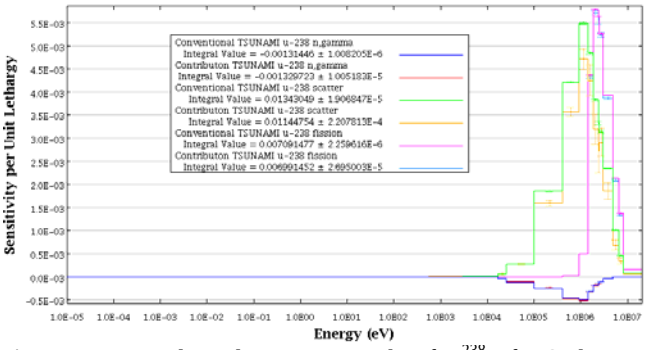

Fig. 4 Energy-dependent sensitivity data for ^{238}U for Godiva problem case from conventional TSUNAMI-3D and the TSUNAMI-3D contributon accumulator.

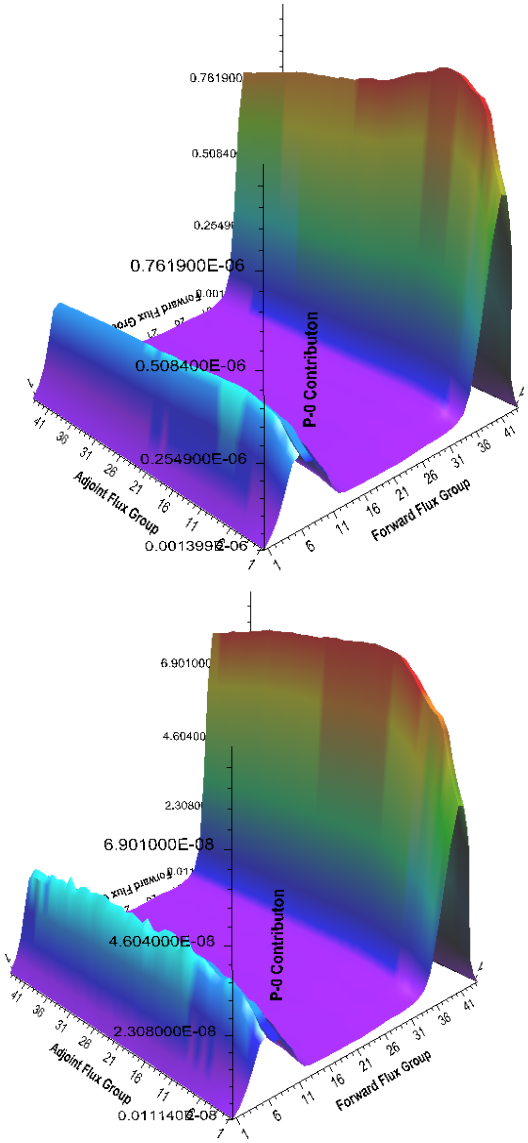

Fig. 5 Forward–adjoint P_0 flux product matrices for forward energy group "Group" and adjoint energy group "Group-Prime" from conventional TSUNAMI-3D (top) and the TSUNAMI-3D contributon accumulator (bottom) for the MCT-001 test problem.

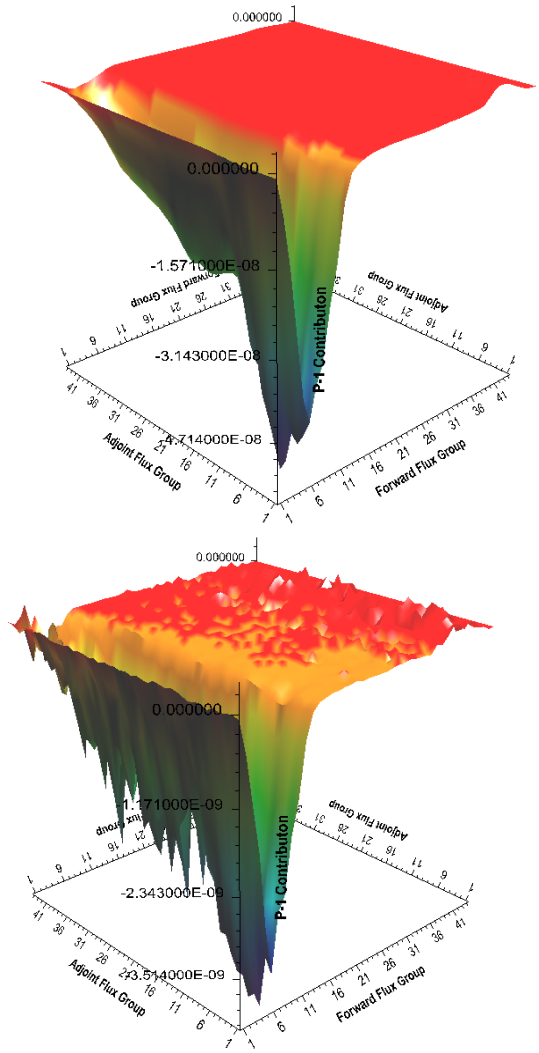

Fig. 6 Forward–adjoint P_1 flux product matrices for forward energy group "Group" and adjoint energy group "Group-Prime" from conventional TSUNAMI-3D (top) and the TSUNAMI-3D contributon accumulator (bottom) for the MCT-001 test problem.

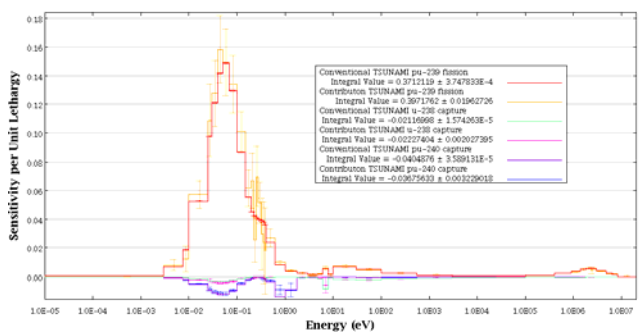

Fig. 7 Energy-dependent sensitivity data for the MCT-001 test problem from conventional TSUNAMI-3D and the TSUNAMI-3D contributon accumulator.

VI. Contributon Figure of Merit Optimization Study

The contributon calculations presented in the previous section were obtained using TSUNAMI calculations that

simulated one contribution particle at the site of every forward particle collision. It is possible to sample more than one contributon particle at the site of every collision by increasing the number of energy groups and directions that are sampled for each collision. For example, increasing the number of energy groups sampled from one to two causes TSUNAMI to create one contributon in each of two randomly sampled energy groups; further increasing the number of sampled directions from one to two causes TSUNAMI to simulate a total of four contributon particles. For cases with complex flux product matrices, it can be advantageous to sample more contributon energy groups and directions at the site of every forward collision in lieu of simulating more forward particles. On the other hand, high-leakage systems are less likely to benefit from simulating more contributons as they are likely to leak out of the system without contributing much to the adjoint flux accumulator.

A parametric study was performed for the two test problems in which the number of contributon energy groups and directions sampled at each forward particle collision was varied, and its effect on the figure of merit of sensitivity coefficients for several key nuclides was examined. The figure of merit for these nuclide sensitivity coefficients is defined as

$$FoM = \frac{1}{\sigma^2 * Time} \quad . \tag{6}$$

Table 1 and **Table 2** show the effect of varying the contributon energy group and direction sampling on the figure of merit for the total nuclide sensitivity coefficients of ^{235}U and ^{238}U, respectively, in the Godiva test problem. As shown in the tables, increasing the number of contributon energy groups and directions universally lowers the efficiency of the contributon calculations for the Godiva test problem. The relative simple symmetric, homogenous, fast-spectrum and high-leakage nature of the Godiva problem makes sampling extra contributon particles at the site of every collision unnecessary. In fact, sampling extra contributons at every collision lowers the efficiency of the sensitivity coefficient calculation, as these contributons are likely to leak from the system without contributing much to the adjoint flux accumulator.

Table 1 Figures of merit for the total nuclide sensitivity of ^{235}U in the Godiva test problem

		Number of contributon energy groups sampled for each forward collision			
		1	2	5	10
Number of contributon directions sampled for each forward collision	1	3898.11	2918.31	2486.63	1093.45
	2	3210.12	2870.93	1078.57	615.33
	5	1791.97	1501.79	510.80	282.32
	10	1133.41	829.94	278.95	145.42

Table 2 Figures of merit for the total nuclide sensitivity of ^{238}U in the Godiva test problem

		Number of contributon energy groups sampled for each forward collision			
		1	2	5	10
Number of contributon directions sampled for each forward collision	1	794.25	620.03	548.28	248.86
	2	661.21	634.42	241.03	142.44
	5	388.33	335.61	113.65	64.02
	10	248.74	185.07	63.25	33.61

Two reference cases were simulated using the conventional TSUNAMI forward–adjoint calculation methodology, and their total nuclide sensitivity coefficient figures of merit were compared to those from the single contributon per collision case. One of the reference cases was simulated using a 1-cm flux mesh size and the other used a 0.25-cm flux mesh size. **Table 3** shows the ratios of the figures of merit from the reference cases to the contributon figures of merit. As shown in the table, the conventional TSUNAMI methodology is more efficient than the contributon methodology for the initial 1-cm mesh case, but the contributon methodology becomes more efficient as the mesh size is refined to 0.25 cm. These results suggest that the contributon methodology can provide superior efficiency when compared with the traditional TSUNAMI methodology for moderately sized problems that demand a very fine mesh or large problems that require even a moderate mesh.

Table 3 Ratio of the figures of merit of the total nuclide sensitivities from the conventional TSUNAMI cases to the figures of merit from the contributon cases

	U-235	U-238
1-cm Mesh	2.038	2.976
0.25-cm Mesh	0.670	1.015

Table 4, **Table 5**, and **Table 6** show the effect of varying the contributon energy group and direction sampling on the figure of merit for the total nuclide sensitivity coefficients of ^{239}Pu, ^{1}H, and ^{238}U, respectively, in the MCT-001 test problem. Unlike in the Godiva test problem, increasing the number of contributons that are simulated at each forward collision can (but does not always) cause an increase in the figures of merit for the total nuclide sensitivity coefficients. This occurs because the MCT-001 test problem is much more complicated than the Godiva test problem from both a geometric, compositional, and flux spectrum standpoint. The MCT-001 test problem contains several isotopes of plutonium and uranium as well as small amounts of transuranic nuclides, and the thermal nature of the flux spectrum in this problem causes the resonance cross sections of these nuclides to have a large impact on the TSUNAMI sensitivity coefficients. Sampling more contributon particles allows one to more thoroughly account for the impact of these resonances. For example, sampling more

contributon energy groups per forward collision causes more contributons to be born at or near resonance energies, and sampling more contributon directions per forward collision allows for more resonance energy neutrons (in the moderator for example) to be scattered back into fuel regions. However, the figures of merit do not scale linearly with additional contributon sampling at each collision – as seen in **Tables 4** through **6**, sampling more contributon energy groups and directions can both increase and decrease the figures of merit. There appears to be a strong nuclide-dependent correlation between the total sensitivity coefficients and how contributon particle energies and directions are sampled. Optimizing the contributon particle birth process could potentially speed up the contributon calculations for complex systems such as MCT-001.

Table 4 Figures of merit for the total nuclide sensitivity of ^{239}Pu in the MCT-001 test problem

		Number of contributon energy groups sampled for each forward collision		
		1	2	5
Number of contributon directions sampled for each forward collision	1	0.0780	0.0583	0.0299
	2	0.0561	0.0341	0.0203
	5	0.0258	0.0183	0.0086

Table 5 Figures of merit for the total nuclide sensitivity of ^{1}H in the MCT-001 test problem

		Number of contributon energy groups sampled for each forward collision		
		1	2	5
Number of contributon directions sampled for each forward collision	1	0.000032	0.000191	0.000120
	2	0.000205	0.000118	0.000004
	5	0.000074	0.000010	0.000005

Table 6 Figures of merit for the total nuclide sensitivity of ^{238}U in the MCT-001 test problem

		Number of contributon energy groups sampled for each forward collision		
		1	2	5
Number of contributon directions sampled for each forward collision	1	0.01162	0.00841	0.00871
	2	0.00732	0.00562	0.00466
	5	0.00707	0.00696	0.00325

Acceleration and/or parallelization of the contributon calculation are greatly needed if the contributon methodology is to be used routinely in production calculations. Some optimization techniques have been explored elsewhere but have not been tested in TSUNAMI-3D.[8)] The contributon figures of merit for the MCT-001 test problem were between 1,000 and 300,000 times smaller than the corresponding figures of merit from the convention TSUNAMI forward–adjoint calculation. This drastic drop in the contributon figures of merit is believed to be due to the highly scattering, thermal nature of the MCT-001 test problem, in which low energy forward particles that have long lifetimes spent scattering in the moderator can produce enormous amounts of contributons and slow down the TSUNAMI simulation. Despite the much slower runtime, the fact that the contributon calculation does not require a flux mesh is a great advantage in this test problem. The conventional TSUNAMI forward–adjoint calculation demands a very fine flux mesh to produce correct sensitivity coefficients and requires more than 30 gigabytes of RAM for its calculation. The contributon calculation only requires 32 megabytes of RAM for its calculation and has the potential to be an alternative to the traditional TSUNAMI methodology baring the previously mentioned acceleration issues.

VII. Conclusion

A new methodology for computing eigenvalue sensitivity coefficients has been developed and implemented in TSUNAMI-3D. Good agreement with classical forward–adjoint techniques has been demonstrated, and the potential for mesh-less contributon calculations has been recognized. With appropriate sampling optimization and parallelization, the contributon technique provides an opportunity for continuous-energy calculations in TSUNAMI-3D. Additionally, the contributon estimator provides the opportunity to extend TSUNAMI-3D to additional types of sensitivity calculations, such as kinetics parameters.

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