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EIGENVALUE CONTRIBUTON ESTIMATOR FOR SENSITIVITY CALCULATIONS WITH TSUNAMI-3D

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Introduction

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

1. TSUNAMI-3D

The TSUNAMI-3D analysis sequence, based on the KENO V.a Monte Carlo code, 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 V.a. When the mesh fluxes are requested, a uniform cubic mesh of user-defined size is distributed throughout the entire system model. 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,

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 [2].

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 an appropriate spatial size 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.

2. Eigenvalue contributon approach

To reduce the need for user input and the large amounts of computer memory required by the current TSUNAMI-3D methodology, a new technique to simultaneously obtain the product of the forward and adjoint angular flux moments with Monte Carlo techniques has been developed and implemented into a prototypic 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 [4]. 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}. The contributon provides equivalent information to forward–adjoint product for each location and energy at which the forward flux solution is sampled. Spatial refinement of the forward–adjoint product is inherent to the methodology, and the need for meshing is eliminated.

3. Theoretical development

A method for the generation of 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

$$\phi_{j,g,z} = \frac{\sum_{k=1}^{K} \sum_{\substack{t \\ g_t = g \\ z_t = z}} w_{k_t} l_{k_t,\hat{\Omega},z} R_j(\hat{\Omega})}{V_z \sum_{k=1}^{K} w_{k_0}}, \tag{2}$$

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,

$R_j(\hat{\Omega})$ = 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,

K = total number of particles in the generation.

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

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

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,

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

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

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

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

4. Results

The methodology outlined above was implemented into a prototypic TSUNAMI-3D computational sequence. Two simple test problems were selected such that the data could easily be verified against one-dimensional models with data generated with TSUNAMI-1D.

The selected test problems were critical experiments selected from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [5] and are identified as follows:

1. HEU-MET-FAST-001 – The Godiva highly-enriched uranium bare sphere.
2. LEU-COMP-THERM-033 Case 1 – A spherical model of well–moderated homogeneous mixture of $U(2)F_4$ and paraffin. This model will be referred to as LCT-033 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 computed with TSUNAMI-1D and the contributon version of TSUNAMI-3D are shown in Figs. 1 and 2, respectively. It can be observed in the figures 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 Godiva test problem from TSUNAMI-1D and the TSUNAMI-3D contributon accumulator are shown in Figs. 3 and 4 for ^{235}U and ^{238}U, respectively. Excellent agreement is observed for the corresponding curves between the two methodologies.

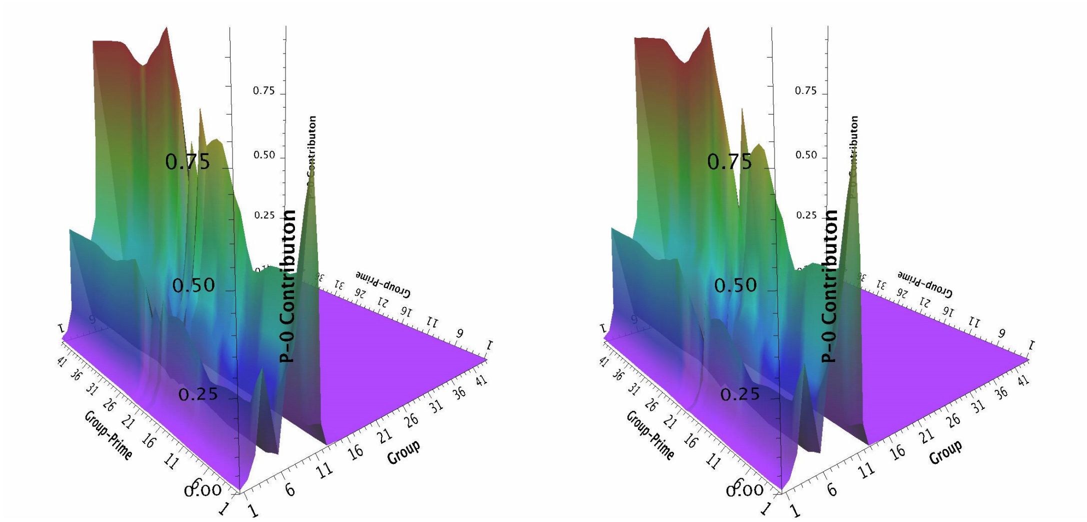

Figure 1. Forward–adjoint P_0 flux product matrices for forward energy group "Group" and adjoint energy group "Group-Prime" from TSUNAMI-1D (left) and TSUNAMI-3D contributon accumulator (right) for the Godiva test problem.

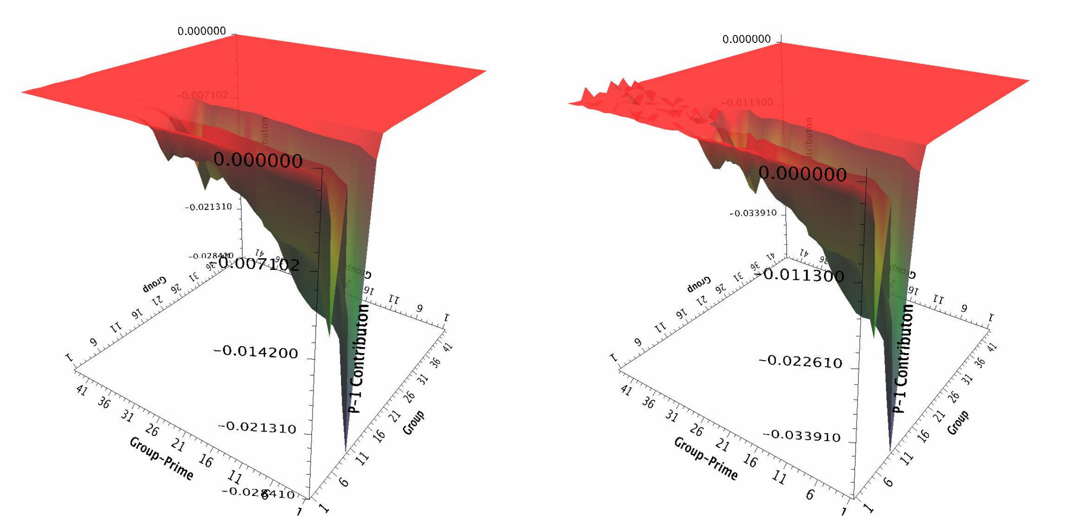

Figure 2. Forward–adjoint P_1 flux product matrices for forward energy group "Group" and adjoint energy group "Group-Prime" from TSUNAMI-1D (left) and TSUNAMI-3D contributon accumulator (right) for the Godiva test problem.

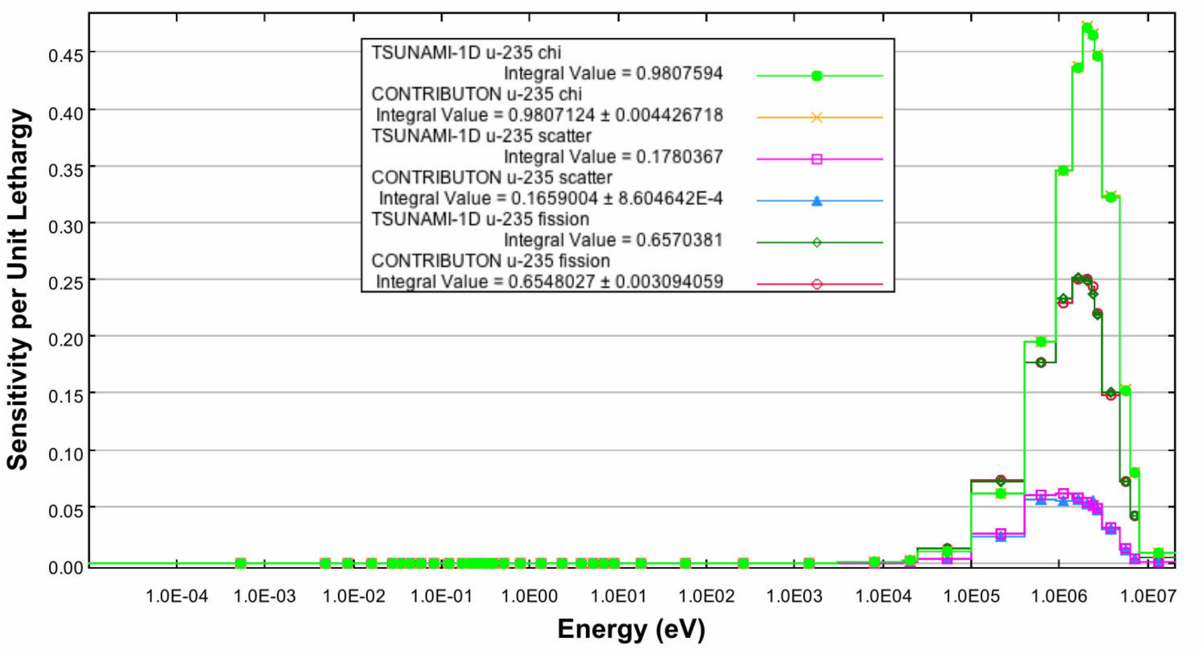

Figure 3. Energy-dependent sensitivity data for ^{235}U for Godiva test problem from TSUNAMI-1D and TSUNAMI-3D contributon accumulator.

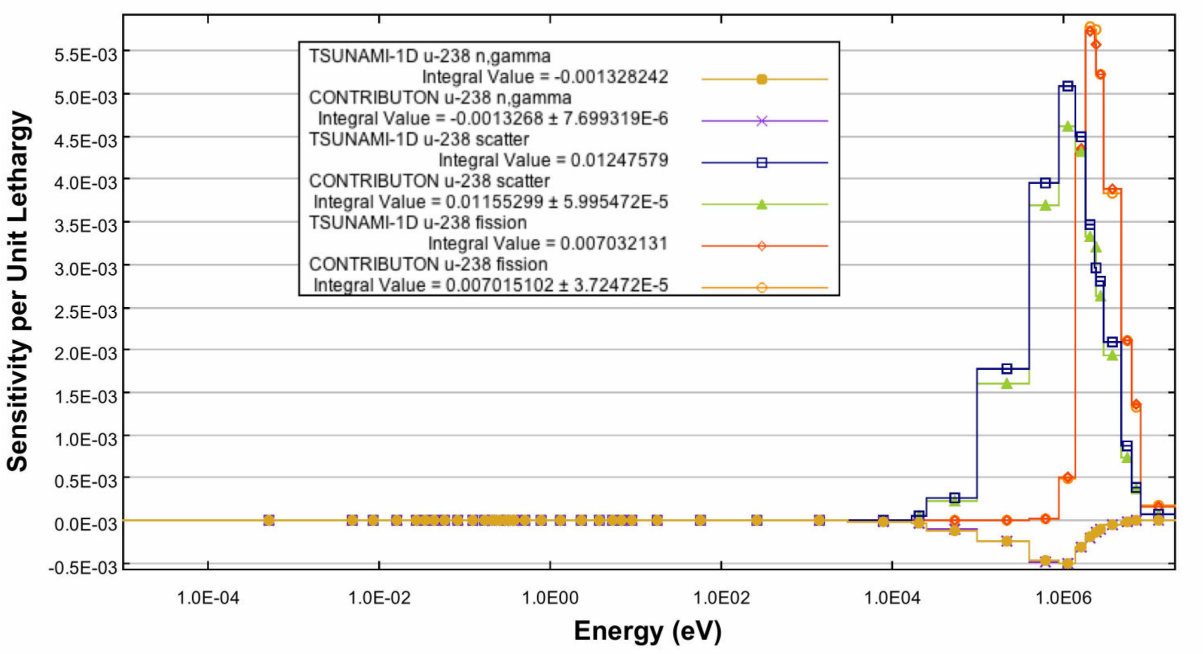

Figure 4. Energy-dependent sensitivity data for ^{238}U for Godiva problem case from TSUNAMI-1D and TSUNAMI-3D contributon accumulator.

For the LCT-033 test problem, P_0 and P_1 forward–adjoint flux product matrices computed with TSUNAMI-1D and the contributon version of TSUNAMI-3D are shown in Figs. 5 and 6, respectively. It can be observed in the figures 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 LCT-033 test problem from TSUNAMI-1D and the TSUNAMI-3D contributon accumulator are shown in Fig. 7. Excellent agreement is observed for the corresponding curves between the two methodologies.

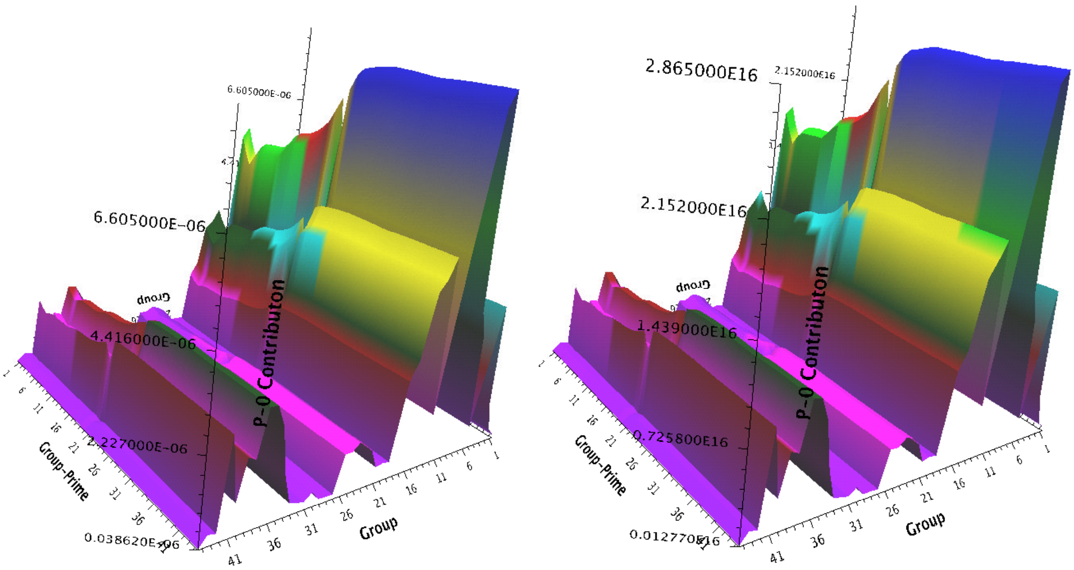

Figure 5. Forward–adjoint P_0 flux product matrices for forward energy group “Group” and adjoint energy group “Group-Prime” from TSUNAMI-1D (left) and TSUNAMI-3D contributon accumulator (right) for LCT-033 test problem.

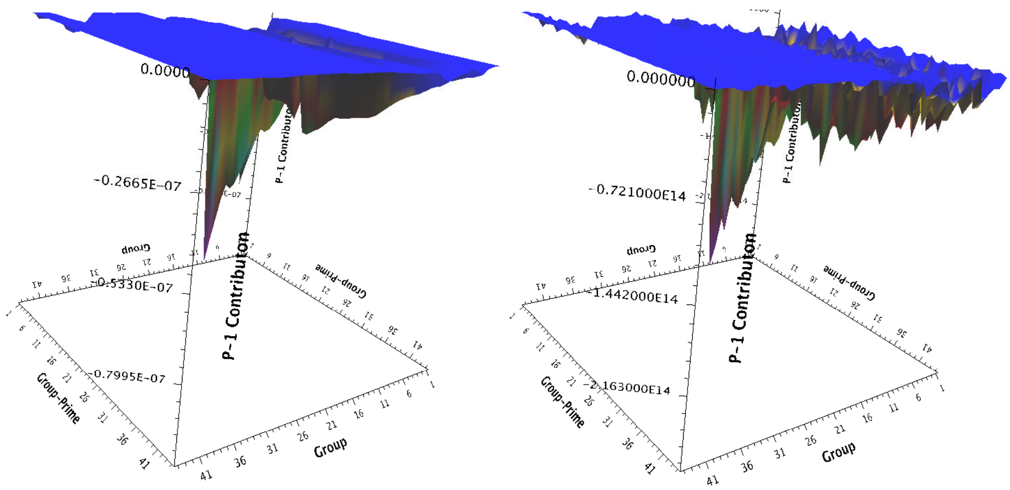

Figure 6. Forward–adjoint P_1 flux product matrices for forward energy group “Group” and adjoint energy group “Group-Prime” from TSUNAMI-1D (left) and TSUNAMI-3D contributon accumulator (right) for LCT-033 test problem.

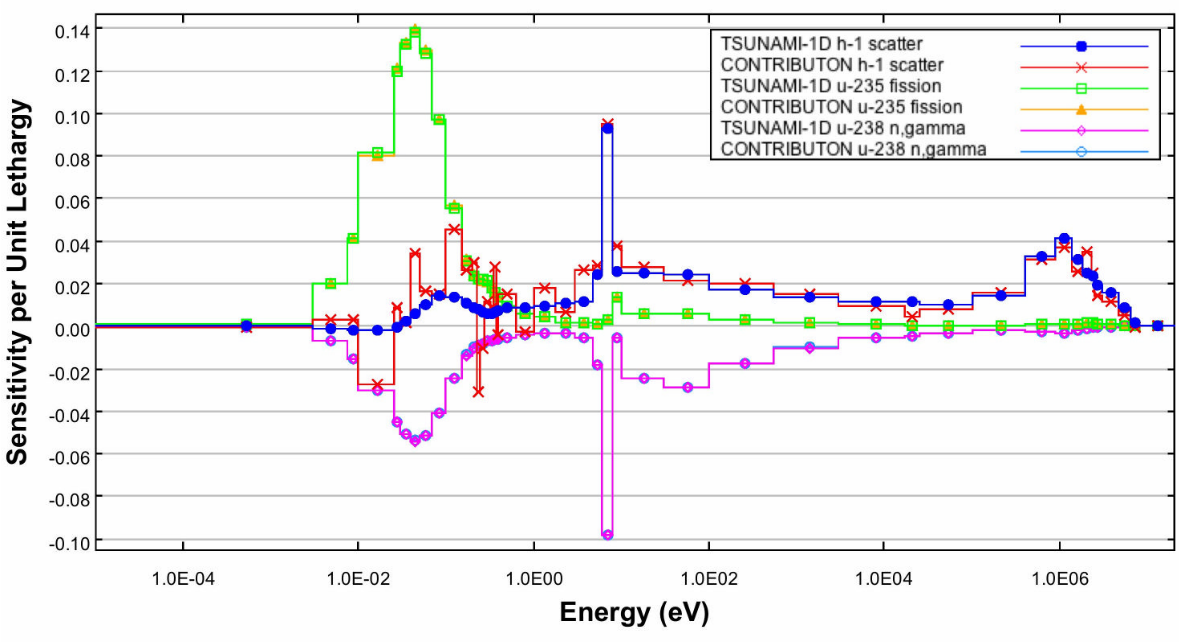

Figure 7. Energy-dependent sensitivity data for LCT-033 test problem from TSUNAMI-1D and TSUNAMI-3D contributon accumulator.

5. Conclusions

A new methodology for computing eigenvalue sensitivity coefficients has been developed and implemented in a prototypic version of TSUNAMI-3D. Excellent agreement with classical forward–adjoint techniques has been demonstrated.

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