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IMPROVEMENTS IN KENO V.a TO SUPPORT TSUNAMI-3D SENSITIVITY CALCULATIONS

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ABSTRACT

Improvements in the KENO V.a Monte Carlo code to support sensitivity calculations are described in this paper. The calculation of angular moments and spatially resolved fluxes using a mesh accumulator are explained. The uses of the features to produce accurate sensitivity coefficients are explored in a series of example calculations. With limited user intervention, sensitivity coefficients that are consistent with direct perturbation results can be generated for complex systems.

Key Words: TSUNAMI, KENO, Moment, Mesh, Sensitivity

1 INTRODUCTION

The **T**ools for **S**ensitivity and **Un**certainty **A**nalysis **M**ethodology **I**mplementation (TSUNAMI) software released with SCALE 5 in June of 2004 includes the TSUNAMI-3D sensitivity analysis sequence, which computes the sensitivity of k_{eff} to the multigroup cross-section data for each reaction of each nuclide on an energy-dependent basis. TSUNAMI-3D computes sensitivity coefficients using adjoint-based first-order linear perturbation theory. The forward and adjoint neutron transport solutions required to produce the sensitivity coefficients are computed with the KENO V.a Monte Carlo code. Perturbation theory requires the angular moments of the forward and adjoint flux solutions, which were not available in KENO V.a prior to the development of the sensitivity analysis sequence. Furthermore, the angular moments must be adequately resolved spatially to obtain an accurate inner product of the forward and adjoint solutions to compute the sensitivity coefficients.

To support sensitivity calculations with TSUNAMI-3D, angular moment calculational techniques were developed and implemented into KENO V.a. To produce adequate spatial resolution of the flux solutions, a simple automated mesh feature was implemented into KENO V.a. Descriptions of the new Monte Carlo techniques and examples of their use in sensitivity calculations are presented in this paper.

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2 METHODS

In adjoint-based perturbation theory, the products of the angular moments of the flux solutions from the forward and adjoint calculations are computed for each region of the system model. Once these products are computed for each region, the sensitivity coefficients, which give the expected change in the system (k_{eff}) due to changes in the constituent cross-section data, can be analytically determined for each region. The sensitivity coefficients for the individual regions can be summed to determine the sensitivity of the system as a whole to a particular cross-section value. The keys to successful implementation of the procedure are to (1) produce accurate angular moments of the forward and adjoint flux solutions and (2) provide adequate spatial resolution of the flux solutions such that variations across the system are captured.

The ability to accumulate angular flux moments with KENO V.a has been documented elsewhere [1], and will be only briefly reviewed in Sect. 2.1 as a means of establishing the context for other material. The ability to accumulate fluxes with spatial refinement over a simple computational mesh has recently been added to KENO V.a and is discussed in Sect. 2.2.

2.1 Angular Flux Moments

To compute sensitivity coefficients using adjoint-based perturbation theory, angular variations in the flux solutions are represented in terms of moments that correspond to the Legendre expansion of the group-to-group transfer arrays in the cross-section data. For three-dimensional geometry models, the fluxes are represented by a spherical harmonics expansion of the angular flux solution. With KENO V.a, techniques have been developed to accumulate the moments directly from each individual neutron track or to bin the individual neutron tracks into an angular quadrature and then expand the quadrature solution to moments after the calculation is complete. With either method, the angular representation of a particular track can be computed in terms of a transformed angular coordinate system, which allows the accumulation of the angular moments in terms of a spherical coordinate system instead of the Cartesian system used for neutron tracking.

The use of the transformed coordinate system is necessitated by the large geometry regions commonly used in Monte Carlo models. In the case of a single finite fuel region in a vacuum, the Cartesian representation of the angular variation of the flux is exactly zero for the system as a whole. For example, the first moment of a particle exiting the system along the x-axis in the positive direction would be of equal magnitude and opposite sign as an equivalent particle exiting the system along the x-axis in the negative direction. The net moment for the system is the sum of the moments of the individual particles and is zero. However, the computation of the moments of each of these particles in terms of a spherical coordinate system from the center of the fuel results in equal magnitude and equal signed moments for both particles and a nonzero moment for the sum of the two.

The transformation to a spherical coordinate system determines the direction the particle is transporting relative to a given reference point. KENO V.a allows for user control of this reference point, which is identified as the “center” of the transform in the code input. The default value for the center of the transform is the centroid of all fissile material in the system model, but the user can override this default value and input translation of the transform center for any individual geometry region.

In deterministic transport codes, where the flux solutions are converged within a fine computational mesh, the transform from a Cartesian to spherical coordinate system is not necessary to obtain nonzero flux moments for individual computational regions. The use of the Cartesian system is permitted by the small size of each computational cell. In the case of the system discussed above, two cells on the positive and negative *x*-faces would individually have nonzero moments. In perturbation theory, the product of the moments for the forward and adjoint solutions are computed for each computational cell. The first moment of the forward solution would be positive at the $+x$ face and negative at the $-x$ face. For the adjoint solution, the first moment would be negative at the $+x$ face and positive at the $-x$ face. Thus, the product of the forward and adjoint solutions have the same sign for the cells at both the $+x$ and $-x$ faces. The nonzero product of the moments leads to nonzero contributions to the sensitivity coefficients from the group-to-group transfer arrays in each cell, and the sum of the sensitivity coefficients for the systems is also nonzero.

2.2 Mesh Flux Accumulator

The necessity of obtaining spatially resolved flux solutions for adjoint-based perturbation theory calculations has been demonstrated in previous work [1]. In examples presented in Ref. 1, the geometry was manually subdivided to provide additional regions in the Monte Carlo model for flux accumulation. However, for complex systems, the task of manually subdividing the geometry to adequately resolve the flux solution may be impracticable, or at least undesirable. The commonly used array feature in KENO V.a allows for simplified modeling of systems with repeated units in a regular pattern. However, the flux accumulator in KENO V.a stores the fluxes for all instances of the same unit in the same location. The flux per unit volume computed for a unit that is repeated in the model is the sum of the fluxes for all occurrences of the unit divided by the volume of the unit and the number of times the unit appeared in the system model. The resulting flux is the average flux for the unit throughout the model. For sensitivity calculations, the average flux for all occurrences of the unit in the model typically does not provide accurate products of the forward and adjoint solutions. The flux must be further resolved spatially, and axial as well as radial refinement is typically required. These refinements could be accomplished by manually defining a number of instances of the repeated unit, each of which could have further internal refinements, and then placing the repeated definitions of the unit in the array in a manner that minimizes the flux variation across any individual unit. Again, the process is likely not desirable to a user.

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 based on the position of the tally within the outermost or "global" unit of the model. In the case of a unit repeated multiple times in an array, the flux solution is not averaged over all occurrences of the unit in the entire system model but is averaged only over those occurrences, or partial occurrences, of the unit within a given mesh interval. 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 that contain a given region. Sensitivity coefficients are then computed for that region using the forward and adjoint flux products summed over the mesh intervals.

A two-dimensional view of a mesh flux accumulator for an array of fuel pins is shown in Fig. 1, where the fuel is red, the gap is white, the clad is grey, the moderator is blue, and the boundaries of the mesh flux accumulator are shown in yellow. Here, the fluxes for a single fuel pin, repeated 36 times in an array, are accumulated over a cubic mesh whose side is 1.375 times the pitch of the array. The mesh size is chosen to illustrate how the mesh operates when a mesh interval crosses a geometry region. Individual mesh accumulators are established for each of the fuel, gap, clad, and moderator regions of the fuel pin in the array. The four accumulators are shown in Fig. 2. The interior of each box, outlined in yellow in Fig. 2, represents a unique storage location for the flux solution, including the scalar flux, higher-order angular moments, or angular quadrature, depending on the user-selected options. Not shown in the figures is the third dimension of the mesh flux accumulator, which also divides this model axially on the same interval as the radial division shown.

When tracking an individual particle with the mesh flux accumulator, the normal tracking procedure of KENO V.a is unchanged. A particle is transported until a collision or geometric boundary crossing occurs, and the distance for the track-length flux accumulator is determined. A track length can traverse no more than one geometry region; otherwise, a crossing would occur. However, the track can traverse more than one mesh interval. The flux is tallied in the mesh intervals in which it occurred, with a track-length estimator based on the distance traversed by the track in each mesh interval.

As an example, the fuel regions contained in a particular mesh interval are shown in Fig. 3. Prior to the calculation, the combined volume of the fuel regions and partial regions bounded by this mesh interval is analytically computed. As the transport solution progresses, the track lengths or partial track lengths occurring in any of the fuel material bounded by this interval are tallied in the mesh flux accumulator. Once the tracking procedure is complete, the flux solution is divided by the volume of fuel that is bounded by this mesh interval to give the flux per unit volume occurring in all instances of this fuel region that are bounded by this mesh interval. This regionally and spatially dependent flux solution is accumulated as angular moments for each energy group, including the 0^{th} moment or scalar flux. Fluxes are also accumulated separately for the gap, clad, and moderator regions occurring in this same mesh interval.

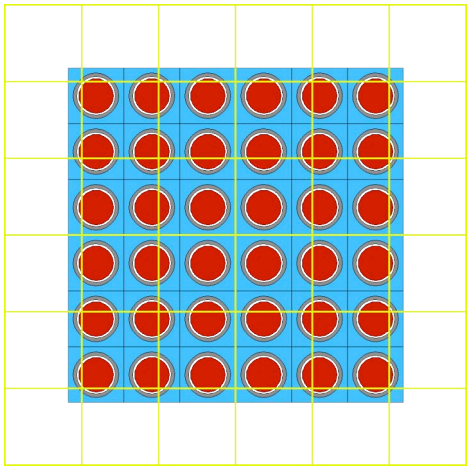

Figure 1. Illustration of mesh flux accumulator on an array of fuel pins

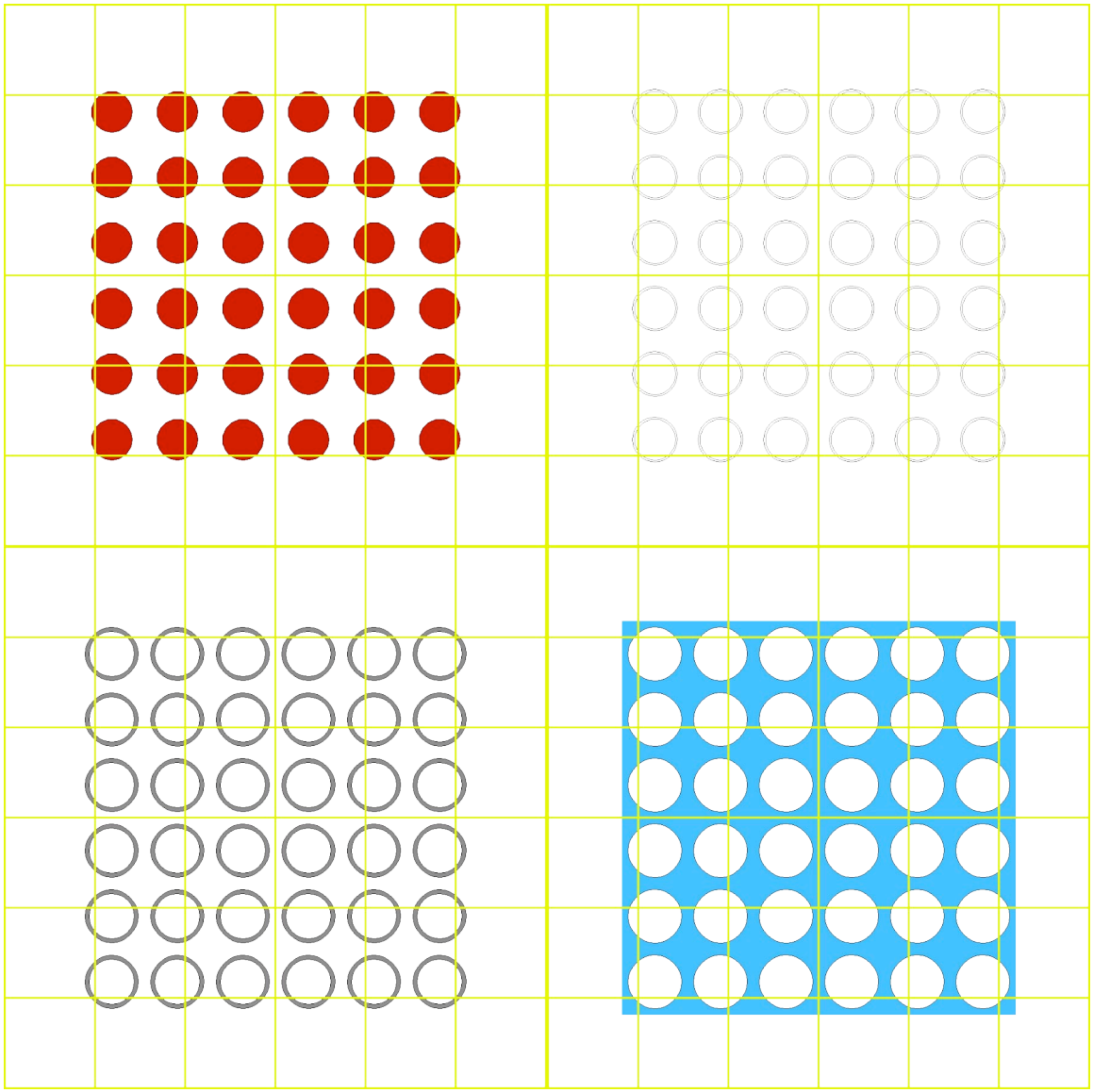

Figure 2. Mesh flux accumulators for the fuel, gap, clad, and moderator regions of the array of fuel pins

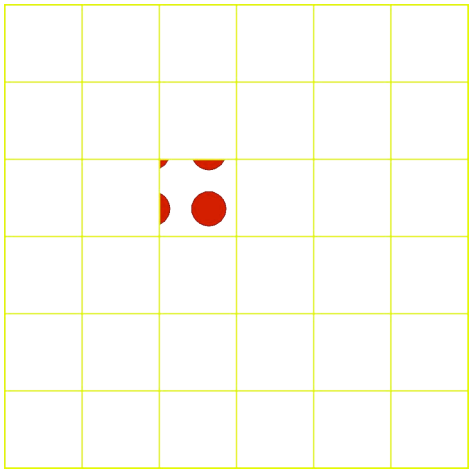

Figure 3. Fuel regions contained in a single mesh interval

3 EXAMPLE SYSTEM

To demonstrate the use of the angular moment and mesh flux accumulators in sensitivity calculations, a sample problem was selected from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [2]. The selected system is a critical configuration of mixed-oxide (MOX) fuel pins in a partially flooded tank and is identified as case 1 from evaluation MIX-COMP-THERM-011. In the critical assembly, 169 RAPSODIE fuel pins with 25.8 wt % PuO_2 in MOX with UO_2 enriched to 60 wt % in ^{235}U were assembled in a hexagonal arrangement with a triangular pitch of 1.9 cm. The height of the fissile material in a fuel pin is 34.55 cm, but the critical configuration was partially flooded and the active fuel height below the moderator is 30.43 cm. The partial flooding of the core leaves 4.12 cm of fuel extending above the moderator. A cutaway view of this system, as modeled in KENO V.a, is shown in Fig. 4. In this figure, the water is shown in green, and the MOX fuel is shown in dark blue. Cladding and other materials, not described here, are also shown in other colors.

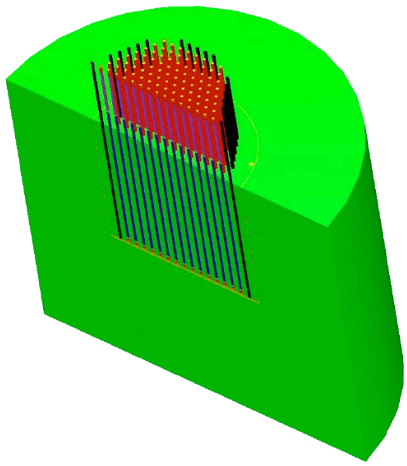

Figure 4. Cutaway view of MIX-COMP-THERM-011 case 1

3.1 Direct Perturbation Results

The validity of the energy-integrated sensitivity coefficients can be confirmed through the use of central difference direct perturbation sensitivity calculations. Through this technique, the sensitivity of k_{eff} to the number density of particular nuclide can be obtained. This sensitivity of k_{eff} to the number density is equivalent to the sensitivity of k_{eff} to the total cross section, integrated over energy. Because the total cross-section sensitivity coefficient tests much of the data used to compute all other sensitivity coefficients, it is considered an adequate test for verification. For each sensitivity coefficient examined by direct perturbation, the k_{eff} of the system is computed first with the nominal values of the input quantities, then with a selected input value increased by a certain percentage, and then with the value decreased by the same percentage. The direct perturbation sensitivity coefficient of k_{eff} to some input value α is computed as

$$S_{k,\alpha} = \frac{\alpha}{k} \times \frac{dk}{d\alpha} = \frac{\alpha}{k} \times \frac{k_{\alpha^+} - k_{\alpha^-}}{\alpha^+ - \alpha^-} \tag{1}$$

where α^+ and α^- represent the increased and decreased values of the input quantity, α, respectively, and k_{α^+} and k_{α^-} represent the corresponding values of k_{eff}. Statistical uncertainties in the computed values of k_{eff} are propagated to uncertainties in direct perturbation sensitivity coefficients by standard error propagation techniques [3] as

$$\sigma_S = \left(\left(\frac{\left(\sigma_{k^+}^2 + \sigma_{k^-}^2\right)}{\left(k^+ - k^-\right)^2} + \frac{\sigma_k^2}{k^2} \right) \times \left(\frac{k^+ - k^-}{k} \right)^2 \right)^{1/2} \times \frac{\alpha}{\alpha^+ - \alpha^-} \tag{2}$$

For this model, direct perturbation sensitivity coefficients were computed for ^{235}U in the MOX fuel and ^{1}H in the water moderating the MOX fuel lattice using 2% perturbations in the number densities. These direct perturbation sensitivity coefficients are 0.056 ± 0.005 and 0.363 ± 0.005, respectively. Note that due to the small magnitude of the ^{235}U sensitivity, which is larger than that of ^{239}Pu in this MOX system, accurate prediction with direct perturbation is difficult. Each of the direct perturbation calculations was performed with 30,000 neutrons per generation for 1503 generations, with 100 initial generations skipped, producing over 42 million histories. Still, the uncertainty in the ^{235}U sensitivity coefficient is approximately 9%. The larger magnitude of the ^{1}H sensitivity value leads to an uncertainty of approximately 1%. Although not examined for this paper, the use of additional direct perturbations greater or less than 2% variations in the number densities would provide more insight into the true behavior of these systems.

3.2 TSUNAMI-3D Results

The experiment described above was modeled with TSUNAMI-3D, using different combinations of options for the placement of the center of the coordinate transform and the mesh

flux accumulator. In all cases, the angular flux moments were expanded to first order. Nine calculations were conducted to form a matrix of results with three different angular transform options and three different mesh flux accumulator options. The three options for the transform are the code default that places the transform center at the centroid of the fuel; a user-defined transform where the transform center is translated in the $-z$ direction to the center of the fuel that is flooded; and the calculation of the angular moments without the use of the transform, such that the moments are computed in reference to the Cartesian coordinates. The three options for the mesh flux accumulator are the use of no mesh, such that only region-averaged fluxes are used; spatially resolved fluxes on a 10-cm mesh, which is approximately one-third of the fuel height; and spatially resolved fluxes on a 3-cm mesh, which is approximately one-tenth of the fuel height.

The energy-integrated sensitivities of k_{eff} to the total cross sections from the TSUNAMI-3D calculations are shown in Table I and represented graphically with the direct perturbation results in Fig. 5. The results for ^{235}U for all TSUNAMI-3D cases agree with the direct perturbation results within two standard deviations. As discussed above, the small magnitude of this sensitivity coefficient creates difficulties in obtaining accurate direct perturbation values; however, some general observations regarding these results can be made. The small scattering cross section for ^{235}U minimizes the influence of the angular moments, which can be affected by changes in the center of the transform. For this system, which is well moderated and well reflected, the spectrum of the scalar flux changes little as a function of position in the fuel except for fast leakage at the fuel/reflector interface. For this thermal system, k_{eff} is largely insensitive to the ^{235}U cross section at fast energies, and the product of the forward and adjoint scalar fluxes can be accurately produced without spatial refinement of the flux solution. Where the center of the transform is modified or the flux solution is further spatially refined with a mesh, the ^{235}U sensitivity is only marginally affected. The energy-dependent sensitivity profiles for ^{235}U fission, capture, and scatter for the case with no transform and no mesh and the case with the transform based on the center of flooded MOX fuel with a 3-cm mesh are shown in Fig. 6. Here, the most significant difference between corresponding sensitivity profiles for the two systems can be seen for scatter at fast energies with other small differences in fission and capture.

Due to the higher-order scattering cross sections, the sensitivity of k_{eff} to ^{1}H is affected by the choice of the center for the coordinate transform and the spatial refinement of the flux solution. Although the energy shape of the scalar flux is largely constant throughout the system, the angular moments, especially for fast energies, vary significantly from the center of the core, where the flux is isotropic at all energies, to the edge of the core, where the fast flux is exiting the core with no fast return from the reflector. This variation in the energy shape of the flux solution across the system requires the use of spatial refinement to obtain accurate products of the forward and adjoint solutions. As shown in Table I and Fig. 5, the value of the sensitivity of k_{eff} to the total cross section for ^{1}H can vary substantially depending on the choice of mesh and transform.

For the “Center of MOX Fuel, No Mesh” case, the center of the transform is placed at the center of the fissile material. However, the fuel rods extend 4.12 cm above the top of the moderator. Without moderation, this fuel is largely nonreactive. The use of this nonreactive fuel in the placement of the center of the moment calculation causes the transform to be performed in reference to a point that is 2 cm above the center of the active flooded fuel. The exclusion of a mesh flux accumulator from this model eliminates any spatial refinement of the solution. As a

result of these two inadequacies in the input specification, the sensitivity for ^{1}H differs from the direct perturbation result by 17% and by 12% outside of one standard deviation.

In the "Center of Flooded MOX Fuel, No Mesh" case, the center for the transform has been translated 2.06 cm in the –*z* direction to the centroid of the active flooded fuel. Although spatial refinement is still omitted from the solution, the translation of the center for the transform improves the accuracy of the moment calculation and leads to an improved estimation of ^{1}H sensitivity. The sensitivity for ^{1}H differs from the direct perturbation result by 3% and agrees within one standard deviation.

Table I. TSUNAMI-3D results

Size of Flux Mesh → **Placement of Transform Center↓**	**No Mesh**	**10-cm Mesh**	**3-cm Mesh**
Center of MOX Fuel	^{235}U: 0.0583 ± 0.0003 ^{1}H: 0.3003 ± 0.0139	^{235}U: 0.0618 ± 0.0005 ^{1}H: 0.3788 ± 0.0147	^{235}U: 0.0617 ± 0.0004 ^{1}H: 0.3817 ± 0.0094
Center of Flooded MOX Fuel	^{235}U: 0.0619 ± 0.0004 ^{1}H: 0.3736 ± 0.0147	^{235}U: 0.0604 ± 0.0005 ^{1}H: 0.3571 ± 0.0147	^{235}U: 0.0614 ± 0.0004 ^{1}H: 0.3709 ± 0.0094
No Transform	^{235}U: 0.0567 ± 0.0003 ^{1}H: 0.2669 ± 0.0137	^{235}U: 0.0605 ± 0.0005 ^{1}H: 0.3580 ± 0.0147	^{235}U: 0.0614 ± 0.0004 ^{1}H: 0.3707 ± 0.0094

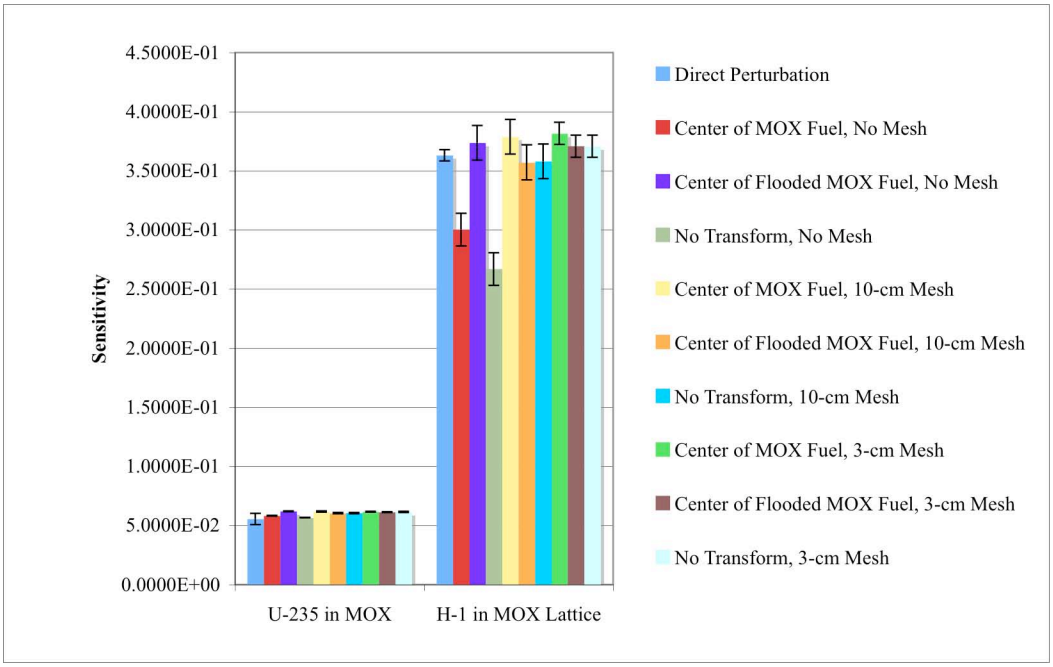

Figure 5. Direct perturbation and TSUNAMI-3D results

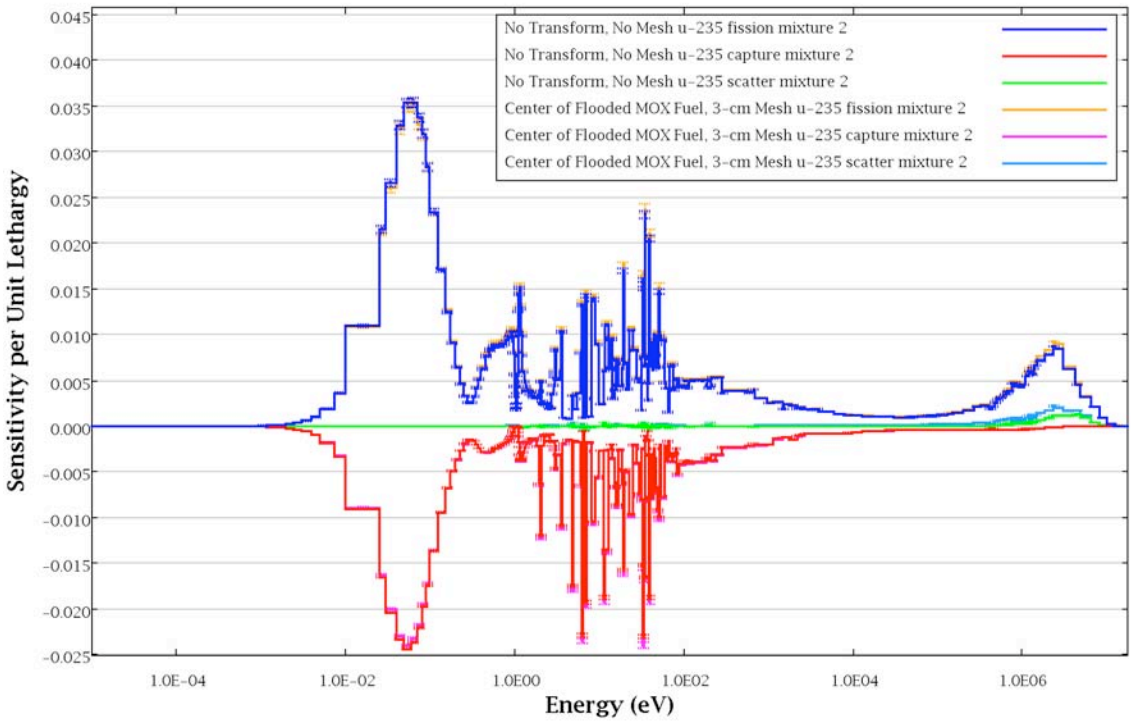

Figure 6. ^{235}U sensitivity profiles for fission, capture, and scatter

In the "No Transform, No Mesh" case, the angular flux moments are computed in reference to the Cartesian coordinate system, and no spatial refinement is used. In this case, the sensitivity for ^{1}H differs from the direct perturbation result by 27% and by 21% outside of one standard deviation. The case produces the greatest disagreement with the direct perturbation results.

The "Center of MOX Fuel, 10-cm Mesh" case provides some spatial refinement of the flux solution and performs the angular transform relative to the centroid of all the fuel. In this case, the spatial refinement provides improved results relative to the "Center of MOX Fuel, No Mesh" case, but the angular moments are not transformed correctly. The sensitivity for ^{1}H differs from the direct perturbation result by 4.3% and agrees within one standard deviation. Translating the transform to the center of the active fuel in the "Center of Flooded MOX Fuel, 10-cm Mesh" case leads to improved results where the sensitivity for ^{1}H differs from the direct perturbation result by 1.7% and agrees within one standard deviation. Removal of the angular transform leads to similar results where the sensitivity for ^{1}H differs from the direct perturbation result by 1.4% and agrees within one standard deviation. It is interesting to note that removal of the transform leads to results similar to those achieved by correctly translating the transform. In this case, because the size of the mesh is approximately one-third the fuel height, the product of the forward and adjoint angular flux moments, as used in the sensitivity calculations, can be accurately computed using either spherical coordinates computed with the transform or Cartesian coordinates computed without the transform. As demonstrated by the poor results for the "No Transform, No Mesh" case, this removal of the transform is appropriate only where adequate spatial resolution is provided.

The spatial resolution is further improved by reducing the mesh size to 3 cm and examining the three angular moment options. For the "Center of MOX Fuel, 3-cm Mesh," "Center of Flooded MOX Fuel, 3-cm Mesh," and "No Transform, 3-cm Mesh" cases, the sensitivities for ^{1}H differ from the direct perturbation result by 5.0, 2.0, and 2.1%, respectively, and the three sensitivities agree with the direct perturbation result within one standard deviation, except for the first result, which differs by 1% outside of one standard deviation. The larger magnitude of these differences, relative to the 10-cm mesh cases, likely indicates that the sensitivity of k_{eff} to the ^{1}H density in the moderator is not linear. The direct perturbation value is computed for perturbations of 2% in the ^{1}H density and may underpredict the sensitivity of k_{eff} to smaller perturbations. Further investigation with larger and smaller perturbations would be useful. The adjoint perturbation theory used in TSUNAMI-3D predicts only the linear sensitivity of k_{eff} to the cross section at the value of the number density.

The energy-dependent sensitivity profiles for ^{1}H scatter and capture are shown in Fig. 7 for the "No Transform, No Mesh" and "Center of Flooded MOX Fuel, 3-cm Mesh" cases. These two cases produce the poor and good agreement with the direct perturbation results, respectively. It can be observed in Fig. 7 that the sensitivity profiles for scatter differ substantially at fast energies and differ little at intermediate and thermal energies. The capture profiles differ little at any energy. The difference in the scatter profiles at fast energies is due to the combined effect of the accurate calculation of the angular moments through the correct translation of the transform and the fine spatial resolution of the fluxes, especially the higher-order angular moments.

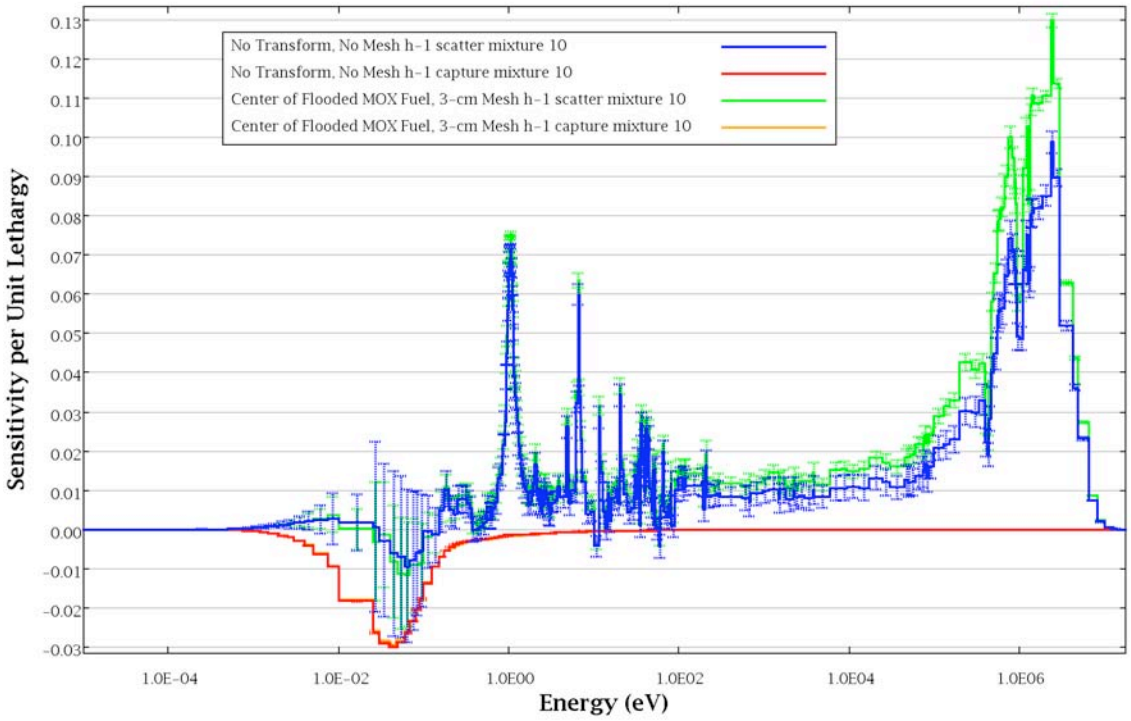

Figure 7. ^{1}H sensitivity profiles for capture and scatter

3.3 Resource Requirements

The results presented in the previous section demonstrate that good results can be achieved by using the angular moments relative to the Cartesian coordinate system with a fine mesh flux accumulator. However, the spatial refinement of the flux solution increases the need for computational resources. Without a mesh flux accumulator, this model contains 92 computational regions. The number of storage locations required for the flux solutions is 92 regions × 238 energy groups × 4 moments (P_0, P_1^{-1}, P_1^0 and P_1^1) × 3 statistical accumulators (current generation, sum of generations, sum of squares of generations), which results in 262,752 storage locations. Using the 3-cm mesh flux accumulator, the flux is accumulated for 51,228 mesh intervals. This requires 146,307,168 storage locations for the flux solution. In the current version of TSUNAMI-3D, the SAMS code that folds together the forward and adjoint solutions to produce the sensitivity coefficients requires approximately double the storage as KENO V.a.

4 CONCLUSIONS

Enhancements to the KENO V.a Monte Carlo code to produce the angular moments and provide spatial resolution of the flux solution have been described. The uses of these new code features in the TSUNAMI-3D sequence have been demonstrated in the accurate calculation of sensitivity coefficients. It has been demonstrated that with adequate spatial resolution of the flux solution, accurate sensitivity coefficients can be produced without the use of the coordinate transform in the angular moment calculation. Where adequate spatial resolution cannot be achieved due to computational restraints, the careful placement of the center of the coordinate transform is essential to the accurate computation of the angular moments, which leads to accurate sensitivity coefficients.

5 FUTURE WORK

Ongoing research is focused on reduction of the computational requirements and user intervention for accurate sensitivity coefficient generation. The feasibility of sampling an importance function, equivalent to an adjoint solution, simultaneous with the sampling of the forward solution is under investigation. This technique is similar to the contributon responses investigated for fixed source calculations [4], but has not been fully tested for eigenvalue calculations.

6 ACKNOWLEDGMENTS

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