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Advances in Sensitivity Analysis Capabilities with SCALE 6.0 and 6.1*

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The sensitivity and uncertainty analysis sequences of SCALE compute the sensitivity of k_{eff} to each constituent multigroup cross section using perturbation theory based on forward and adjoint transport computations with several available codes. Versions 6.0 and 6.1 of SCALE, released in 2009 and 2010, respectively, include important additions to the TSUNAMI-3D sequence, which computes forward and adjoint solutions in multigroup with the KENO Monte Carlo codes. . Previously, sensitivity calculations were performed with the simple and efficient geometry capabilities of KENO V.a, but now calculations can also be performed with the generalized geometry code KENO-VI. TSUNAMI-3D requires spatial refinement of the angular flux moment solutions for the forward and adjoint calculations. These refinements are most efficiently achieved with the use of a mesh accumulator. For SCALE 6.0, a more flexible mesh accumulator capability has been added to the KENO codes, enabling varying granularity of the spatial refinement to optimize the calculation for different regions of the system model. The new mesh capabilities allow the efficient calculation of larger models than were previously possible. Additional improvements in the TSUNAMI calculations were realized in the computation of implicit effects of resonance self-shielding on the final sensitivity coefficients. Multigroup resonance self-shielded cross sections are accurately computed with SCALE's robust deterministic continuous-energy treatment for the resolved and thermal energy range and with Bondarenko shielding factors elsewhere, including the unresolved resonance range. However, the sensitivities of the self-shielded cross sections to the parameters input to the calculation are quantified using only full-range Bondarenko factors.

KEYWORDS*: *Sensitivity, KENO, SCALE, TSUNAMI

I. Introduction

TSUNAMI is a suite of computational tools within the SCALE code system in which individual components each perform a specific task. [1] The TSUNAMI-1D, TSUNAMI-2D and TSUNAMI-3D analysis sequences, respectively, compute the sensitivity of k_{eff} to energy-dependent cross-section data for each reaction of each nuclide in a system model described in one-dimensional (1D), two-dimensional (2D), or three-dimensional (3D) geometry. [2] The 1D transport calculations are performed with XSDRNPM discrete ordinate codes, the 2D transport calculations are performed with the 2D arbitrary geometry lattice physics code NEWT, and the 3D calculations are performed with KENO V.a or KENO-VI. [3] The energy-dependent sensitivity data are stored in a sensitivity data file (SDF) for subsequent analysis. Additionally, the TSUNAMI sequences use the multigroup cross-section-covariance data to compute the uncertainty in each system's k_{eff} value due to the cross-section uncertainties.

TSAR (Tool for Sensitivity Analysis of Reactivity Responses) computes the sensitivity of the reactivity change between two k_{eff} calculations, using SDFs from TSUNAMI-1D, -2D, and/or -3D. TSAR also computes the uncertainty in the reactivity difference due to the cross-section-covariance data.

TSUNAMI-IP (TSUNAMI Indices and Parameters) uses the SDFs generated from TSUNAMI-1D, -3D, or TSAR for a series of systems to compute correlation coefficients that determine the amount of shared uncertainty between each target application and each benchmark experiment considered in the analysis. TSUNAMI-IP offers a wide range of options for more detailed assessment of system-to-system similarity and gap analysis.

TSURFER (Tool for S/U Analysis of Response Functions Using Experimental Results) is a bias and bias uncertainty prediction tool that implements the generalized linear least-squares approach to data assimilation and cross-section data adjustment. The data adjustments produced by TSURFER are not used to produce adjusted cross-section data libraries for subsequent use; rather, they are used only to predict biases in application systems.

Each of the data analysis tools relies on accurate SDFs generated from TSUNAMI-1D, -2D or -3D. As use of these methods becomes more widespread, it is important to enable efficient generation of sensitivity data, especially in the 3D analysis tool, which can accurately represent the full geometric and energy detail of benchmark experiments and safety systems. Many improvements in these tools were realized in SCALE 6.0, which was released in January 2009, and in SCALE 6.1, scheduled for release in the fall of 2010. Some of the updates to the TSUNAMI tools are detailed below.

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II. Generalized Geometry for TSUNAMI-3D

For SCALE 6.0, TSUNAMI-3D was extended to include not only the orthogonal solid geometry capabilities of KENO V.a, but also the generalized geometry capabilities of KENO-VI. The new capability has extended the types of systems for which sensitivity data can be generated with SCALE to include virtually any system of interest to criticality safety or reactor physics practitioners. The TSUNAMI-3D_K6 sequence can generate the sensitivity of k_{eff} to nuclide-, reaction-, and energy-dependent cross section data for any system that can be modeled with the KENO-VI predefined body shapes, which include cones, cuboids, cylinders, dodecahedrons, elliptical cylinders, ellipsoids, hexagonal cylinders, hoppers, parallelepipeds, planes, rhombohedra, spheres, and wedges. Each body can be arbitrarily rotated and combined with other bodies. Additionally, KENO-VI supports any body that can be described with quadratic equations and bodies can contain other bodies as *holes*. Bodies can be combined in repeating arrays in the form of cuboids, hexagonal prisms, or dodecahedra. For example, with the KENO V.a-based TSUNAMI-3D_K5 sensitivity analysis sequence, it was quite difficult to model systems such as hexagonally pitched arrays. These are now easily modeled with KENO-VI, as shown in **Figure 1**.

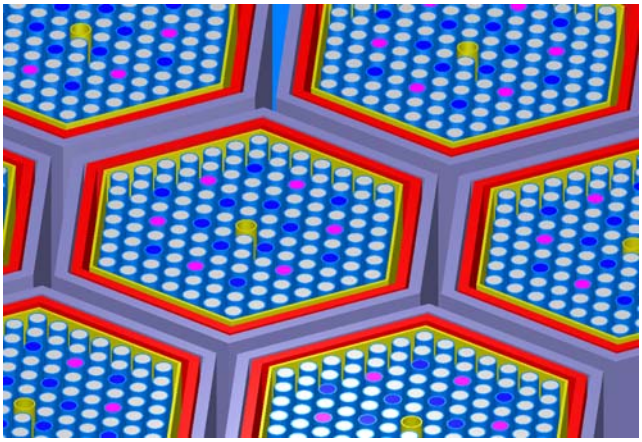

Fig. 1 TSUNAMI-3D_K6 model of hexagonally pitched fuel assemblies.

III. Spatial Resolution of Forward and Adjoint Flux Solutions

To adequately resolve the spatial dependence of the angular moments of the forward and adjoint KENO flux solutions used to generate sensitivity coefficients in TSUANMI-3D, a mesh flux accumulator is commonly used. The meshing options available in both KENO V.a and KENO-VI were substantially improved for SCALE 6.0 and further improved for SCALE 6.1. The initial version of the spatial mesh accumulators in SCALE 5.0 and 5.1 was limited to mesh intervals of a uniform size superimposed across the entire geometry. It is often desirable to create mesh geometries in which the grid intervals can vary depending on the importance or mean free path of the region. For example, it is typically necessary to use a fine grid within the fueled regions of a model, but a coarser grid is acceptable in a reflector, void or more remote regions. In SCALE 6.0 and 6.1, the grid geometry capabilities developed for the MAVRIC[4)] automated variance reduction shielding sequences were applied to KENO, meaning grid geometry can be defined using arbitrarily placed planes oriented along the x-, y- and z-axes.

The differences in the meshing algorithms are demonstrated with the critical experiment PU-SOL-THERM-014 case 22 from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* distributed through the International Criticality Safety Benchmark Evaluation Program.[5)] This experiment consists of an array of three plutonium solution tank suspended in air in a large concrete room, as shown in **Figure 2**. The solution tanks, shown in dark blue, have an outer diameter of 30 cm, whereas the room has a length of 15 m.

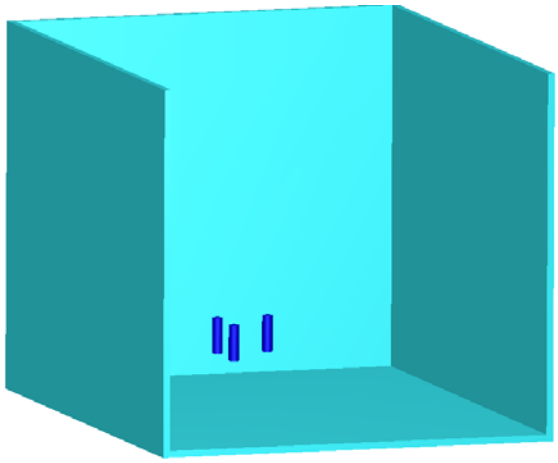

Fig. 2 TSUNAMI-3D_K5 model of PU-SOL-THERM-014-022.

To provide adequate spatial resolution in the solution tanks, a grid size of 3 cm is recommended. With SCALE 5.1, the only meshing option was to extend a uniform 3-cm grid throughout the geometry, requiring approximately 80,000,000 mesh intervals. For TSUNAMI-3D calculations, fluxes are accumulated for each mesh interval for each energy group, for each spherical harmonic moment, and for statistics. For a 238-group calculation with a third order spherical harmonics expansion (16 flux moments), 11,424 values are required for each mesh interval. The total RAM required for this calculation would be approximately 300 GB.

Where the planar mesh of SCALE 6.0 is applied, each x-, y- and z-plane is explicitly defined, as shown in **Figure 3**. An xy-slice of this grid geometry was generated with the MeshView tool and SCALE and is shown in **Figure 4**. Note that in the figure, not all closely spaced grid lines are clearly seen due to the resolution of the image. Using this grid geometry, 136,740 grid intervals are defined for this model, and approximately 500 MB of RAM are required for each of the forward and adjoint KENO calculations.

```
read gridgeometry 1
   xplanes
     -750 -700 -650 -600 -550 -500 -450 -400 -350 -331 -325 -322 -319
     -316 -313 -311 -310 -307 -304 -301 -298 -295 -292 -291 -271 -261
     -241 -221 -201 -180 -175 -172 -169 -166 -163 -160 -160 -157 -154
     -151 -148 -145 -142 -139 -100 -50 0 50 100 150 200 250 300 350
     400 450 500 550 600 650 700 750
   end
   yplanes
     -585 -550 -500 -450 -400 -350 -300 -250 -200 -150 -116 -110 -107
     -104 -101 -98 -96 -95 -92 -89 -86 -83 -80 -77 -76 -56 -36 -16 4
     24 40 43 44 46 49 52 55 58 61 64 64 67 70 84 100 150 200 250 300
     350 400 450 500 550 585
   end
   zplanes
     -540 -500 -450 -406 -386 -366 -346 -345 -342 -339 -336 -333 -330
     -327 -326 -324 -321 -319 -316 -313 -310 -307 -306 -304 -300 -286
     -250 -200 -150 -100 -50 0 50 100 150 200 250 300 350 400 450 500
     550 570
   end
end gridgeometry
```

Fig. 3 Grid geometry for PU-SOL-THERM-014 case 22.

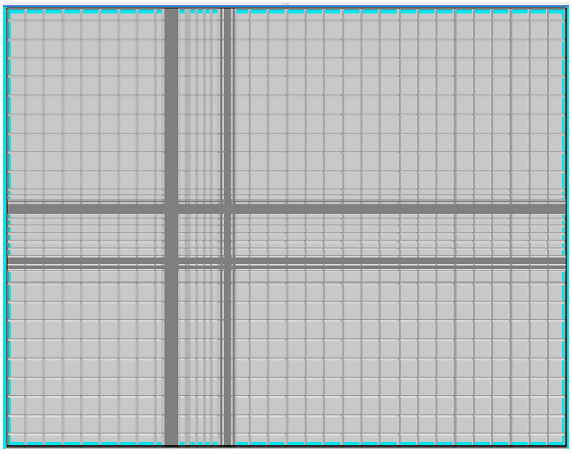

Fig. 4 Top down xy view of SCALE 6.0 planar grid for PU-SOL-THERM-014 case 22.

The sensitivity of k_{eff} to ^{1}H for this model is highly dependent on adequate spatial resolution. As shown in **Figure 5**, the non-mesh value does not agree well the reference direct perturbation solution, but the model using the mesh shown in Figure 4 does provide good agreement, within the statistical uncertainties, which are not shown in the figure.

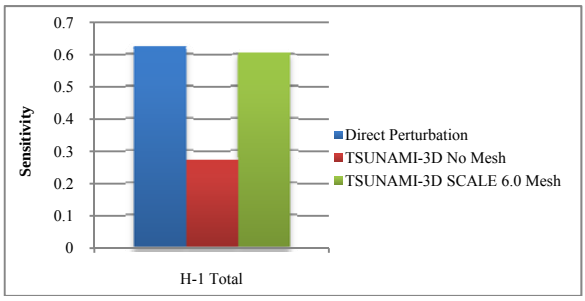

Fig. 5 Energy-integrated sensitivity of k_{eff} to 1H total cross section for PU-SOL-THERM-014 case 22.

With SCALE 6.1 the mesh definitions are further improved such that intervals can be more easily defined. As shown in **Figure 6**, the number of planes between a minimum and maximum, inclusive, is defined. A similar feature was available in SCALE 6.0, but only one interval was allowed in each direction. With SCALE 6.1 use of this shorthand feature to refine the geometry through specific regions, such as the fuel tanks in PU-SOL-THERM-014 case 22, is now possible.

```
read gridgeometry 1
   xlinear 30 -750 750
   xlinear 15 -331 -291
   xlinear 15 -179 -139
   ylinear 24 -585 585
   ylinear 15 -116 -76
   ylinear 15 44 84
   zlinear 22 -540 570
end gridgeometry
```

Fig. 6 SCALE 6.1 multiple interval definitions for grid geometry.

IV. Mesh Volume Calculation

For sensitivity calculations the volume of each region of the model within each mesh interval must be available. In SCALE 5.1 the regular grid and predictable geometry of KENO V.a enabled an analytic calculation of the required mesh volumes. With SCALE 6.0, which includes more dynamic mesh capabilities and support for generalized geometry, the mesh volumes are stochastically computed using randomly placed points. With SCALE 6.0, the default sampling is that 5000 points are placed in sets of 1000 batches. The mesh volumes and their uncertainties are computed and propagated to the sensitivity coefficients. Where additional sampling is desired, the user can adjust the sampling with the KENO *volume* block, in which the number of *points* and number of *batches* can be specified, as shown in **Figure 7**. With SCALE 6.0 this control over the volume calculation is available with TSUNAMI-3D_K6. For TSUNAMI-3D_K5 calculations, only the fixed sampling of 5000 points in 1000 batches is available.

```
read volume
  type=random
  batches=4000
  points=25000
end volume
```

Fig. 7 KENO volume block for specifying stochastic volume sampling.

With SCALE 6.1 the *volume* block is available in both TSUNAMI-3D_K5 and _K6. Additionally, the default sampling strategy has been improved to increase the number of points based on the volume of the system. The default number of points is based on a function of the total volume as the model, as shown in Equation 1 below. When applied to PU-SOL-THERM-014 case 22, approximately 150,000,000 volume points are sampled for each of 1000

batches, providing a sampling density of approximately 0.08 points/cm^3/batch.

$$points = \frac{volume}{ln\left(volume/5000\right)} \quad (1)$$

Additionally, the user can override the default sampling density with the SCALE 6.1 *volume* block keyword *sample_den*. With this new parameter, the sampling density in units of points/cm^3 is directly input by the user.

V. Implicit Effect of Resonance Self-Shielding Calculations

The adjoint-based perturbation methodology implemented in TSUNAMI to calculate sensitivity coefficients was originally developed for fast reactor applications in which the effect of resonance self-shielding in the multigroup cross-section data is minimal.[6] To provide an accurate estimation of the sensitivity coefficients for systems in which resonance self-shielding is important, the sensitivity coefficients require additional terms to account for the first-order implicit effect of perturbations in the material number densities or nuclear data upon the shielded group-wise macroscopic cross-section data.[7] For example, in a water-moderated, low-enriched-uranium system, the resonance self-shielded multigroup cross section for ^{238}U(n,γ) is dependent on the fine-structure of the flux, which in impacted by ^{1}H elastic scattering. Thus, the sensitivity of k_{eff} to ^{1}H elastic scattering has an implicit component, associated with perturbations in the spectral fine-structure for self-shielding the multigroup ^{238}U(n,γ) cross section, as well as an explicit component associated with its impact on the multigroup transport solution.

The implicit effect was demonstrated with a simple test case based on an unreflected rectangular parallelepiped consisting of a homogeneous mixture of UF_4 and paraffin with an enrichment of 2% in ^{235}U. The H/^{235}U atomic ratio is 294:1. The dimensions of the experiment were 56.22 cm × 56.22 cm × 122.47 cm.[8] For the purposes of this exercise, this experiment was modeled as a sphere with a critical radius of 38.50 cm, and computations were performed using TSUNAMI-1D analysis sequence.

The importance of the implicit effect is demonstrated in **Figure 8**, which provides energy-integrated sensitivity coefficients for each nuclide, detailing the implicit, explicit and complete (sum of implicit and explicit) terms as well as the expected results computed with direct perturbations of the systems. It can be observed that without the proper calculation of the implicit components in the resonance self-shielding calculation, the TSUNAMI results do not provide good agreement with the direct perturbation reference solutions.

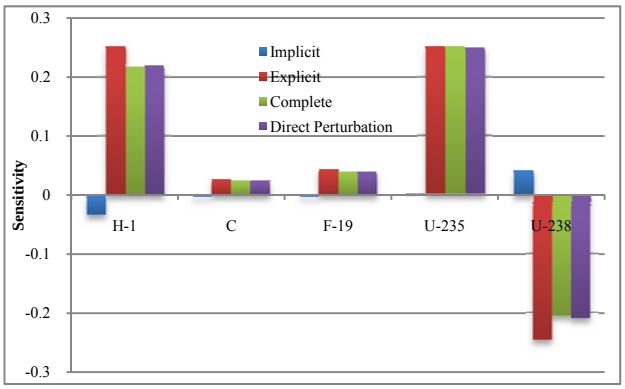

Fig. 8 Components of SCALE 6.0 energy-integrated sensitivity coefficients for UF4 test case.

With SCALE 5.1 automatic differentiation techniques were applied to the suite of resonance self-shielding codes used in TSUNAMI to compute the sensitivity of resonance self-shielded cross sections to the data used in their computation such as number densities and Dancoff factors.[9] This reference implementation included differential versions of the pointwise deterministic code CENTRM used for self-shielding in the resolved resonance and thermal regions and the Bondarenko factor code BONAMI to treat the unresolved resonance region. The differential versions of these codes are denoted as CENTRMST and BONAMIST. Because CENTRMST computes the sensitivity of each pointwise flux for each zone of the unit cell model to each nuclide present, it may require substantial computer resources, depending on the type of system analyzed. Additionally, limitations in the automatic differentiation tool used in the development of CENTRMST prevent dynamic memory allocation in the differential parts of the code, often requiring user intervention to adjust allocation settings in the code input. CENTRMST also demands long run times, often requiring more time for implicit sensitivity generation than was required for all other steps in the calculation.

For SCALE 6.0, it was desirable to alleviate the issues associated with CENTRMST by producing an accelerated technique that required no user intervention. Full-range Bondarenko factors were developed for the SCALE ENDF/B-VI.8 and ENDF/B-VII.0 238-group cross section libraries such that BONAMIST could be applied to generate implicit sensitivity terms across the full energy range. CENTRM is still applied to generated accurate cross sections in the resolved resonance region, but the implicit terms applied to these groups are generated in BONAMIST. Both methods can produce equivalent results, as shown in **Figure 9**, but the CPU time required for the implicit self-shielding calculation is reduced in the new approach, as shown in **Table 1**.

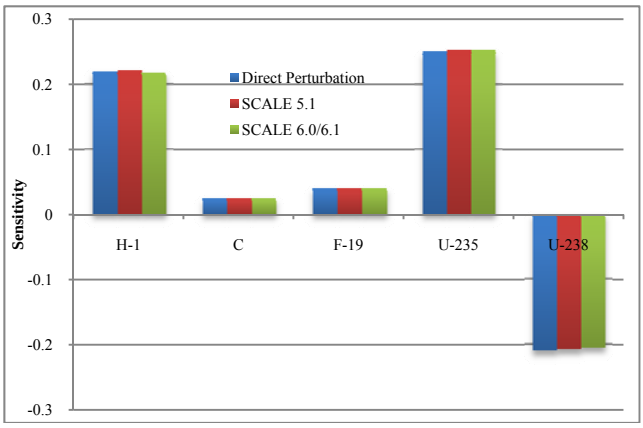

Fig. 9 Comparison of SCALE 5.1, SCALE 6.0 and direct perturbation energy-integrated sensitivity coefficients for homogeneous UF_4 test case.

Table 1 CPU time (seconds) required to execute TSUNAMI-1D for the UF_4 and spent fuel pin test problems

	UF_4		Spent Fuel Pin	
	SCALE 5.1	SCALE 6.0	SCALE 5.1	SCALE 6.0
Cross-section preparation	23.95	5.40	708.45	50.59
Transport solutions	59.57	45.61	11.72	22.30
Sensitivity calculations	1.10	1.33	5.68	6.80
Total	84.62	52.34	725.85	79.69

To further demonstrate the speedup, a more complex test case of a fuel pin from a burnup credit shipping cask model was selected.[10,11] This fuel pin represented a Westinghouse 17 × 17 optimized fuel assembly with an initial enrichment of 4 wt % ^{235}U burned to 40 GWd/MTU and cooled for 5 years. From the depletion calculations using the STARBUCS sequence of SCALE, fuel compositions for the following nuclides were retained for the criticality calculations: ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{243}Am, ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, ^{109}Ag, ^{133}Cs, ^{147}Sm, ^{149}Sm, ^{150}Sm, ^{151}Sm, ^{152}Sm, ^{143}Nd, ^{145}Nd, ^{151}Eu, ^{153}Eu, and ^{155}Gd. The fuel burnup calculations model the depletion of the ^{235}U and the in-growth of plutonium and selected fission product nuclides. When applying the SCALE 6.0 analysis techniques to a 1D fuel pin with these isotopes, the calculation time is substantially reduced, as shown in Table 1.

VI. Conclusions

The sensitivity and uncertainty analysis tools of SCALE provide unique capabilities to produce the sensitivity of quantities of interest to energy-dependent cross-section data. Important developments were realized in SCALE 6.0 and 6.1 that enable users to more easily analyze larger and more complex systems, especially with improved meshing algorithms and improved implicit sensitivity computation.

Acknowledgement

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