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ENHANCEMENTS IN CONTINUOUS-ENERGY MONTE CARLO CAPABILITIES FOR SCALE 6.2

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ABSTRACT

SCALE is a widely used suite of tools for nuclear systems modeling and simulation that provides comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, radiation shielding, and sensitivity and uncertainty analysis. For more than 30 years, regulators, industry, and research institutions around the world have used SCALE for nuclear safety analysis and design. SCALE provides a "plug-and-play" framework that includes three deterministic and three Monte Carlo radiation transport solvers that are selected based on the desired solution. SCALE includes the latest nuclear data libraries for continuous-energy and multigroup radiation transport as well as activation, depletion, and decay calculations. SCALE's graphical user interfaces assist with accurate system modeling, visualization, and convenient access to desired results. SCALE 6.2 provides several new capabilities and significant improvements in many existing features, especially with expanded continuous-energy Monte Carlo capabilities for criticality safety, shielding, depletion, and sensitivity/uncertainty analysis, as well as improved fidelity in nuclear data libraries. A brief overview of SCALE capabilities is provided with emphasis on new features for SCALE 6.2.

Key Words: **SCALE, KENO, Monaco, Continuous-Energy, Eigenvalue, Shielding**.

1. INTRODUCTION

SCALE [1] is a widely used suite of tools, including recent nuclear data, for nuclear systems modeling and simulation that provides comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, spent fuel and radioactive source term characterization, radiation shielding, and sensitivity and uncertainty analysis. SCALE was developed and is being maintained within the Reactor and Nuclear Systems Division of the Oak Ridge National Laboratory (ORNL). For more than 30 years, regulators, industry, and research institutions around the world have used SCALE for nuclear safety analysis and design. SCALE provides a "plug-and-play" framework that includes three deterministic and three Monte Carlo radiation transport solvers that can be selected based on the desired solution, including hybrid deterministic/Monte Carlo methods for optimized performance. SCALE includes the latest nuclear data libraries for continuous-energy (CE) and multigroup (MG) radiation transport as well as activation, depletion, and decay calculations. All of SCALE's nuclear data are generated with the AMPX code system [2], also developed at ORNL, for a truly independent methodology. SCALE's graphical user interfaces assist with accurate system modeling and visualization and provide

convenient access to the desired results. SCALE 6.2, projected for release in 2014, provides several new capabilities and significant improvements in existing features, including expanded CE Monte Carlo capabilities for criticality safety, shielding, depletion, and sensitivity/uncertainty analysis, as well as improved fidelity in nuclear data libraries.

SCALE provides separate Monte Carlo capabilities for eigenvalue neutronics and fixed-source coupled neutron-gamma calculations, in the KENO and Monaco codes, respectively [3,4]. Although the eigenvalue and fixed-source capabilities are provided in separate codes, many capabilities are shared between them, including physics methodology and geometry packages.

1.1. Continuous-Energy Physics

The CE treatment in SCALE provides high-resolution solution strategies with explicit physics representation. The CE data represent thermal scattering kernels using free-gas and S(α,β), with explicit point-to-point data provided through the thermal region. The resolved resonance region is represented by pointwise data where the energy point density is optimized for each reaction within each nuclide. Data in the unresolved resonance region are represented by probability tables, and data above the unresolved region implement pointwise data with explicit point-to-point representation for secondary particles. The SCALE CE physics package provides nontransport data handling to support various flux, reaction rate, and point detector tallies and to allow for depletion and sensitivity analyses. In addition, CE data are converted from double-differential data in a center-of-mass format to data in the laboratory system in a process wherein fast lookup tables are generated during the library generation.

1.2. Geometry Packages

Two variants of KENO provide identical solution capabilities with different geometry packages. KENO V.a uses a simple and efficient geometry package that is sufficient for modeling many systems of interest to criticality safety and reactor physics analysts. KENO-VI and Monaco use the SCALE Generalized Geometry Package, which provides a quadratic-based geometry system with much greater flexibility in problem modeling. Both packages are based on solid bodies that are organized into reusable objects called “units” that are constructed of material “regions.” Units can be conveniently arranged in rectangular or hexagonal “arrays” of repeating units. Additionally, nesting is available such that one unit can contain another unit as a “hole” or an array, which can be nested inside of a unit, which itself can be repeated in another array. There is no limit to the number of nesting levels available, so very complex systems can be quickly generated.

Additionally, KENO and Monaco implement “grid geometry” for accumulating data or communication of data into or out of a calculation. Grid geometries can be used for source or biasing parameter specifications as well as for tallying results from a calculation.

2. EIGENVALUE ANALYSIS ENHANCEMENTS

KENO V.a and KENO-VI perform eigenvalue calculations for neutron transport primarily to calculate multiplication factors and flux distributions of fissile systems in both CE and MG mode. Both codes allow explicit geometric representation with their respective geometry packages.

KENO provides an MG adjoint capability, which is especially useful for sensitivity analysis. KENO implements standard variance reduction techniques such as implicit capture, splitting, and

Russian roulette.

The initial fission source distribution in KENO can be specified with nine options. These options include the default option of a uniform distribution throughout the fissile material; an axially varying distribution input by the user or defined as cos(z) or $(1\text{-}\cos[z])^2$, where z is the axial position; several options to initialize the source at a given position, within a given volume, within a given unit, or within a unit at a specified array index; or to specifically provide the coordinates of each starting point.

KENO approximates the real k_{eff} variance using an iterative approach, lagging the covariance data between generations [5]. Historical indicators of source convergence include a χ^2 test for the normality of k_{eff} and plots of k_{eff} by active and inactive generations. KENO reports a best estimate of k_{eff} that is computed as the k_{eff} at the minimum variance of k_{eff} based on generations skipped and generations run. Track-length tallies for scalar flux and angular flux moments needed for sensitivity analysis are also available. Additionally, tallies are provided for reaction rates. Matrix k_{eff} calculations provide an additional method of calculating the k_{eff} of the system. Cofactor k_{eff} and source vectors, which describe the contribution to the system k_{eff} from each unit, hole, or array, are also available.

KENO has been substantially improved for SCALE 6.2, especially for CE calculations, source convergence diagnostics and acceleration, and parallel capabilities. A summary of these improvements is provided below.

2.1. Reduction in Memory Requirement of CE Internal Storage

Continuous-energy calculations in SCALE 6.0–6.1 have been performed using a unionized energy grid, where material-dependent cross-section data are generated for each user-defined mixture on a uniform neutron-energy grid as the calculation begins. Consider, for example, a uranyl nitrate solution, where the well-behaved ^{1}H cross sections generally have very few energy points; these cross sections must be refined to the same energy resolution as ^{238}U, which has approximately 200,000 energy points. Refinement of the ^{1}H cross sections results in a significant increase in the memory footprint of the data. This cross-section duplication and the resulting increase in the data memory footprint scales with the number of materials in a system because each cross section is fully duplicated in memory for each material where it is used. For example, a model with spent nuclear fuel with 18 axial zones would require 18 copies of each cross section on the unionized grid, one for each use of the same data in the model. This data format causes even basic criticality safety models to require many gigabytes of memory, and applications with multiple spent fuel mixtures could easily exceed 100 GB of memory, making the tool of limited practical value.

To mitigate the problems with previous implementations, an interpolated cross-section calculation capability has been introduced as an option in KENO to disable the use of the unionized energy grid for materials in a mixture. This new option provides a dramatic reduction in memory requirements that can be more than an order of magnitude, depending on the materials used in the model, with a runtime penalty of a few percent. Similarly, data for various reactions of the same nuclide, which were previously also mapped to a unionized energy grid, may now optionally be kept on distinct reaction-specific energy grids, providing an additional 10% to 20% reduction in memory requirements.

Internal storage of CE cross-section data has been converted from double precision to single precision (i.e., energy remains in double precision), which results in a further 15% to 45% reduction in memory footprint, depending on the problem, with no loss of precision in computed results. Optimizations in the storage of the kinematics data result in a 5% to 30% memory reduction, and optimizations of in-memory access to nuclear data result in another 3% to 15% memory reduction. These and other refinements in data storage and use strategies have enabled the modeling of critical systems with many regions of spent fuel using approximately 2 GB of memory.

2.2. Fission Source Convergence Diagnostics

Prior to SCALE 6.2, KENO provided only plots of k_{eff} by generation and average k_{eff} for visual inspection of fission source convergence, followed by a χ^2 statistical assessment of convergence. SCALE 6.2 has implemented fission source convergence diagnostic techniques in KENO to provide improved confidence in the computed results and to potentially reduce the simulation time for cases with already-converged fission sources. Confirming the convergence of the fission source distribution is especially useful for avoiding the false convergence of k_{eff}, which can be caused by insufficient sampling of important portions of the system [6].

KENO source convergence diagnostics rely on Shannon entropy statistics [6] of mesh-based fission source data. In order to accumulate the fission source on a grid, multiple grid-geometry support has been added to KENO. Formerly, KENO supported only a single grid definition for either mesh-flux calculations for use in sensitivity and uncertainty analysis or for fission source accumulations for use in criticality alarm system analysis. The multiple-mesh capability added to SCALE 6.2 enables accumulation of these quantities on different grids and also enables the accumulation of fission source data for convergence diagnostics. Figure 1 illustrates convergence of the eigenvalue and fission source distribution for a challenging source convergence benchmark problem [7]. These results illustrate the usefulness of Shannon entropy to identify fission source convergence in a scenario where the k_{eff} results falsely suggest convergence. KENO source convergence diagnostics indicate that the fission source becomes stationary in 5,018 generations for this model problem, but an examination of only the eigenvalues falsely suggests convergence in less than 1,000 generations.

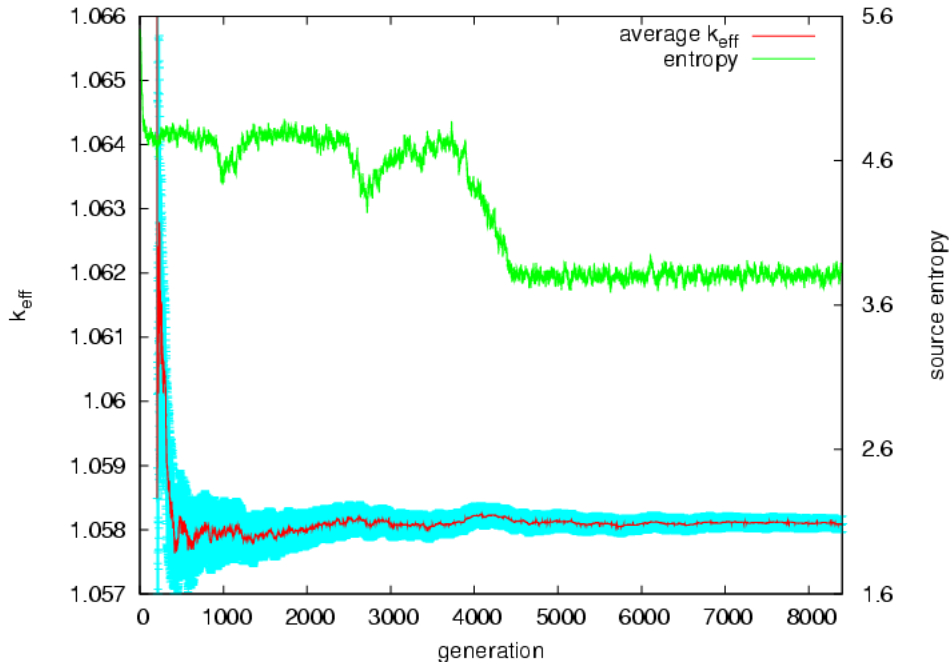

Figure 1. Shannon entropy and average k_{eff} variations for the given model problem.

2.3. Doppler Broadening Rejection Correction

The implementation of Doppler Broadening Rejection Correction (DBRC) techniques provides further improvements in the accuracy of KENO calculations by implementing a more accurate model for neutron scattering with heavy isotopes at elevated temperatures [8]. As shown in Table 1, DBRC in KENO results in a reactivity correction of approximately 300 pcm relative to the default methodology for a 1200K light water reactor (LWR) fuel pin, consistent with that predicted using Monte Carlo N-Particle Extended (MCNPX) [9].

Table 1. Effect of DBRC for an LWR fuel pin at 1200K

Case	Default	DBRC	Difference (pcm)
MCNPX	1.31137 +/- 9E-5	1.30791 +/- 9E-5	-346
KENO VI	1.31029 +/- 15E-5	1.30730 +/- 15E-5	-299

2.4. Problem-Dependent Doppler Broadening

In SCALE 6.0–6.1, CE calculations are performed only at temperatures available on the data libraries by selecting the library temperature that is nearest to the desired temperature for the calculation. Previously, when temperatures of isotopes in the KENO model were different from those present on the CE library, KENO would select the nearest temperature, which can be several hundred degrees from the desired temperature and may produce results that vary significantly from those that would be produced at the correct temperature. CE data libraries distributed with SCALE are provided with only about five temperatures of data per isotope.

A finite difference method has been implemented to provide problem-dependent temperature corrections by Doppler broadening the pointwise data in the resolved resonance region and the probability tables in the unresolved resonance region when the cross sections are loaded for the calculation [10]. The eigenvalues computed for a typical fresh pressurized water reactor (PWR) pin cell using the nearest selected CE temperature and problem-dependent CE temperature treatments are shown in Figure 2. The previous approach of rounding to the nearest temperature in CE calculations is seen to produce unrealistic, step-like behavior in the problem eigenvalue estimates and eigenvalue biases that exceed 1000 pcm in some cases.

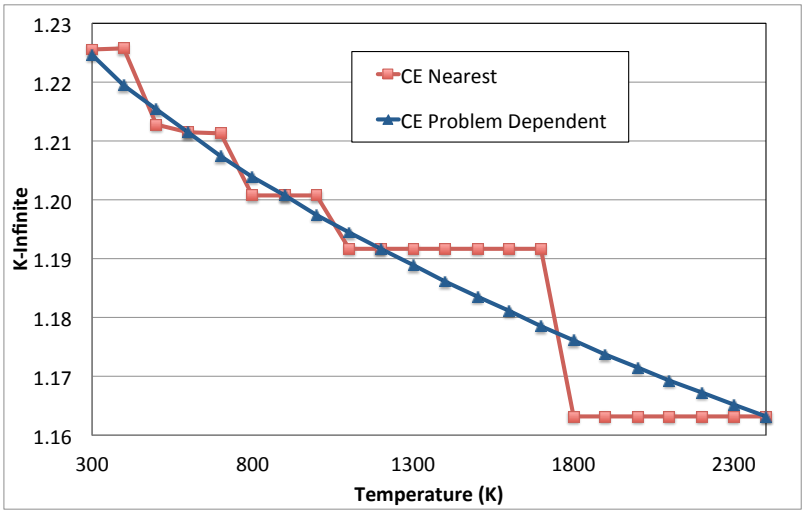

Figure 2. Eigenvalues computed for a PWR pin cell with different temperature treatments.

2.5. Hybrid Method for Starting Source Distribution

The *Sourcerer* sequence introduced in SCALE 6.2 uses the solution from the Denovo [11] discrete-ordinates code (through the DEVC sequence) as the starting fission source distribution in a KENO Monte Carlo calculation. Initial studies [12,13] have shown that using a starting fission distribution that is similar to the true fission distribution can both reduce the number of skipped generations required for fission source convergence and significantly improve the reliability of the final k_{eff} result.

For many criticality safety applications, the additional step of performing a deterministic calculation to initialize the starting fission source distribution is not necessary. However, for challenging criticality safety analyses, such as as-loaded spent nuclear fuel transportation packages with a mixed loading of low- and high-burnup fuel, even a low-fidelity deterministic solution for the fission source produces more reliable results than the typical starting distributions of uniform or cosine functions over the fissionable regions, as demonstrated in a recent study [14]. In that study, a cask containing 24 spent fuel assemblies was examined using a uniformly distributed starting source and a deterministically calculated starting source. Multiple KENO simulations were run (with different random number seeds) for various numbers of skipped cycles, and the number of calculations that produced incorrect k_{eff} estimates was tabulated. As shown in Figure 3, using a precomputed deterministic starting source can significantly increase the k_{eff} reliability of the eigenvalue calculation.

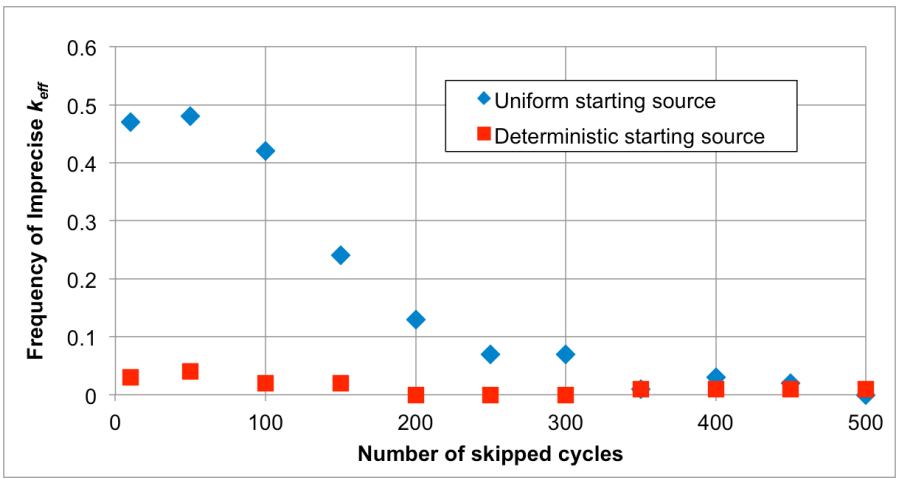

Figure 3. Fraction of results failing to agree with the reference k_{eff} value by within three standard deviations for KENO calculations with different starting sources (Figure 4 from Ref. [14]).

2.6. Distributed Memory Parallelism via MPI

In addition to the numerous improvements to the reliability and accuracy of KENO V.a and KENO-VI calculations, parallel computation capabilities have been implemented to provide reductions in wall clock time, especially for S/U analysis or Monte Carlo depletion on computer clusters. By introducing a simple master-slave approach via Message Passing Interface (MPI) [15], KENO runs different random walks concurrently on the replicated geometry within the same generation. The fission source and other tallied quantities are gathered at the end of each generation by the master process, where they are either processed for final edits or prepared for the next generation of particle histories.

The parallel performance of KENO as used in a CE calculation for a graphite-moderated reactor model is shown in Figure 4. These tests were conducted on a heterogeneous Linux cluster where the size of the nodes varies from 4 to 16 cores with differing processor speeds, much like SCALE users may encounter in practice. Tests were conducted with systematically increasing numbers of particles per generation, and various combinations of options were enabled to develop the distributions of speedups for each number of MPI processes shown in the figure. With larger numbers of particles per generation, KENO provides nearly linear speedup on the 64 processors tested here and has been successfully demonstrated on hundreds of processors.

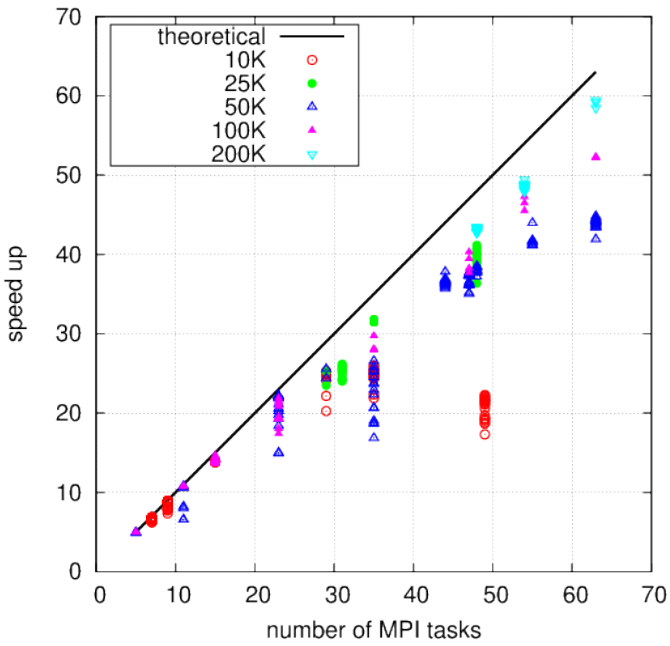

Figure 4. Speedup for parallel KENO-VI calculations for a graphite-moderated reactor model.

The parallel capabilities have recently been demonstrated in a series of high-fidelity physics test simulations for the AP1000® PWR [16]. A typical model used in this work was generated with 688,000 units and was simulated with 50 billion particle histories on 180 cores of a computational cluster, exercising many of the enhancements available in an early release of SCALE 6.2. Sample relative power distribution generated in this study is shown in Figure 5.

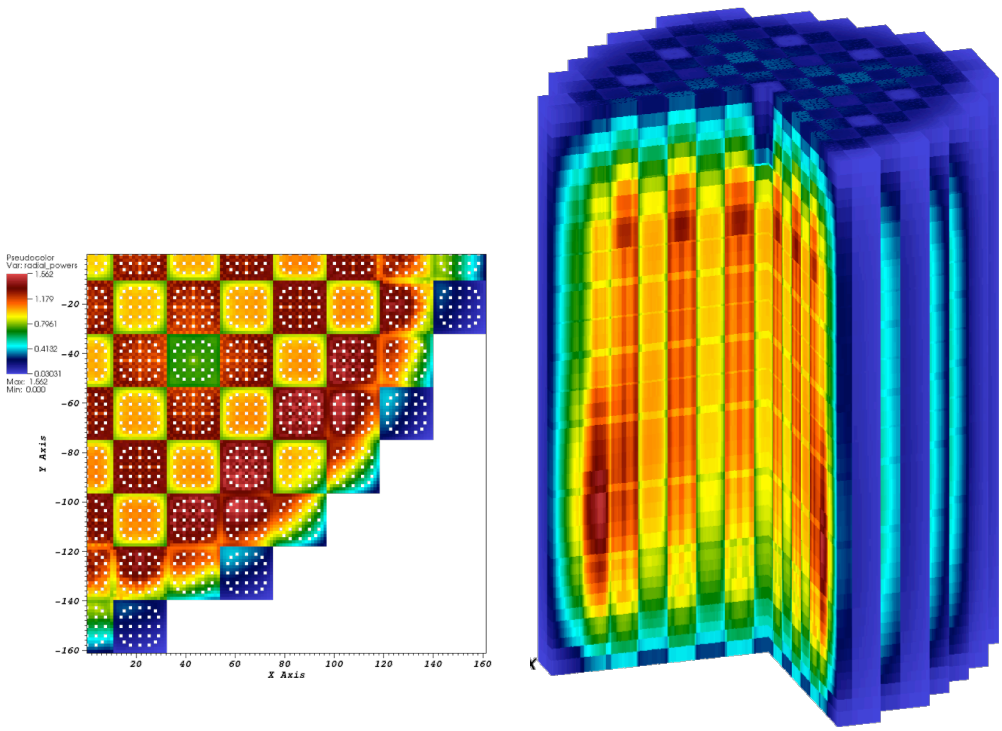

Figure 5. Relative power distribution in the AP1000® PWR.

3. SHIELDING ANALYSIS ENHANCEMENTS

Monaco is a fixed-source Monte Carlo shielding code that calculates neutron and photon fluxes and response functions for specific geometry regions, point detectors, and mesh tallies [4]. Monaco contains variance reduction capabilities to maximize the efficiency of shielding calculations, including source biasing and weight windows, which can be automated via the Monaco with Automated Variance Reduction using Importance Calculations (MAVRIC) sequence. MAVRIC performs radiation transport on problems that are too challenging for standard, unbiased Monte Carlo methods. The intention of the sequence is to calculate fluxes and dose rates with low uncertainties in reasonable times, even for deep penetration problems. MAVRIC automatically performs a coarse mesh, three-dimensional, discrete-ordinates calculation using Denovo to determine the adjoint flux as a function of position and energy and uses this adjoint flux information to construct a space- and energy-dependent importance map (i.e., weight windows) for biasing during particle transport and a mesh-based biased source distribution. MAVRIC then passes the importance map and biased source distribution to Monaco to be used during the Monte Carlo shielding calculation.

Prior to SCALE 6.2, the MAVRIC/Monaco capabilities relied on the MG approach for radiation transport. The MG approach is suitable for many applications but can be problematic for others. For example, for deep penetration shielding through iron, the MG-averaged cross section for capture resonances may not accurately represent the true transmission of neutrons due to fine "windows" through (i.e., minima in) the cross section. Additionally, MG calculations cannot adequately resolve discrete gamma emission lines, such as those of ^{60}Co. The CE treatment introduced in SCALE 6.2 allows for improved solution fidelity by enabling Monaco calculations to use SCALE CE physics. The generation of CE nuclear data and the implementation of CE physics in Monaco are based on a first-principles approach, where the simulation is represented as realistically as possible. This approach will lead to higher-fidelity results, but runtimes may be substantially increased over more approximate methods.

3.1. SCALE CE Modular Physics Package

A new package, called the SCALE Continuous-Energy Modular Physics Package (SCEMPP), was developed to serve as the CE collision physics engine. SCEMPP models particle collisions in a material and generates any emerging or secondary particle(s) that result from the collision, essentially acting as an event generator for SCALE. SCEMPP has Fortran and C++ application programming interfaces (APIs) in order to support both legacy and future developments in SCALE. The CE Resource package is another new feature in the SCALE code development to read and store all the nuclear data from AMPX CE particle libraries and to transfer information via APIs. Communication through APIs, unlike traditional input/output operations in SCALE, and SCEMMP's generic modular structure enable a flexible and yet powerful integration of capabilities supporting SCALE modernization efforts. In addition to creating collision particles, SCEMPP provides nontransport data, such as reaction responses or point detector data, to Monaco to enable dose calculations and point detector tally estimates.

3.2. CE MAVRIC/Monaco

CE calculations in Monaco use SCEMPP for particle transport, and the currently available features in Monaco have been improved to enable MG and CE calculations with a consistent and user-friendly input. CE Monaco can operate in neutron, photon, and neutron-photon coupled particle transport modes. All of the available tally types in Monaco have been improved to use us-

er-defined energy structures and particle types (neutron and photon). MAVRIC always requires an MG library to enable variance reduction calculations with the Denovo S_n code. However, the final Monaco calculation in the MAVRIC sequence can now be performed with either MG or CE physics.

One area where the impact of MG physics is detrimental is the transport of monoenergetic photons. In MG physics, all photons within a group use the same group-averaged cross section. Consider a ^{60}Co source and a tungsten shield. The cross sections for the two ^{60}Co line sources are listed in Table 2 for different cross-section libraries. The small differences in cross section can make large differences in the transmission through the shield. Considering the cross sections in Table 2, the attenuation ($e^{-\mu x}$) through just 5 cm of tungsten for either energy line can vary by 30%.

Table 2. Total macroscopic cross section in tungsten (cm^{-1}).

	Incident Energy	
Data Library	1.173230 MeV	1.332490 MeV
SCALE CE	1.03353	0.94864
SCALE 47-group	1.09066	0.92743
SCALE 19-group	1.05167	0.89289

For line photon sources in deep penetration shielding problems, the difference in fluxes and dose rates between MG and CE can be quite large. Consider a radioactive transport package consisting of steel and tungsten (71.12 cm outer diameter and 91.44 cm height). Predicted dose rates outside the package due to a 1 Ci ^{60}Co source in the inner cavity (16.51 cm diameter and 50.8 cm height) using the 19-group cross sections can be two to three times higher than the CE predictions, as shown in Figure 6. Dose rates with the 47-group cross sections are closer to CE but can still be about 50% higher than the CE dose rates.

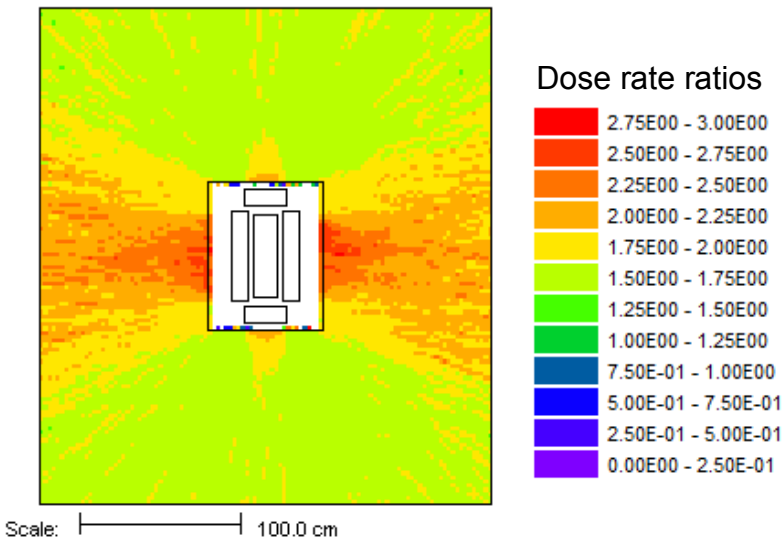

Figure 6. Simple transportation package geometry and ratio of the 19-group MG computed dose rates to the CE dose rates.

4. MONTE CARLO DEPLETION ENHANCEMENTS

SCALE 6.1 provided MG Monte Carlo depletion that coupled SCALE MG cross-section processing capabilities with KENO and Oak Ridge Isotope Generation and Depletion Code (ORIGEN) via the Transport Rigor Implemented with Time-Dependent Operation for Neutronic Depletion (TRITON) sequence [17]. In addition to the existing MG capability, a new CE-based KENO/ORIGEN Monte Carlo depletion capability has been developed for SCALE 6.2 and can be utilized by simply changing the input library specification [18]. CE depletion is especially useful for models with complex geometry that present difficulties in obtaining accurate resonance self-shielded MG data and for models with many depletion regions where run time to generate and store the resonance self-shielded cross-section data for each material is prohibitive.

TRITON performs CE depletion calculations using ORIGEN to update region-wise nuclide inventories at each burnup step by integrating cross-section data with the flux spectrum for each depletion region. In addition to the reaction cross-section data utilized in the Monte Carlo calculation, energy-dependent fission product yield data and additional activation cross sections must be integrated with the scalar flux at each depletion step. In MG mode, resonance self-shielded cross-section data are generated prior to the KENO calculation. SCALE provides MG Monte Carlo depletion by integrating the scalar flux with the resonance self-shielded multigroup cross-section data with a utility module outside the KENO Monte Carlo calculation. The predictor-corrector methodology is implemented for depletion.

In some cases, MG depletion suffers from the inadequacies of the MG approximations, such as inadequate group structure or inability to properly shield the cross sections for the problem using the one-dimensional resonance self-shielding modules available in SCALE. Additionally, the requirement to update the resonance self-shielding at each depletion step can present a large computational burden that makes calculations impractical or impossible because the storage of independent sets of MG data for thousands of depletion materials can require excessive amounts of memory. To alleviate issues associated with the MG technique while maintaining components of the current depletion infrastructure of SCALE, a few-group microscopic reaction cross-section calculation capability is now available for CE calculations in KENO.

Results are shown below in Table 3 for an Organization for Economic Cooperation and Development (OECD) benchmark based on destructive isotopic assay data for used LWR fuel [19]. Here the percentage differences from the calculated (C) to experimental (E) values are shown to be similar between MG and CE calculations on the same KENO models. However, for CE depletion, it is not necessary to compute and track resonance self-shielded cross sections for each depletion region separately. For models with hundreds or thousands of depletion regions, the previously described advancements in CE calculations provide substantially reduced memory requirements, enabling high-fidelity calculations that were not previously possible.

Table 3. C/E -1 (%) for OECD depletion benchmark.

	MG	CE		MG	CE
^{234}U	-0.5	-1.3	^{99}Tc	0.5	1.1
^{235}U	-3.8	-4.8	^{101}Ru	1.2	1.6
^{236}U	1.7	2.1	^{103}Rh	3.1	2.8
^{238}U	-0.6	-0.6	^{133}Cs	0.7	1.0
^{238}PU	-11.9	-11.7	^{143}Nd	0.4	0.4
^{239}Pu	0.2	-1.4	^{145}Nd	-0.7	-0.4
^{240}Pu	-0.3	-2.3	^{147}Sm	3.4	2.9
^{241}Pu	-1.6	-1.5	^{149}Sm	-38.5	-38.9
^{242}Pu	-1.9	-0.2	^{150}Sm	-4.9	-4.2
^{241}Am	-4.1	-4.1	^{151}Sm	-24.0	-24.9
^{243}Am	-1.6	0.8	^{152}Sm	-1.5	-1.8
^{237}Np	5.3	4.4	^{153}Eu	2.2	2.3

5. SENSITIVITY AND UNCERTAINTY ANALYSIS ENHANCEMENTS

Sensitivity coefficients describe the fractional change in a system response that is induced by changes to system parameters and nuclear data. The Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) code within the SCALE code system makes use of eigenvalue sensitivity coefficients for an extensive number of criticality safety applications, such as quantifying the data-induced uncertainty in the eigenvalue of critical systems, assessing the neutronic similarity between different critical systems, and guiding nuclear data adjustment studies [20].

With SCALE 6.2, the MG eigenvalue sensitivity and uncertainty analysis methods that use KENO for transport analysis are extended to provide CE capabilities through the implementation of the Contribution-Linked Eigenvalue Sensitivity/Uncertainty Estimation via Tracklength Importance Characterization (CLUTCH) and Iterated Fission Probability (IFP) methods [21]. CLUTCH is an efficient methodology that has been demonstrated to provide high-fidelity results with manageable run times and memory requirements, and both of these state-of-the-art sensitivity methods make CE sensitivity calculations easier to learn and use than MG in several ways; for example, CE calculations do not require resonance self-shielding calculations to determine implicit sensitivity effects, the simulation of a separate adjoint transport calculation, or the use of a flux mesh for tallying fluxes and flux moments.

The use of CE physics allows for improvements in sensitivity coefficient accuracy compared to MG. Table 4 compares the accuracy of the total nuclide sensitivity coefficients estimated by each sensitivity method for the MIX-COMP-THERM-004-001 system from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [22]. The MG analysis produced a ^{238}U total nuclide sensitivity that disagreed with the reference direct perturbation sensitivity by 2.80 effective standard deviations (σ_{eff}); sensitivities of the CE methods (IFP and CLUTCH) were within almost one standard deviation of the reference sensitivity coefficients for all of the nuclides examined. Table 4 also provides the amount of computational memory required by each method for the sensitivity coefficient calculations. These memory requirements were obtained by subtracting the memory requirements of each eigenvalue-only calculation from the memory requirements of each sensitivity coefficient calculation. As seen in Table 4, the CLUTCH method excels in terms of memory usage and can readily compute sensitivities for complex systems on a typical personal computer with 8 GB of RAM.

Figure 7 compares the figures of merit, (time × variance)$^{-1}$, for the nuclide sensitivity coefficients presented in Table 4. Figure 7 indicates that the CE sensitivity calculations are of a comparable efficiency to the MG calculations and that in some cases the CE CLUTCH method is more efficient than the MG method. This is remarkable because of the use of CE physics, which can impose relatively long cross-section lookup times, and indicates the efficiency of the CLUTCH method.

Table 4. MIX-COMP-THERM-004-001 total nuclide sensitivity coefficient comparison [21].

Material	Reference	MG TSUNAMI	CE TSUNAMI	
			IFP	CLUTCH
H_2O	0.2935 ± 0.0179	0.2805 ± 0.0088 (-0.65 σ_{eff})	0.2733 ± 0.0052 (-1.08 σ_{eff})	0.2793 ± 0.0065 (-0.75 σ_{eff})
^{238}U	-0.0061 ± 0.0003	-0.0050 ± 0.0002 (2.80 σ_{eff})	-0.0055 ± 0.0003 (1.16 σ_{eff})	-0.0057 ± 0.0001 (1.14 σ_{eff})
^{239}Pu	0.1262 ± 0.0087	0.1264 ± 0.0014 (0.02 σ_{eff})	0.1188 ± 0.0020 (-0.83 σ_{eff})	0.1190 ± 0.0001 (-0.83 σ_{eff})
^{240}Pu	-0.03777 ± 0.00350	-0.03750 ± 0.00011 (0.08 σ_{eff})	-0.03738 ± 0.00060 (0.11 σ_{eff})	-0.03743 ± 0.00002 (0.10 σ_{eff})
^{241}Pu	0.00589 ± 0.00042	0.00599 ± 0.00004 (0.24 σ_{eff})	0.00567 ± 0.00014 (-0.50 σ_{eff})	0.00579 ± 0.00003 (-0.24 σ_{eff})
Memory Usage		13,785 MB	10,643 MB	63 MB

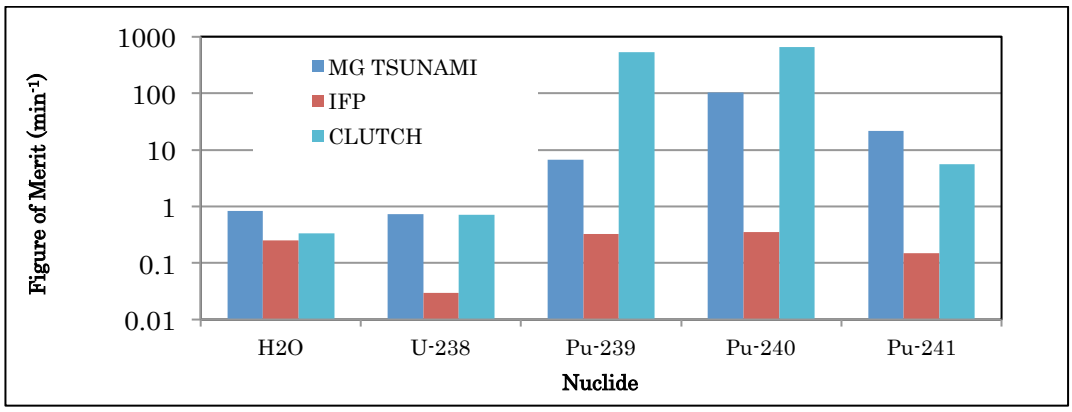

Figure 7. MIX-COMP-THERM-004-001 total nuclide sensitivity figure of merit comparison.

6. NUCLEAR DATA ENHANCEMENTS

AMPX is a cross-section processing software package that has been developed at ORNL for more than 30 years and is completely independent of any other cross-section processing software package [2]. AMPX is used to process Evaluated Nuclear Data Format (ENDF) nuclear data evaluations, as well other data sources that use the ENDF format, and to provide nuclear data

libraries for the SCALE radiation transport package. AMPX provides CE, MG, and covariance data libraries for SCALE.

Investigations into the CE data generated by the AMPX code system for deployment with SCALE 6.0–6.1 revealed a need for improvement in the S(α,β) treatment, especially for forward-peaked kinematics. For thermal moderators such as hydrogen in H_2O, ENDF evaluations give detailed angular and exit energy information for incoherent elastic scattering. Information is given in the form of an S(α,β) function, where α is the momentum transfer and β is the energy transfer. AMPX uses the information from the ENDF/B evaluation to reconstruct the double differential scattering distribution. Prior to the development of the CE capabilities in SCALE, AMPX was primarily used to produce MG libraries, and AMPX collision kinematics distributions were provided as a function of cosine moment distributions instead of CE distributions. To support the CE capability development in SCALE, AMPX modules were developed to post-process the cosine moment distributions and to recreate the original CE collision kinematics distributions. Once the CE distributions were reconstructed, the marginal and conditional probability distributions for exit angles and energies were generated (i.e., a "legacy" CE kinematics distribution approach). For the CE libraries distributed with SCALE 6.0–6.1, AMPX used this legacy procedure to generate CE double-differential data from the cosine moment distributions. Following the release of SCALE 6.1, investigations revealed that this procedure introduced nonphysical structure in the thermal scattering law data for water that resulted in a bias for some benchmark calculations. Based on the investigation, the AMPX collision kinematics processing procedures have been updated and modernized to produce CE probability distributions directly from the CE collision kinematics distributions, thereby eliminating the cosine moment distribution processing step. The SCALE ENDF/B-VII.0 data libraries have been regenerated using the new AMPX processing procedures, and the benchmark testing results with SCALE 6.2 show substantially improved results with the new CE data libraries; an example matrix is shown in Figure 8. Select critical benchmark results for thermal mixed oxide systems are provided in Figure 9, where it may be observed that the bias in the SCALE 6.2 CE results is reduced relative to SCALE 6.1. Additional details are provided in preliminary documentation of the validation of SCALE 6.2 [23]. The impact of this update for burned fuel can be as much as 1000 pcm.

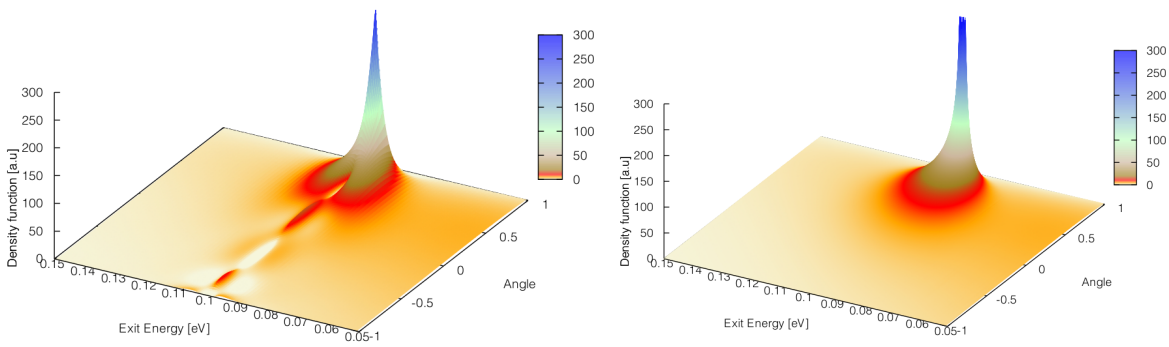

Figure 8. ENDF/B-VII.0 CE collision kinematics for 0.1 eV neutron incident on ^1H in H_2O for SCALE 6.0–6.1 (left) and SCALE 6.2 (right).

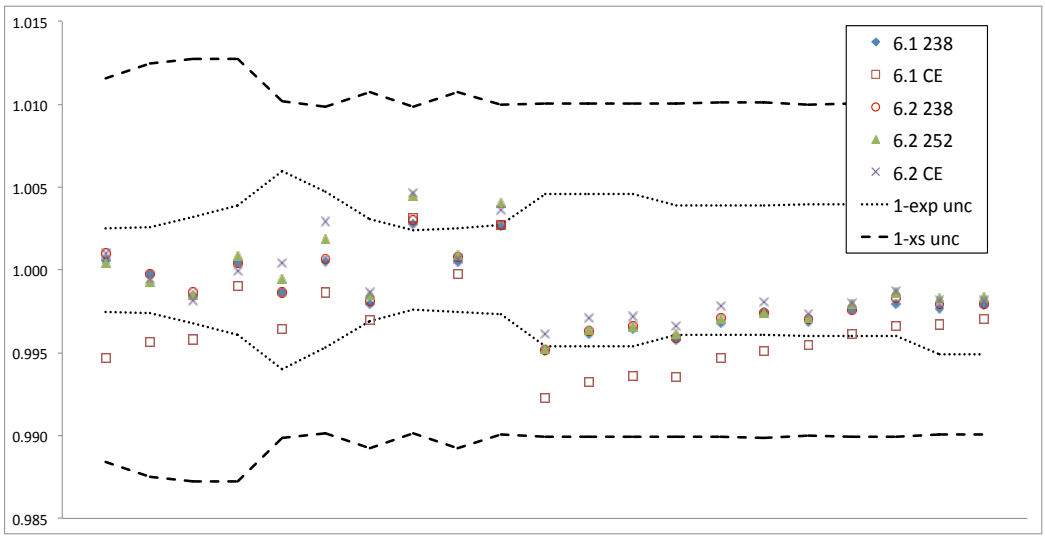

Figure 9. SCALE calculated/experimental results for ICSBEP thermal mixed oxide critical systems for SCALE 6.1 and 6.2 beta with 238 group, 252 group and CE energy resolution and 1σ standard deviations for experimental and cross section uncertainties.

In addition to updates in the kinematics data, the probability tables that provide CE treatment in the unresolved resonance range have been improved, primarily through the inclusion of additional energy resolution and error correction. Testing with the new probability tables has shown reduced biases for systems that are sensitive to the intermediate energy range.

7. CONCLUSIONS

SCALE 6.2 continues a 30-year legacy of nuclear systems modeling and simulation by providing comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, spent fuel and radioactive source term characterization, radiation shielding, and sensitivity/uncertainty analysis. The new capabilities within SCALE 6.2 provide significant advances over the previous versions, especially the expanded CE Monte Carlo capabilities for criticality safety, shielding, depletion, sensitivity and uncertainty analysis, and improved CE data.

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