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OVERVIEW OF 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, licensees, 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 CE Monte Carlo capabilities for criticality safety, shielding, depletion, and sensitivity and uncertainty analysis. A brief overview of SCALE capabilities is provided with emphasis on new features for SCALE 6.2.

1 INTRODUCTION

SCALE 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 is developed and maintained within the Reactor and Nuclear Systems Division of the Oak Ridge National Laboratory (ORNL). For more than 30 years, regulators, licensees, 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 (CE) and multigroup (MG) 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 CE Monte Carlo capabilities for criticality safety, shielding, depletion, and sensitivity and uncertainty analysis. A brief overview of SCALE capabilities is provided with emphasis on new features for SCALE 6.2.

2 CAPABILITY ENHANCEMENTS

SCALE 6.2 provides a number of capability enhancements relative to previous releases. Several key enhancements are briefly described here with references to numerous other extended papers that provide additional details.

2.1 Criticality Safety

The KENO Monte Carlo neutron transport codes for eigenvalue problems have realized a number of enhancements for SCALE 6.2. A comprehensive review of the CE treatment in KENO has led to a number of improvements providing reduced biases and a substantially reduced memory footprint [1]. Parallel computation capabilities have been added to KENO to provide faster results on multicore PCs and Linux clusters, with speed up as a function of the number of processors, as shown in Fig. 1. Fission source convergence diagnostic techniques have been implemented to provide improved confidence in the computed results, and an innovative hybrid technique in the new Sourcerer sequence sets the starting source distribution with an automated deterministic calculation to provide improved reliability for challenging calculations such as as-loaded transportation and storage configurations of used nuclear fuel [2].

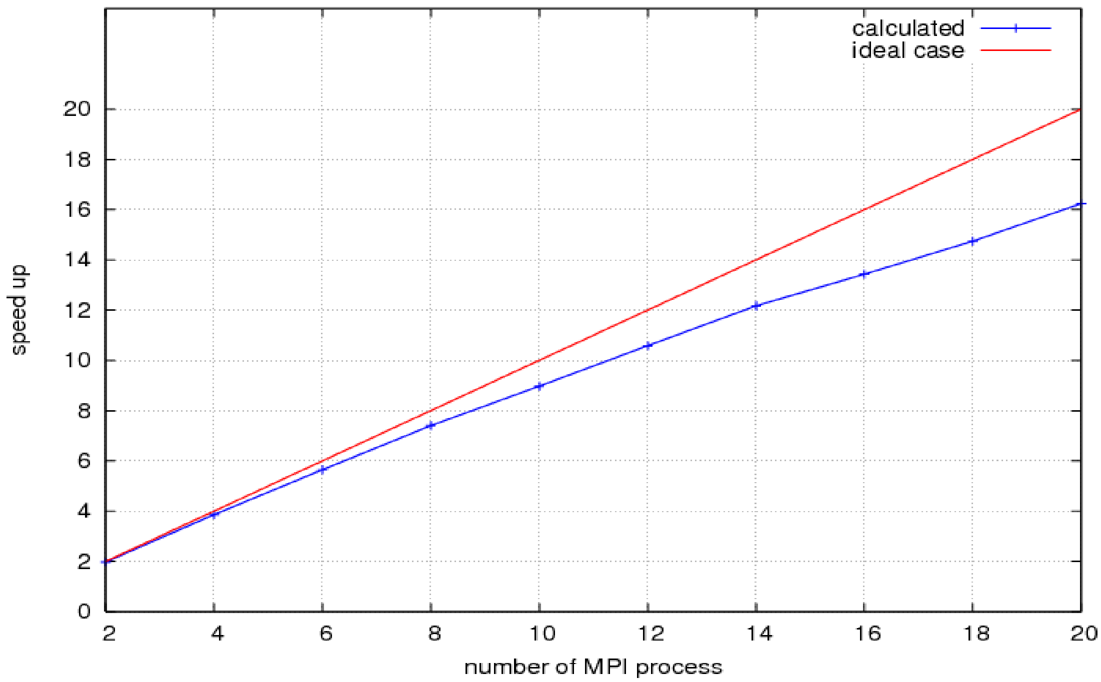

Figure 1. Speedup of KENO calculations as a function of number of processors

Additional improvements in the initialization of the problem-dependent fission spectrum data provide improved reliability in CE calculations, and the implementation of Doppler Broadening Rejection Correction (DBRC) techniques provides further enhancements for calculations with elevated temperatures [3]. As shown in Table I, DBRC in KENO presents 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 with MCNPX by the originators of the methodology [4].

Table I. Effect of DBRC for a 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

2.2 CE Depletion

SCALE 6.1 provided MG Monte Carlo depletion that coupled SCALE MG cross-section processing capabilities with KENO and ORIGEN (Oak Ridge Isotope GENeration). A new CE-based KENO/ORIGEN Monte Carlo depletion capability has been developed and can be utilized by simply changing the input library specification [5]. 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. Results for a benchmark based on destructive isotopic assay data for sample MKP109-P of assembly D047 irradiated in the Calvert Cliffs pressurized water reactor to a burnup of 44 GWd/MTU are shown below in Table II [6]. Here the percent 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, CE calculations provide substantially reduced memory requirements, enabling high-fidelity calculations that were not previously possible.

Table II. C/E -1 (%) for Calvert Cliffs sample MKP109-P

	MG KENO	CE KENO
U-234	4.1	3.2
U-235	5.3	4.6
U-236	1.8	1.4
U-238	-0.1	-0.1
Pu-238	-10.4	-10.2
Pu-239	7.0	9.1
Pu-240	3.2	1.8
Pu-241	0.8	1.5
Pu-242	-7.5	-8.2
Np-237	2.3	3.1
Am-241	-6.5	-5.8
Cs-133	0.8	0.7
Cs-135	4.8	4.2
Cs-137	-3.3	-3.3
Nd-143	2.1	2.1
Nd-144	-3.2	-3.1
Nd-145	-3.0	-3.1
Nd-146	0.2	0.3
Nd-148	0.0	-0.1
Nd-150	2.6	2.5

2.3 Radioactive Source Term Characterization

SCALE includes the ORIGEN code and its comprehensive depletion, activation, decay, gamma-ray, and x-ray library with over 2,200 nuclides. ORIGEN and its nuclear data libraries have been updated to provide convenient modular interfaces within SCALE, and these interfaces also provide easy access to ORIGEN’s robust capabilities by other software packages [7].

2.4 CE Fixed-Source Radiation Transport

The SCALE fixed-source Monte Carlo capability with automated variance reduction has been enhanced to enable CE calculations [1]. The new CE capabilities provide enhanced solution fidelity while still implementing the unique acceleration techniques of the FW-CADIS

(Forward-Weighted Consistent Adjoint Driven Importance Sampling) methodology for deep penetration shielding and criticality accident alarm system modeling.

In the early 1990's, several experiments measuring the energy spectrum of ^{252}Cf neutrons after leaking from a sphere of iron were performed [8]. Two sets of measurements were made – one by the Czechoslovakian National Research Institute (NRI) and the other by the Skoda Company. The calculated energy spectrum of flux using MG Monaco, MCNP and CE Monaco is compared to the two sets of original experimental measurements, as shown in Fig. 2. The flux calculations from all three codes match the experimental results well. Compared to what the experiments measured, the codes predict larger swings in the flux near the resonances in the 0.01-1 MeV range. It is possible that the experiments or detectors did not have the energy resolution required to show these details. Note that CE Monaco agrees quite closely with the MCNP calculation, improving agreement over the previously available MG results from Monaco.

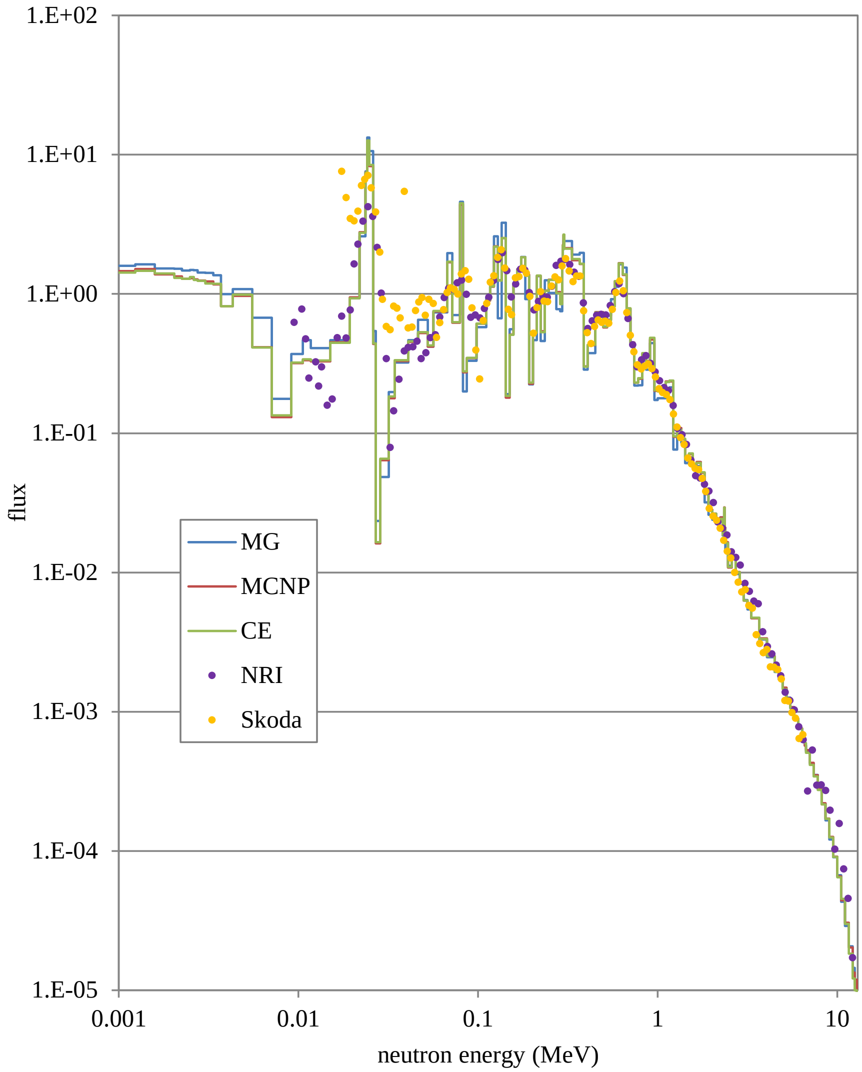

Figure 2. Flux results for the iron sphere transmission experiment

2.5 Sensitivity and Uncertainty Analysis

The MG TSUNAMI eigenvalue sensitivity and uncertainty analysis methods that use KENO for transport analysis are extended to provide CE capabilities through the implementation of the CLUTCH (Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization) methodology and Iterated Fission Probability method [9]. CLUTCH is an efficient methodology that has been demonstrated to provide high-fidelity results with manageable run-times and memory requirements. In addition to avoiding the need for resonance self-shielding calculations with implicit sensitivity effects, CE TSUNAMI calculations provide the capability to tally sensitivities with very fine energy resolution, as shown in Fig. 3.

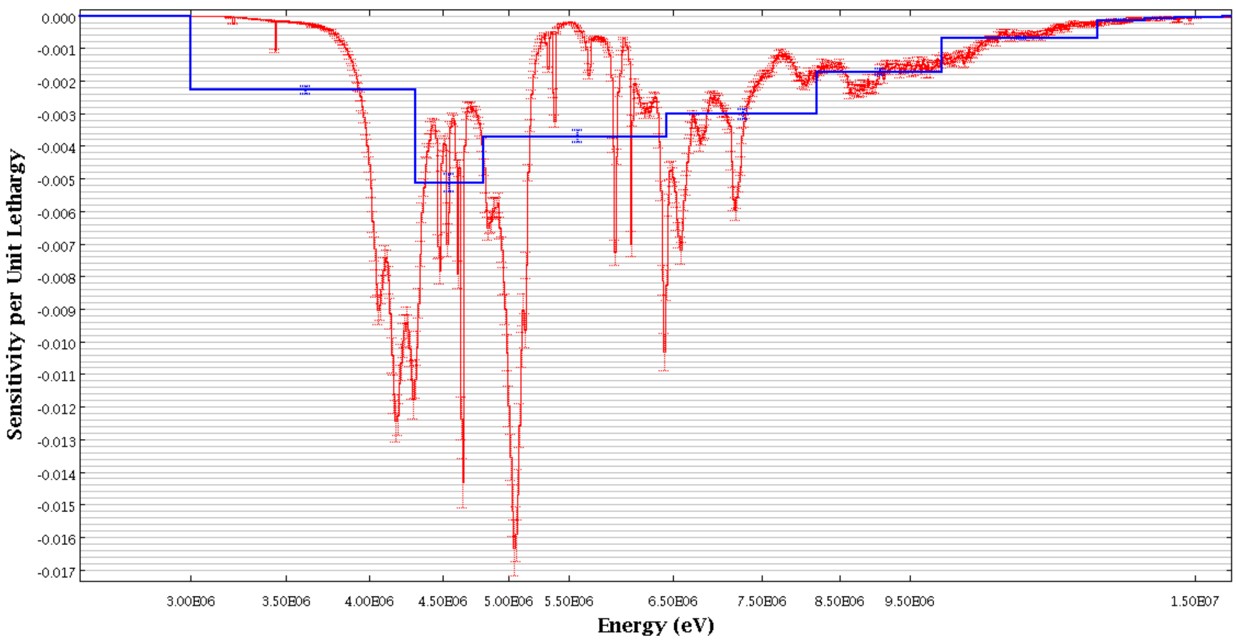

Figure 3. Sensitivity of k_{eff} to ^{16}O capture computed with MG TSUNAMI in 238 groups (blue) and CE TSUNAMI binned in 10,000 groups (red)

A new stochastic uncertainty quantification capability has been added with the SCALE 6.2 Sampler module that implements stochastic techniques to quantify the uncertainty in any computed result from any SCALE sequence due to uncertainties in

- neutron cross sections,
- fission yield and decay data, and
- any user input parameter, such as geometry, material density, isotopic composition, temperature, etc.

Sampler propagates these uncertainties through complex analysis sequences, such as depletion calculations, and provides the variation in the output quantities due to variations in any combination of input data [10]. Correlations between systems with shared uncertainties are also computed, which is especially useful for quantifying correlated uncertainties in benchmark experiments, as required for generalized linear least-squares techniques as implemented by the SCALE module TSURFER [11].

2.6 Additional SCALE Updates

SCALE 6.2 includes a number of other improvements, such as the extension of the maximum allowed number of materials from approximately 2,000 to more than 2 billion. Additionally, some older features are removed such as Evaluated Nuclear Data File (ENDF) Versions V and VI data libraries (i.e., ENDF/B-V and -VI, respectively), the point kernel shielding capability, and a one-dimensional material optimization search sequence.

3 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 [12]. AMPX is used to process ENDF-formatted nuclear data evaluations and provide nuclear data libraries for the SCALE radiation transport package. AMPX provides CE, MG, and covariance data libraries for SCALE. The following summary identifies the recent AMPX updates that have led to improved nuclear data libraries for the SCALE code system.

3.1 CE Data

Investigations into the CE data generated by the AMPX code system for deployment with SCALE revealed a need for improvement in the $S(\alpha,\beta)$ treatment, especially for forward-peaked kinematics. For thermal moderators like 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 $S(\alpha,\beta)$ function, where α is the momentum transfer and β 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 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., “legacy” CE kinematics distribution approach). For the CE libraries distributed with SCALE 6.0 and SCALE 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 non-physical structure in the thermal scattering law data for water that resulted in a bias from 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. Select critical benchmark results for thermal mixed oxide (MOX) systems are provided in Fig. 4, and the bias in the SCALE 6.2 CE results is reduced relative to SCALE 6.1. Additional details are provided in a companion paper on the validation of SCALE 6.2 [13].

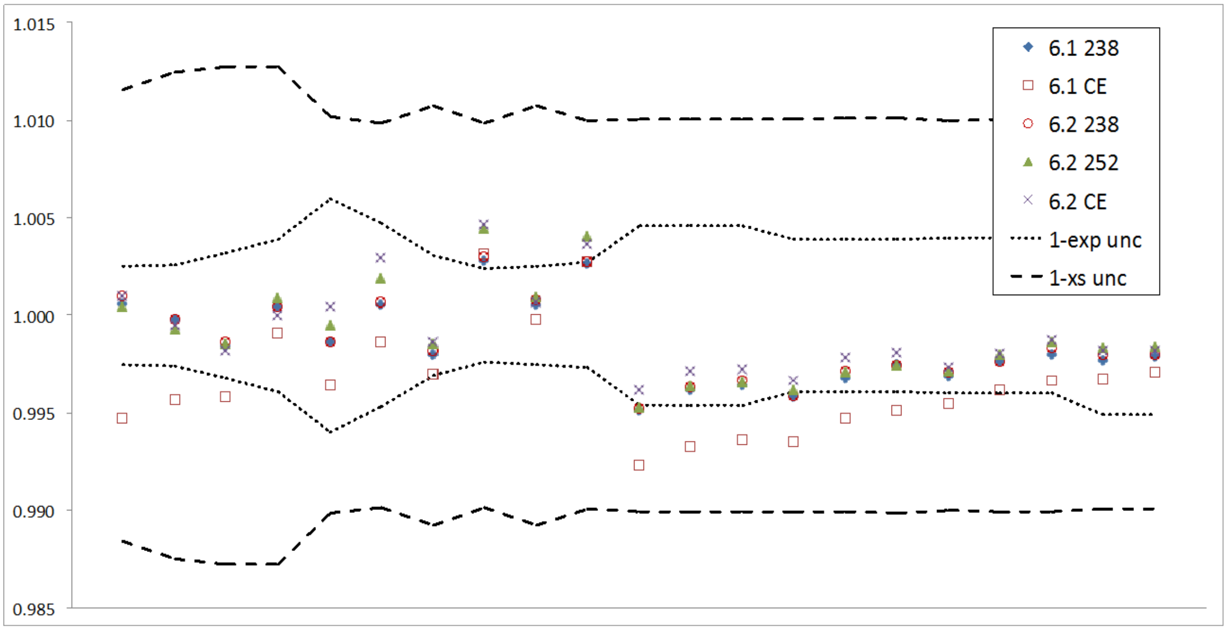

Figure 4. SCALE calculated results for International Criticality Safety Benchmark Evaluation Project (ICSBEP)[14] thermal mixed oxide critical systems

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

3.2 MG Data

With regard to MG analyses, ORNL has performed detailed comparisons between SCALE CE and MG results, and a consistent bias has been observed between the 238-group and CE calculations. Subsequently, a detailed investigation was performed to develop a new group structure that would eliminate the consistent bias observed with the 238-group library, especially for light-water moderated systems. A new 252-group structure has been developed that provides a more detailed representation of the ^{238}U resonance structure, and AMPX has been used to develop a new 252-energy-group ENDF/B-VII.0 neutron cross-section library for SCALE 6.2. In addition to the new group structure, the 252-group library has been generated using a new weighting spectrum with improved resonance self-shielding parameters. Specifically, for actinides and hydrogen in H_2O, a temperature-dependent CE flux spectrum has been generated with the CENTRM module for a PWR pin cell, and the CE flux spectrum has been used to generate the 252-group library. Intermediate resonance parameters (lambdas) for all isotopes have been included in the library, which provides a capability for improved self-shielding with the Bondarenko method [15]. Bondarenko shielding factors, as a function of background cross section and temperature, were computed for all actinides (except ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu) using CE spectra calculated by CENTRM for homogeneous mixtures of the resonance material and hydrogen, corresponding to the respective background cross section. For the nuclides ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu, the Bondarenko factors are based on CENTRM CE calculations for heterogeneous pincell models that span the range of anticipated self-shielding conditions. The thermal cutoff in the 252-group library for thermal moderators and the free-gas approximation has been raised from 3 eV to 5 eV. The new library has been tested by analyzing a wide variety of critical benchmark experiments and by comparing results with CE Monte Carlo results. The 252-group results that are presented in Fig. 4 demonstrate consistent performance w ith the SCALE 6.2 CE results for the thermal MOX critical benchmark experiments. Based on additional studies with the 252-group library, computational benchmark comparisons with CE results at room temperature and elevated temperatures show agreement within 100 pcm in most cases. In addition to the 252-group library, a new ENDF/B-VII.0 broad group library, with approximately 50–70 energy groups, is also under development for SCALE 6.2.

3.3 Additional AMPX Updates

AMPX has also been used to generate prototypic ENDF/B-VII.1 CE, MG, and covariance data libraries. ORNL is in the process of conducting quality assurance (QA) tests of the new ENDF/B-VII.1 libraries prior to their release with SCALE. The ENDF/B-VII.1 library release is planned to occur after the release of SCALE 6.2.

4 QUALITY ASSURANCE

The SCALE QA program has been updated in 2013 to provide an improved means of providing high-quality software and data for the user community. A new QA program has been implemented, which is compliant with ISO 9001 [16], DOE 414.1D [17],the ORNL Standards Based Management System, and is consistent with ASME NQA-1 [18]. With the new SCALE QA program, a streamlined Kanban process is implemented with continual integration of new features and an automated test system that performs approximately 50,000 tests per day on Linux, Macintosh, and Windows operating systems. The QA program provides for rapid introduction of new features for deployment to end users.

5 CONCLUSION

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, and sensitivity/uncertainty analysis and the improved CE and MG data.

6 ACKNOWLEDGMENTS

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