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ENHANCEMENTS IN SCALE 6.1*

B. T. Rearden, L. M. Petrie, D. E. Peplow, M. A. Jessee, D. Wiarda, M. L. Williams, R. A. Lefebvre, J. P. Lefebvre, I. C. Gauld, and S. Goluoglu
Oak Ridge National Laboratory
P.O. Box 2008, Bldg. 5700, Oak Ridge, TN 37831-6170, USA
ReardenB@ornl.gov

ABSTRACT

The SCALE code system developed at Oak Ridge National Laboratory provides a comprehensive, verified and validated, user-friendly tool set 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 with 89 computational modules, including three deterministic and three Monte Carlo radiation transport solvers that are selected based on the desired solution. SCALE's graphical user interfaces assist with accurate system modeling, visualization, and convenient access to desired results. SCALE 6.1 builds on the existing capabilities and ease-of-use of SCALE and provides several new features such as enhanced lattice physics capabilities and multigroup Monte Carlo depletion, improved options and capabilities for sensitivity and uncertainty analysis calculations, improved flexibility in shielding and criticality accident alarm system calculations with automated variance reduction, and new options for the definition of group structures for depletion calculations. The SCALE 6.1 development team has focused on improved robustness via substantial additional regression testing and verification for new and existing features, providing improved performance relative to SCALE 6.0, especially in reactor physics calculations and in the nuclear data used for source term characterization and shielding calculations.

Key Words: SCALE, Modeling, Simulation

1. INTRODUCTION

The SCALE code system consists of easy-to-use analytical sequences, which are automated through control modules to perform the necessary data processing and manipulation of well-established computer codes.[1] Calculations with SCALE are typically characterized by the type of analysis to be performed (e.g., criticality, shielding, or lattice physics) and the geometric complexity of the system being analyzed. The user then prepares a single set of input in terms of recognizable engineering parameters in keyword-based format. The analytical sequence is defined by this single input specification. The SCALE control modules use this information to derive additional parameters and prepare input for each of the functional modules necessary to

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achieve the desired results, especially with the SCALE radiation transport codes that employ discrete ordinates, Monte Carlo, or hybrid methods.

SCALE 6.1 provides several new capabilities such as improved options and capabilities for sensitivity and uncertainty analysis calculations, improved flexibility in shielding and criticality accident alarm system calculations with automated variance reduction, and new options for the definition of group structures for depletion calculations. The SCALE 6.1 development team has focused on improved robustness via substantial additional regression testing and verification for new and existing features, providing improved performance relative to SCALE 6.0, especially in reactor physics calculations and in the nuclear data used for source term characterization and shielding calculations.

2. SCALE CAPABILITIES AND UPDATED FEATURES

The key capabilities and recent updates of the SCALE code system are reviewed in this section. Numerous new and improved features are introduced in SCALE 6.1 to enable improved efficiency and flexibility in analysis, especially in key areas of interest for criticality safety such as sensitivity and uncertainty analysis, burnup credit analysis, and criticality accident alarm system analysis.

2.1 Material Input and Problem-dependent Cross-section Data

A foundation of SCALE is the Material Information Processor Library that allows users to specify materials using easily remembered and recognizable keywords that are associated with mixtures, elements, and nuclides provided in the SCALE Standard Composition Library. An example of material input in a SCALE graphical user interface is shown in Fig. 1. SCALE also uses other keywords and simple geometry input specifications to prepare input for the modules that perform the problem-dependent cross-section processing. Even when performing multigroup calculations, SCALE begins with continuous-energy cross-section data and generates problem-dependent multigroup data based on a pointwise spectrum for the given system. For example, an infinitely dilute multigroup cross section, a self-shielded multigroup cross section, the pointwise cross section, and the problem-dependent flux used to produce the shielded data are plotted in Fig. 2. A keyword supplied by the user selects the cross-section library from a standard set provided in SCALE or designates the reference to a user-supplied library.

For SCALE 6.1, the nuclear masses in the SCALE Standard Composition Library and all cross-section libraries were updated to reflect the most recent evaluations. Nuclear masses are now available for over 3200 nuclides, nearly an order of magnitude more than are available in Evaluated Nuclear Data Files (ENDF).[2]

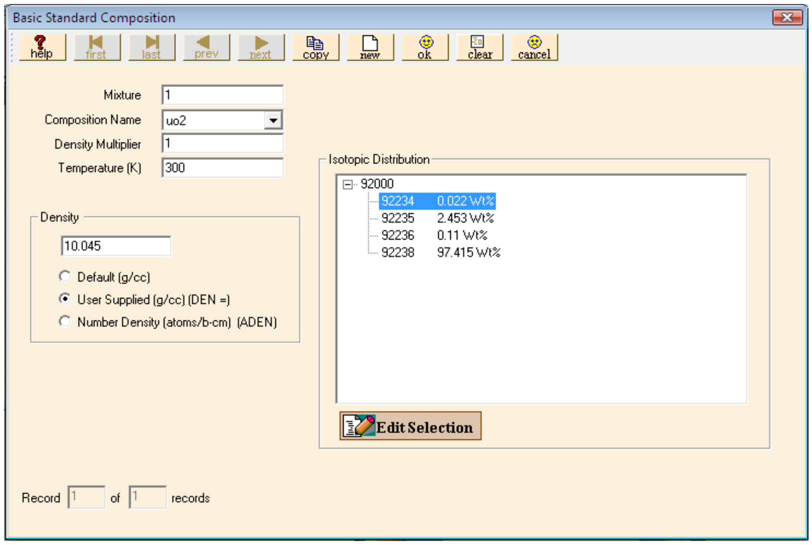

Figure 1. SCALE material input in a SCALE graphical user interface.

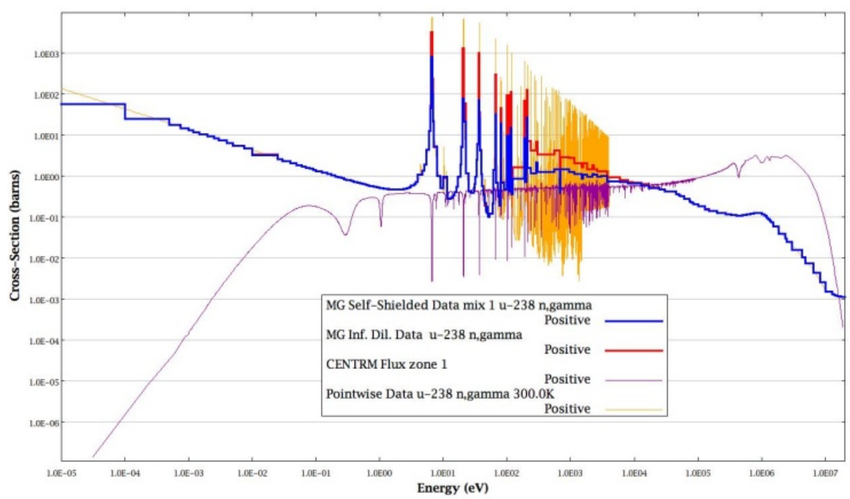

Figure 2. Resonance self-shielding with SCALE.

2.2 Criticality Safety Analysis

The criticality safety analysis sequences provide for the calculation of the neutron multiplication factor of a system, including automated problem-dependent processing of cross-section data, and enable general analysis of a one-dimensional (1D) system model using deterministic transport or three-dimensional (3D) Monte Carlo transport solution using the KENO Monte Carlo codes in multigroup or continuous-energy mode. SCALE also provides capabilities to search on geometry spacing or nuclide concentrations, and provides problem-dependent cross-section processing without subsequent transport solutions for use in executing stand-alone functional modules. A cutaway view of an example SCALE Monte Carlo model is shown in Fig. 3.

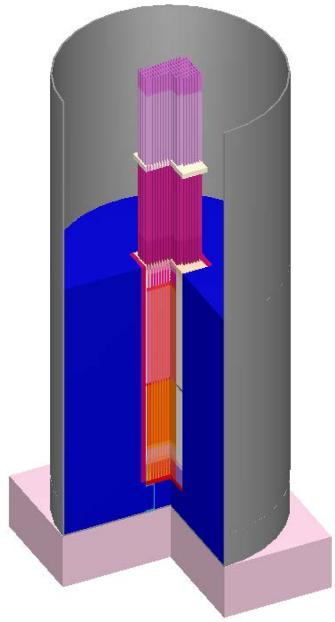

Figure 3. SCALE Monte Carlo model of a mixed oxide critical experiment.

The burnup credit sequence of SCALE assists in performing criticality safety assessments of transport and storage scenarios that apply burnup credit. SCALE automates the generation of spatially varying nuclide compositions in a spent fuel assembly, and the use of these compositions in 3D Monte Carlo analysis of the system. Additional criticality safety tools include a module that produces reaction rates and group collapsed data from Monte Carlo calculations and a tool that performs trending analysis for bias assessment.

For SCALE 6.1 a number of enhancements have been implemented in KENO. The mesh flux and fission source accumulator used in sensitivity analysis and in criticality accident alarm system analysis has been improved with more flexibility in the user definition of mesh intervals and better mesh volume calculations, mesh tracking, and output edits. Mesh fission source data can now be generated in multigroup or continuous-energy mode, and the fission distribution can be visualized, as shown in Fig. 4. Default criticality search parameters have been modified to provide improved convergence to true minimum or maximum values, and region mean free paths can now be computed in continuous-energy mode.

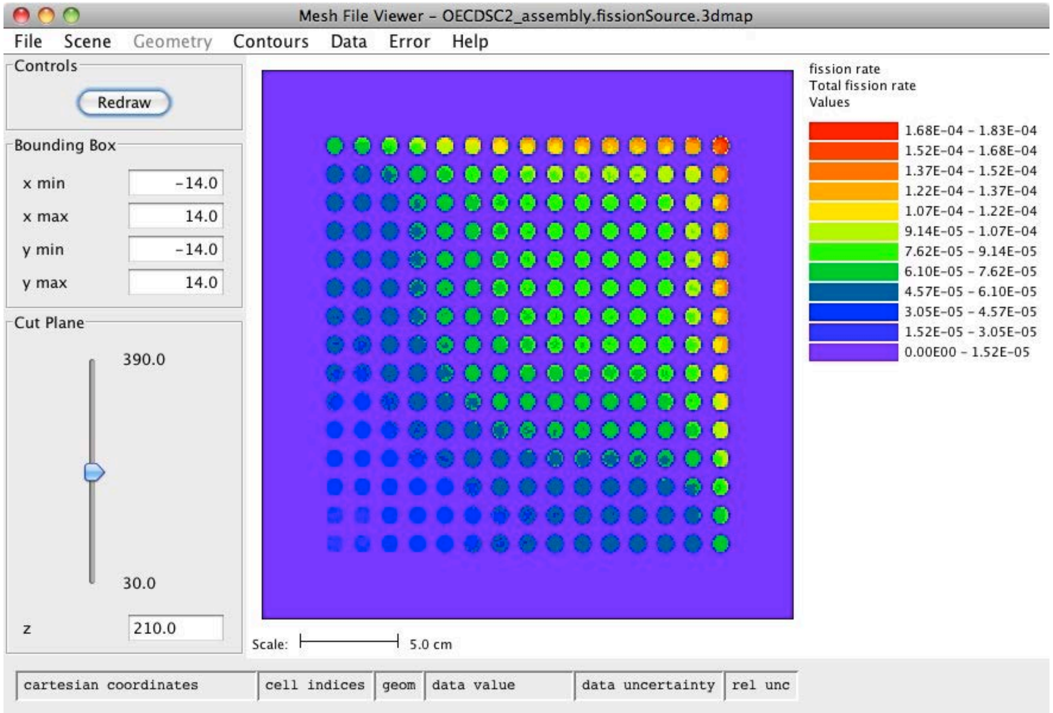

Figure 4. Visualization of a mesh fission source.

2.3 Shielding and Criticality Accident Alarm System Analysis

SCALE's fixed-source radiation transport sequence is designed to apply multigroup fixed-source Monte Carlo to solve problems that are too challenging for standard, unbiased Monte Carlo methods. SCALE uses hybrid (Monte Carlo/deterministic) radiation transport methods to generate a consistent importance map and biased source that are derived from deterministic transport calculations. The two principal hybrid methods are (1) Consistent Adjoint Driven Importance Sampling (CADIS) for optimization of a localized detector (tally) region (e.g., flux, dose, or reaction rate at a particular location) and (2) Forward Weighted CADIS (FW-CADIS) for optimizing distributions (e.g., mesh tallies over all or part of the problem space) or multiple localized detector regions (e.g., simultaneous optimization of two or more localized tally regions). SCALE generates problem-dependent cross-section data and then automatically performs a coarse-mesh, 3D discrete-ordinates transport calculation using Denovo to determine the adjoint flux as a function of position and energy, and to apply the information to optimize the Monte Carlo calculation. An example model and FW-CADIS-based mesh tally for a criticality accident alarm system experiment are shown in Fig. 5. Additionally, SCALE provides general 1D deterministic shielding capabilities.

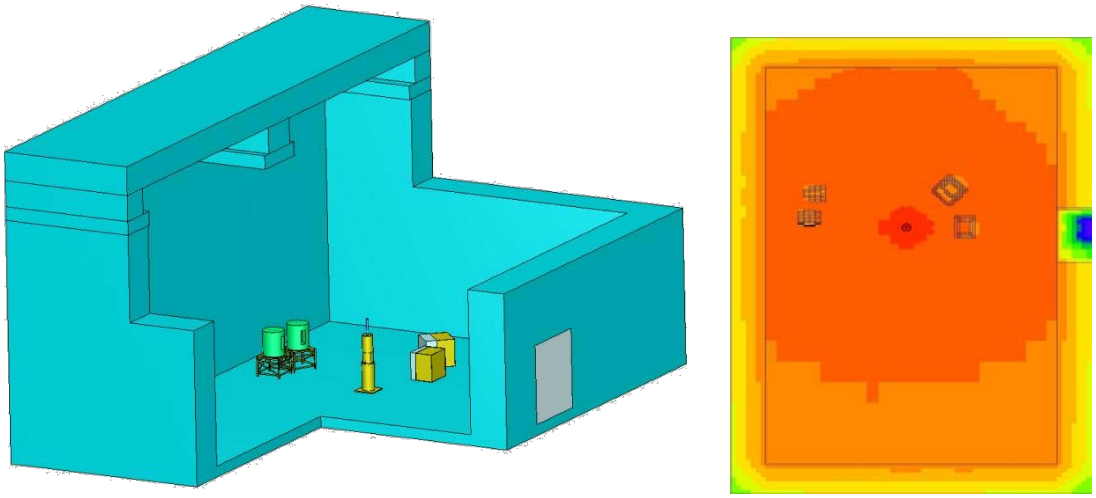

Figure 5. SCALE model of a criticality accident alarm system experiment and mesh tally of the neutron dose rate throughout the facility.

The shielding tools have been updated with a number of enhancements for SCALE 6.1. Multiple sources may now be defined with spatial distributions defined within each source. Energy distributions can be imported from an ORIGEN binary concentration file or from response functions read from a cross-section file. Improvements were also realized in the advanced variance reduction capabilities such as a macro materials option for improved deterministic simulations used to generate variance reduction parameters and increased flexibility in forward-weighting strategies. Cylindrical mesh grids have been added to more accurately capture spatial effects for a shielding calculation for cylindrical geometries such as a spent-fuel shipping cask, and a suite of utilities has been developed to post-process data files.

2.4 Depletion, Decay, and Radioactive Source Term Analysis

The ORIGEN (Oak Ridge Isotope Generation) code applies a matrix exponential expansion model to calculate time-dependent concentrations, activities, and radiation source terms for a large number of isotopes simultaneously generated or depleted by neutron transmutation, fission, and radioactive decay. Provisions are made to include continuous nuclide feed rates and continuous chemical removal rates that can be described with rate constants for application to reprocessing or other systems that involve nuclide removal or feed. ORIGEN includes the ability to utilize multigroup cross sections processed from standard ENDF/B evaluations. Within SCALE, transport codes can be used to model user-defined systems for problem-dependent neutron-spectrum-weighting of cross sections that are representative of conditions within any given reactor or fuel assembly. These cross sections are then converted into a library that can be used by ORIGEN. Time-dependent cross-section libraries may be produced that reflect fuel composition variations during irradiation. An alternative sequence for depletion/decay calculations is ORIGEN-ARP (Automated Rapid Processing), which interpolates pre-generated ORIGEN cross-section libraries versus enrichment, burnup, and moderator density.

The ORIGEN capabilities have been improved substantially for SCALE 6.1. Support is now provided for multigroup cross-section libraries in any group structure, ENDF/B-VII decay libraries, and energy-dependent fission product yields. Cross-section transitions can be included from multiple sources, including JEFF-3.0/A-based multigroup cross-section libraries developed for burnup and activation applications, a library generated by one of the SCALE transport codes, and cross sections input manually by the user via the input file.

2.5 Reactor Analysis

The SCALE lattice physics and depletion sequences provide flexible capabilities to meet the challenges of modern reactor designs and burnup credit analysis by providing 1D pin-cell depletion capabilities, two-dimensional (2D) lattice physics capabilities using a flexible mesh discrete-ordinates code, or 3D Monte Carlo depletion. With each neutron transport option, depletion and decay calculations are conducted with ORIGEN. Additionally, SCALE can produce assembly-averaged few-group cross sections for use in 3D core simulators. Improved resonance self-shielding treatment for nonuniform lattices can be achieved through use of the Monte Carlo code that generates Dancoff factors for generalized 3D geometries.

The lattice physics and depletion capabilities have realized a number of enhancements for SCALE 6.1. The Monte Carlo depletion capabilities have been substantially improved to more accurately compute power distributions and enable additional Monte Carlo functionalities such as source specification, region volume input, and geometry plotting. All sequences were updated to use the improved multigroup functionalities of ORIGEN, and for computer systems with multiple computing nodes, branch calculations can now be run in parallel.

The 2D discrete-ordinates code was enhanced with parallel operation, support for inhomogeneous sources for generalized perturbation theory (GPT) calculations, improvements for high-temperature gas reactor prismatic geometries, and support for coupled n-gamma calculations. Several corrections were also implemented, including improved unstructured coarse-mesh finite diffusion acceleration, grid generation algorithms, results for few-group homogenized cross sections, and output edits.

2.6 Sensitivity and Uncertainty Analysis

SCALE provides eigenvalue sensitivity and uncertainty analysis capabilities for models of 1D, 2D, and 3D systems. It also provides generalized perturbation theory capabilities (new in SCALE 6.1) to compute sensitivities and uncertainties for reactor responses such as reaction rate and flux ratios as well as homogenized few-group cross sections for 1D and 2D system models. SCALE also includes tools to calculate sensitivity coefficients for reactivity differences and for code and data validation capabilities based on sensitivity and uncertainty data. An example plot of energy-dependent sensitivity of k_{eff} to cross-section data for a mixed oxide critical experiment is shown in Fig. 6.

For SCALE 6.1 the 3D Monte Carlo adjoint-based sensitivity and uncertainty analysis capabilities were enhanced through many of the previously described improvements in the Monte Carlo mesh capabilities, a new 2D capability was introduced using the discrete ordinates transport solver, and generalized perturbation theory capabilities are introduced. Additionally, the data assimilation bias assessment tool was updated with improved output edits and plots.

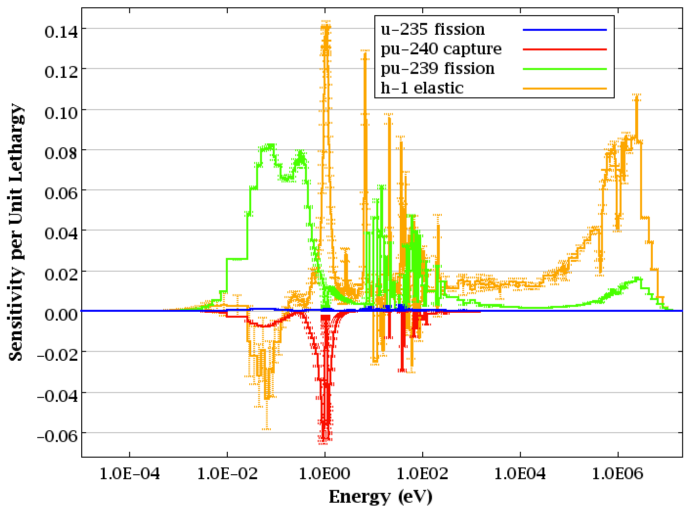

Figure 6. Energy-dependent sensitivity of k_{eff} to cross-section data for a mixed oxide critical experiment.

2.7 Nuclear Data

The cross-section data provided with SCALE include comprehensive continuous-energy neutron and multigroup neutron and coupled neutron-gamma data based on ENDF/B-VI.8 and ENDF/B-VII.0. Additional ENDF/B-V multigroup neutron libraries are also available. The comprehensive ORIGEN data libraries are based on ENDF/B-VII and JEFF-3.0/A and include nuclear decay data, neutron reaction cross sections, neutron-induced fission product yields, delayed gamma-ray emission data, and delayed neutron emission data. The photon yield data libraries are based on the most recent Evaluated Nuclear Structure Data File (ENSDF) evaluations. The libraries used by ORIGEN can be coupled directly with detailed problem-dependent physics calculations to obtain self-shielded problem-dependent cross sections based on the most recent evaluations of ENDF/B-VII. SCALE also contains a comprehensive library of neutron cross-section-covariance data for use in sensitivity and uncertainty analysis. Example plots of multigroup and continuous-energy cross-section data are shown in Fig. 7, and multigroup cross-section-covariance data are shown in Fig. 8.

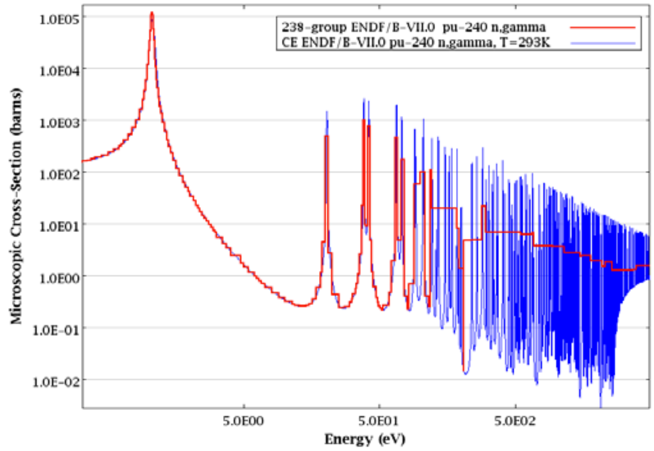

Figure 7. Continuous-energy and multigroup ENDF/B-VII.0 neutron cross-section data for ^{240}Pu n,gamma.

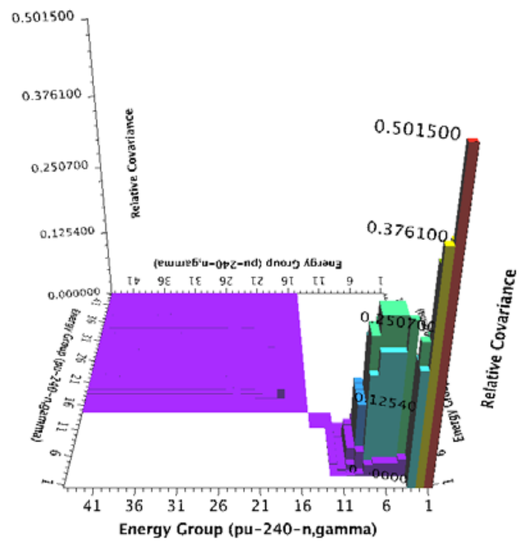

Figure 8. Cross-section-covariance data for ^{240}Pu n,gamma.

Many nuclear data libraries were updated for SCALE 6.1. The unresolved resonance region probability tables for continuous-energy ENDF/B-VI.8 and ENDF/B-VII.0 neutron cross sections for uranium and plutonium isotopes have been improved to provide more accurate results, especially for intermediate-energy systems.

The 238-group ENDF/B-VI.8 and ENDF/B-VII.0 neutron criticality libraries have been updated with an improved weighting function in which the boundary between the 1/E and fission-spectrum-weighting regions has been raised from 67.4 to 820.8 keV. This adjustment improved the performance of spectral calculations for very high-temperature reactor simulations. The multigroup ENDF/B-VI.8 and ENDF/B-VII.0 libraries for coupled n-gamma calculations provide improved gamma yield data. In addition, updated versions of cross-section generation routines using double precision throughout the calculation were used for the library generation.

The ORIGEN data have been updated to include ENDF/B-VII decay and fission yield libraries and JEFF multigroup neutron cross-section libraries in 44-, 47-, 49-, 200-, and 238-group structures. The new decay library contains 2227 nuclides, including 174 actinides, 1149 fission products, and 904 structural activation materials.

The ORIGEN master photon x-ray and gamma-ray library was regenerated using the latest evaluations from the ENSDF. This revision corrects missing gamma lines and incorrect intensities for some nuclides. A total of 982 nuclides were processed from ENSDF data, along with gamma data for an additional 51 nuclides, with no ENSDF evaluation adopted from ENDF/B-VI.

Testing was performed for specific nuclides that had previously been noted in the SCALE 6 Notebook to be missing some lines or to have incorrect intensities. A case for ^{137}Cs was performed to demonstrate that the 662 keV gamma line was assigned correctly to ^{137m}Ba and not ^{137}Cs. Problematic nuclides ^{192}Ir, ^{147}Pm, and ^{241}Pu were checked to ensure that the lines and intensities had been corrected.

Several cross-section utility modules are included to provide users with the capability to edit the cross-section data and reformat user-supplied libraries for use in SCALE.

2.8 Graphical User Interfaces

SCALE includes a number of graphical user interfaces to provide convenient means of generating input, executing SCALE, and visualizing models and data. GeeWiz (Graphically Enhanced Editing Wizard), shown in Fig. 9, is a Windows user interface that provides a control center for setup, execution, and viewing results for most of SCALE's computational sequences. GeeWiz is coupled with the KENO3D interactive visualization program for Windows for solid-body rendering of Monte Carlo geometry models. The OrigenArp user interface for Windows provides for rapid problem setup and plotting of results for spent fuel characterization. The Javapeño (Java Plots Especially Nice Output) multiplatform interface, shown in Fig. 10, provides 2D and 3D plotting of cross-section and cross-section-covariance data, multigroup fluxes and reaction rates, sensitivity data, and pointwise fluxes from resonance self-shielding codes. The MeshView multiplatform interface produces 2D contour views of mesh data and mesh results, and ChartPlot provides for energy-dependent plots of shielding results. The ExSITE tool provides a dynamic multiplatform interface for the sensitivity and uncertainty analysis tools. The USLSTATS (Upper Subcritical Limit Statistics) multiplatform interface allows for trending analysis with integrated plotting, and VIBE (Validation Interpretation and Bias Estimation) assists with interpretation of sensitivity data and couples with the DICE database from the International Criticality Safety Benchmark Evaluation Program.[3] Additionally, several codes provide HTML-formatted output, in addition to the standard text output, to provide convenient navigation through the computed results using most common Web browsers with interactive color-coded output and integrated data visualization tools, as shown in Fig. 11.

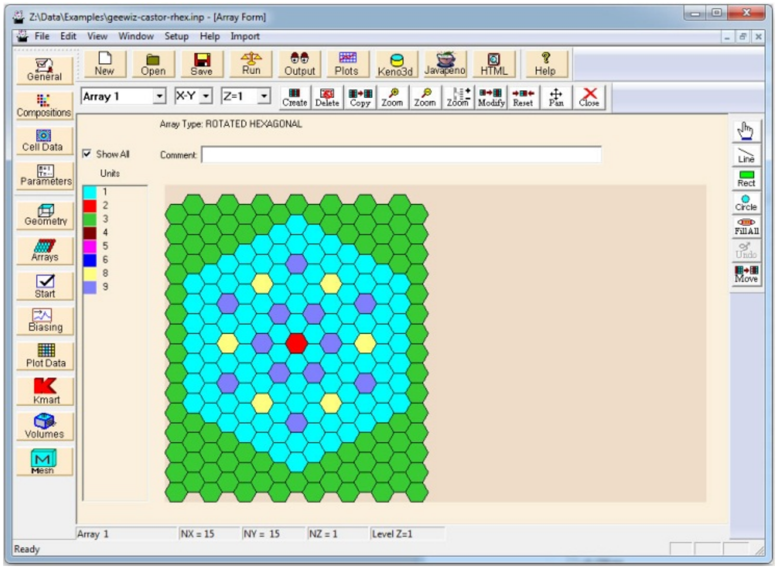

Figure 9. Simplified array data entry with GeeWiz.

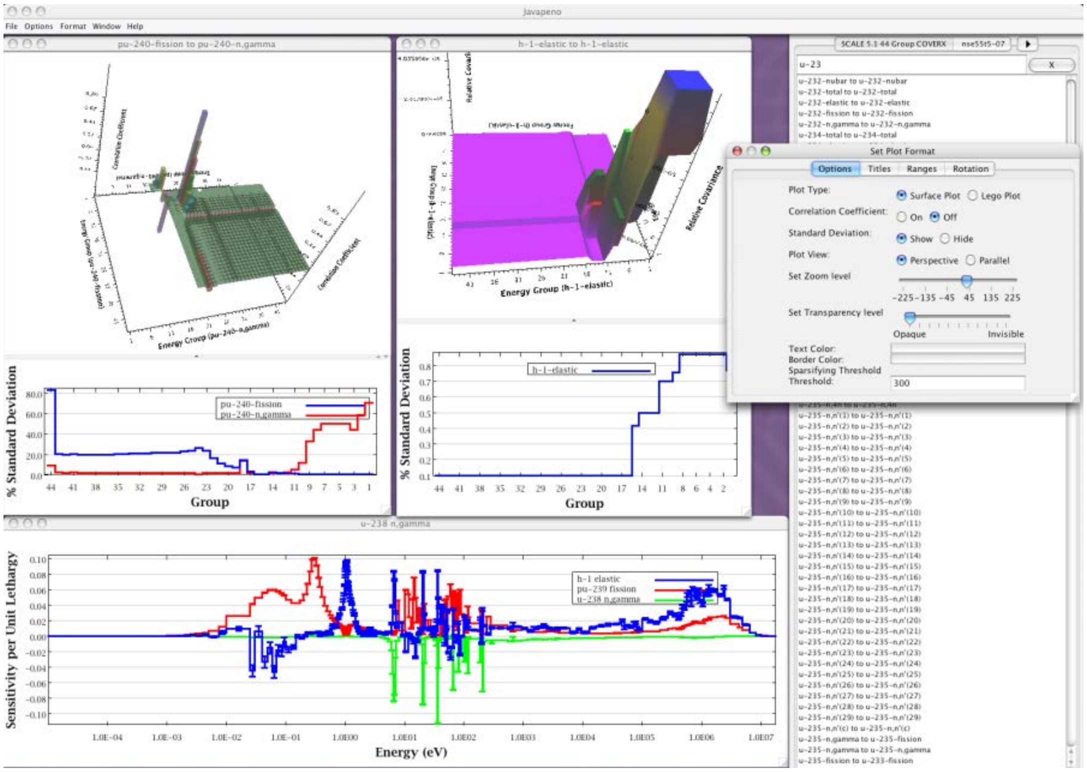

Figure 10. Data visualization with Javapeño.

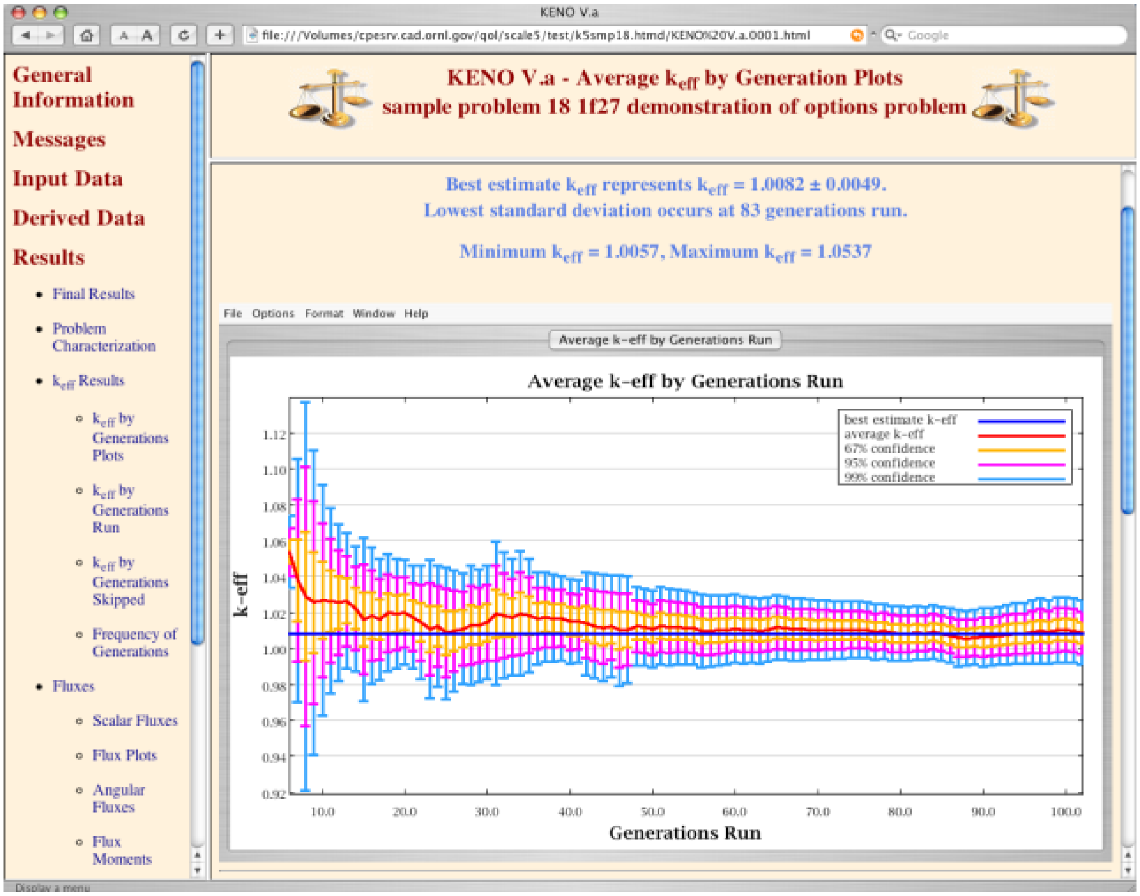

Figure 11. HTML-formatted output from KENO with embedded Javapeño applet.

Many of the SCALE user interfaces have been enhanced for SCALE 6.1. Notably, GeeWiz now fully supports all major SCALE computational sequences and provides a more stable and intuitive work environment. The Javapeño data visualization package now supports plotting SCALE continuous-energy data and ORIGEN data. The ExSITE interface, developed to support sensitivity and uncertainty post-processing calculations, is deployed for the first time, and the VIBE interface for processing and interpreting sensitivity data, shown in Fig. 12, has been updated for compatibility with the latest experimental data from the DICE database distributed with the *International Handbook of Evaluation Criticality Safety Benchmark Evaluations* [3].

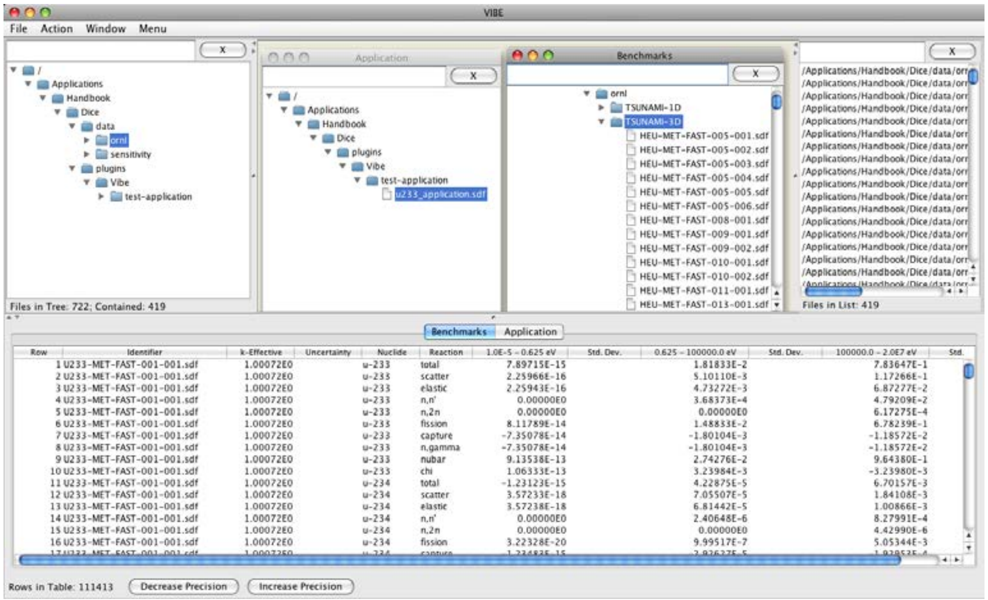

Figure 12. VIBE sensitivity data graphical user interface.

2.9 Infrastructure

SCALE 6.1 is built, tested, and deployed for the following platforms: Linux 32- and 64-bit; Mac OS X (Darwin) 10.6 or newer; Windows XP, Vista, and 7 in 32 and 64-bit; and Itanium (HPUX) 64-bit. A new automated installer, shown in Fig. 13, allows users to easily configure their installation of SCALE to include only the features they desire. The SCALE runtime environment (i.e., batch6.1) has been updated to provide improved flexibility and performance in executing SCALE and verifying proper installation by running sample problems. Additionally, for those wishing to build SCALE from source code, the build configuration has been unified across all platforms and updated to use the CMake build system.

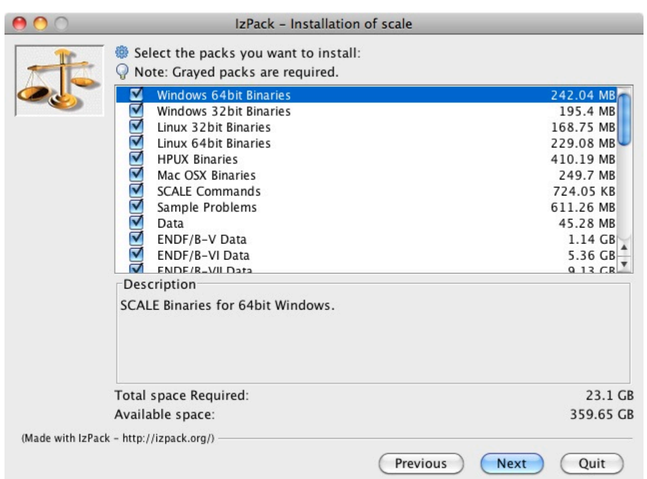

Figure 13. SCALE 6.1 installer.

3. FUTURE DEVELOPMENT

The SCALE team is dedicated to providing advanced features for future releases such as SCALE 6.2. Current projects include significant speedups in 2D lattice physics calculations, the extension of continuous-energy Monte Carlo capabilities to include depletion, sensitivity analysis, and shielding analysis with automated variance reduction. The SCALE nuclear data in continuous-energy, multigroup, and activation/decay libraries will continue to be improved through increased testing. The next version of KENO will include parallel computing capabilities and fission source convergence detection techniques, and the CADIS methodology is being applied to eigenvalue calculations, especially for Monte Carlo depletion.

The entire code system is undergoing extensive refactoring to improve run-time performance and solution fidelity in SCALE 7. The most significant changes in SCALE 7 will be the ability to execute SCALE in parallel on desktops, workstation clusters, and high-performance supercomputers using tens or hundreds of thousands of cores. SCALE 7 will also provide greatly enhanced data management for cross sections, geometry, and depletion data as well as improved solution methodologies and capabilities, especially for reactor physics calculations.

4. CONCLUSIONS

SCALE 6.1 provides a feature-rich set of tools for nuclear safety analysis and design. The SCALE 6.1 development team has focused on improved robustness via substantial additional regression testing and verification. Numerous new and improved features are introduced in SCALE 6.1 to enable improved efficiency and flexibility in analysis.

5. REFERENCES

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2. G. Audi, A. H. Wapstra, and C. Thibault, “The Ame2003 Atomic Mass Evaluation (II),” *Nucl. Phys.*, **A729**, pp. 337–676, December 22, 2003.
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