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NEW CRITICALITY SAFETY ANALYSIS CAPABILITIES IN SCALE 5.1

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Abstract

Version 5.1 of the SCALE computer software system developed at Oak Ridge National Laboratory, released in 2006, contains several significant enhancements for nuclear criticality safety analysis. This paper highlights new capabilities in SCALE 5.1, including improved resonance self-shielding capabilities; ENDF/B-VI.7 cross-section and covariance data libraries; HTML output for KENO V.a; analytical calculations of KENO-VI volumes with GeeWiz/KENO3D; new CENTRMST/PMCST modules for processing ENDF/B-VI data in TSUNAMI; SCALE Generalized Geometry Package in NEWT; KENO Monte Carlo depletion in TRITON; and plotting of cross-section and covariance data in Javapeño.

Introduction

The SCALE (**S**tandardized **C**omputer **A**nalyses for **L**icensing **E**valuation) [1] computer software system developed at Oak Ridge National Laboratory (ORNL) is widely used and accepted around the world for criticality safety analyses. Version 5.1 of the SCALE computer software system developed at ORNL, released in November 2006, contains several significant enhancements for criticality safety analysis.

1. Resonance Self-Shielding Capabilities

The resolved resonance processor modules CENTRM (**C**ontinuous **En**ergy **Tr**ansport **M**odule) and PMC (**P**ointwise **M**ultigroup **C**onverter) have been enhanced in SCALE 5.1. Discrete-level inelastic cross-section data now can be processed by CENTRM/PMC. The pointwise (PW) thermal flux solution in CENTRM can utilize bound thermal-scattering kernels based on ENDF/B S(α,β) data. Down-scattering from inelastic continuum data and thermal up-scattering into the PW range are optionally available by a multigroup treatment. Because CENTRM/PMC calculates a problem-dependent flux profile, it provides a rigorous cross-section treatment that explicitly handles effects from overlapping resonances, fissile material in the fuel and surrounding moderator, anisotropic scattering, and inelastic level scattering.

An efficient two-region solution method has also been added to CENTRM. The two-region approximation usually runs much faster than the discrete-ordinates solution and is adequate for a wide range of standard applications, such as reactor fuel assembly lattices.

Another new feature of CENTRM is the capability to treat nonuniform arrays of absorber bodies. Users can input Dancoff factors computed by Monte Carlo techniques, and the SCALE Material Information Processor Library (MIPLIB) will determine Dancoff-equivalent unit cells for CENTRM calculations.

A new resonance self-shielding option in the SCALE criticality safety calculational sequences can address doubly heterogeneous cells (e.g., pebble bed or prismatic fuel where small micrograins of fuel and moderator matrix are contained in larger spheres or rods) by applying sequential CENTRM/PMC resonance calculations for the low-and high-level heterogeneities. This method computes PW disadvantage factors to obtain cell-homogenized PW cross sections from the low-level unit cell to use in the high-level unit cell resonance-shielding computation.

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2. ENDF/B-VI Cross-Section and Covariance Libraries

SCALE 5.1 includes both continuous energy and multigroup ENDF/B-VI.7 cross-section libraries. The multigroup library is a 238-group general purpose criticality safety library with the same energy group structure as the 238-group ENDF/B-V library in previous versions of SCALE. Users should be aware that the new V6-238 ENDF/B-VI multigroup library in SCALE 5.1 is intended for use only with CENTRM/PMC. It should not be used with NITAWL. The Reich-Moore resonance parameters were omitted from the 238-group ENDF/B-VI library because NITAWL required excessive run times to process them. Because the Reich-Moore parameters are not present, NITAWL will run fairly fast with this library. However, it passes infinitely dilute cross sections to KENO for nuclides that have Reich-Moore parameters in ENDF/B-VI.

For SCALE 5.1, a total of four cross-section covariance libraries are being released; 44GROUPV5COV, 44GROUPV6COV, 44GROUPV5REC, and 44GROUPV6REC. The first two libraries represent a basic set with only the covariance data included in the ENDF/B formal release, about 50 nuclides corresponding to ENDF/B-V and ENDF/B-VI, respectively. The last two represent a recommended set with covariance information for nearly every nuclide in the cross-section library. The recommended sets contain the ENDF/B-V and ENDF/B-VI data plus a large number of nuclides for which covariance information is included based on integral uncertainty data. Each of these libraries contains cross-section covariance information in the SCALE 44 neutron-energy group structure. While conceptually it is possible to process the cross-section covariance information into the SCALE 238 group structure, very little additional information would be available. The capability to use a cross-section covariance group structure that is the same as or a subset of the cross-section library group structure was built into the SCALE sensitivity/uncertainty codes so that these covariance libraries could be used with 238-group calculations. Each of the four covariance libraries described above include all information that was contained in the cross-section uncertainty files. Because many of the specific reactions that contain uncertainty data are not actually used by the TSUNAMI processing codes, the files were thinned to contain only the reactions utilized by TSUNAMI. These reactions include: total, elastic, inelastic, (n,2n), fission, chi, (n,gamma), (n,p), (n,d), (n,t), (n,He-3), (n,alpha), and nu-bar.

3. HTML Output for KENO V.a

An advanced, HyperText Markup Language (HTML)-formatted output interface for KENO V.a has been developed as part of SCALE 5.1. The use of HTML as an alternative output interface for SCALE codes provides the user with a convenient and familiar means of navigating and visualizing data. HTML presents a wide variety of formatting options for differing fonts, colors, and data tables. More advanced technologies such as Java applets and JavaScript are incorporated into the output for advanced navigation and data visualization. In addition to easily navigated and color-coded tables of data, interactive plotting capabilities are available via a new version of Javapeño that executes within the web browser as a Java applet. Javapeño-compatible data files are created by KENO V.a so that the user may view data in colorful, interactive, and customizable plots. Data available for plotting within the HTML interface include k_{eff} by generation, frequency distribution of k_{eff} values (Fig. 1), flux spectra by region, and fission and absorption rates by region (Fig. 2). Future development plans call for adding HTML output to KENO-VI and other SCALE modules.

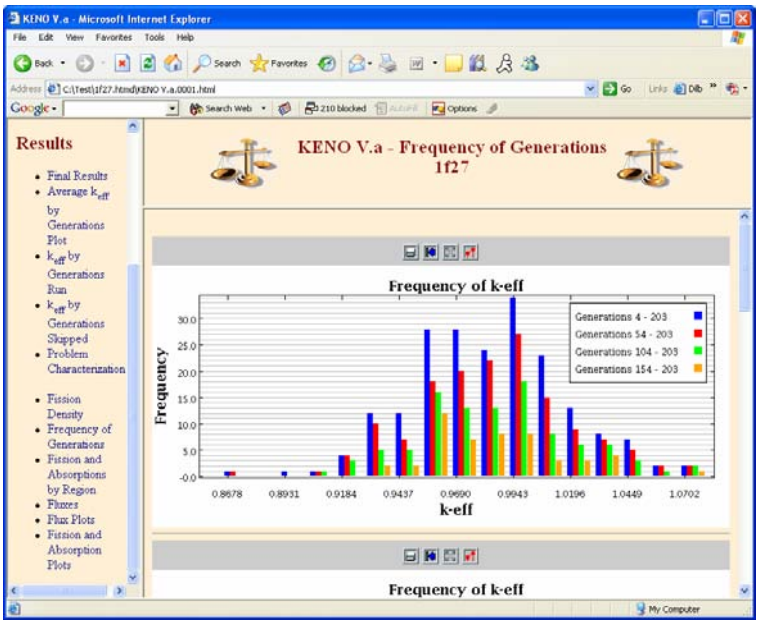

Figure 1. Plot of frequency of k_{eff}.

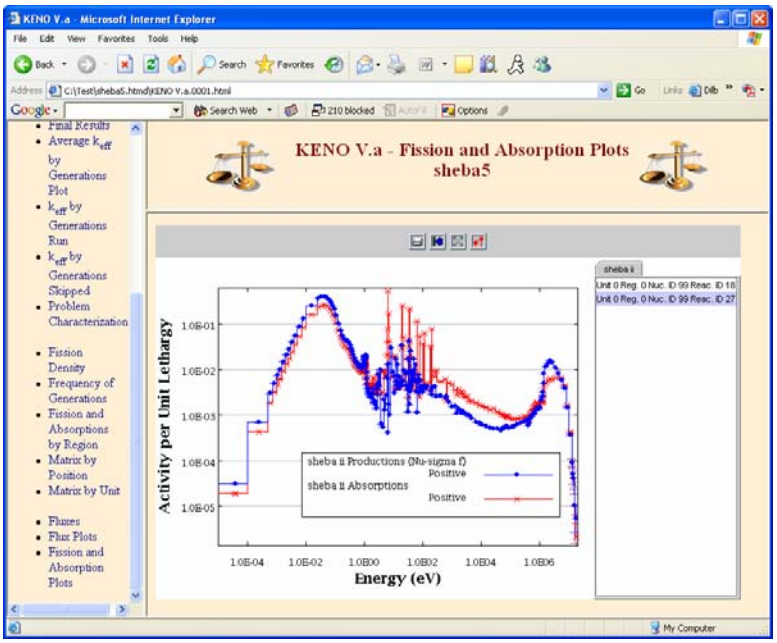

Figure 2. Plot of fission and absorption rates by region.

4. GeeWiz and KENO3D Extensions

GeeWiz (Graphically Enhanced Editor Wizard for SCALE) is the graphical user interface (GUI) that serves as a "command center" for SCALE users. It assists users in setting up, running, and viewing results interactively from an integrated user-friendly environment. It is integrated with KENO3D, Javapeño, and the KENO V.a HTML output. The capability of GeeWiz has been expanded in SCALE 5.1. It is now compatible with the following SCALE sequences: CSAS/KENO V.a, CSAS6/KENO-VI, TSUNAMI-1D and -3D, TRITON/KENO V.a, TRITON6/KENO-VI, STARBUCS, and SMORES.

Keno3D is the three-dimensional (3-D) visualization software designed for interactively viewing KENO V.a and KENO-VI geometry models on Windows computers. A sample KENO3D image is shown in Fig. 3. In SCALE 5.1, it has been enhanced to read TSUNAMI-3D, TRITON/KENO V.a, TRITON6/KENO-VI, and STARBUCS in addition to the traditional CSAS/KENO V.a, CSAS6/KENO-VI sequences.

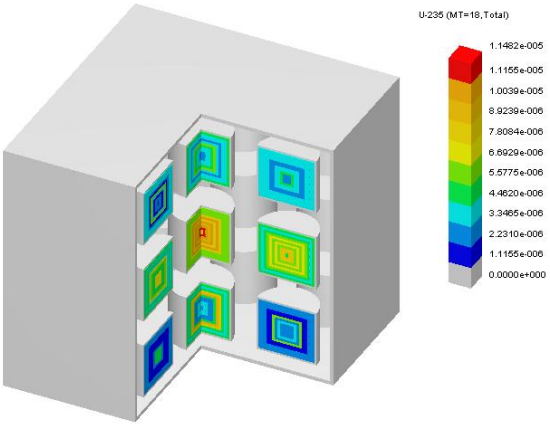

Figure 3. KENO3D image of 1F27 experiment showing fission rates by region.

5. Analytical Calculations of KENO-VI Volumes with GeeWiz/KENO3D

The SCALE KENO-VI program does not calculate volumes for model bodies by default. The reason is that the calculation of volumes in KENO-VI is more difficult than in KENO V.a because of the generalized geometry in KENO-VI that allows body intersections. Although volumes are not needed for the calculation of k_{eff}, they are necessary for the calculation of other parameters such as fluxes and fission densities. They are also required for TRITON6/KENO-VI fuel depletion calculations to correctly normalize the power densities.

The GeeWiz user interface and KENO3D visualization tool have been enhanced to calculate KENO-VI volumes analytically and write those volumes directly to a KENO-VI input file. This new feature is a significant capability that will prove useful for applications that use a KENO-VI model and require accurate volumes for model bodies.

KENO3D has the capability to calculate volumes of individual bodies. Previously, the volume calculation was used internally by KENO3D when performing Boolean operations (e.g., subtracting bodies and intersecting bodies). With the need for accurate volume calculations for KENO-VI geometry models, the volume calculation was extended to calculate the volumes for each medium in the model and to write the volumes to a file that is formatted for reading by KENO-VI or GeeWiz.

The calculation of volumes in KENO3D has been optimized for models where all units and arrays are bounded by rectangular solids. If a unit or array is bounded by a rectangular solid, then each body can be tested to see if its bounding box intersects that of the rectangular solid. For rectangular geometries, if the bounding boxes do not intersect, then the model bodies do not intersect. If the model bodies do not intersect, then the volume of each object as constructed in its unit of origin is simply added to the accumulated volume for that medium.

The intersection of boxes is significantly faster than the intersection of bodies. For a shipping cask model containing approximately 200,000 bodies, the execution time required to accurately calculate volumes was reduced from 30 min to less than 1 s by using the bounding box optimization. With rectangular geometries, when a unit or array bounding box does intersect an object's bounding box, the more-costly calculation using intersections is required for that object. In most practical applications, only a subset of object boundaries intersects unit or array bounds; therefore, execution time would still be reduced by box optimization.

Volumes can be calculated directly with KENO3D; however, as an aid to users, a volume calculation capability was added to the GeeWiz Volume dialog. If the user selects the "Keno3D Volumes" button, KENO3D is called to calculate volumes and create an ASCII volume file formatted for input into SCALE. Subsequently, if the user selects the "Attach Volumes" button, the volume data will be added directly to the media records in every region in the SCALE input file.

6. Enhancements to TSUNAMI

The TSUNAMI (**T**ools for **S**ensitivity and **Un**certainty **A**nalysis **M**ethodology **I**mplementation) capabilities for criticality safety in SCALE 5.1 have been expanded by the availability of ENDF/B-VI cross-section and covariance data as mentioned earlier [2]. Because CENTRM is compatible with ENDF/B-VI data format but NITAWL is not, sensitivity versions of CENTRM and its associated data-processing code PMC, called CENTRMST and PMCST, were developed for SCALE 5.1. These codes process point-wise data from ENDF/B-V and ENDF/B-VI into problem-dependent multigroup cross sections and produce the sensitivity of the multigroup cross sections to data input to their calculation. This sensitivity information is used to produce the implicit portion of the sensitivity coefficients in the SAMS module of SCALE. Another significant improvement is the removal of the limitation on the number of nuclides with resolved-resonance data in the model. In SCALE 5.0, NITAWLST was limited to a maximum of 50 nuclides.

The cross-section covariance data has been expanded for SCALE 5.1. An ENDF/B-VI covariance library was developed for use with ENDF/B-VI cross-section data. Furthermore, only a limited amount of nuclear data uncertainty information is available in both ENDF/B-V and VI. Therefore, SCALE 5.1 provides approximate values for much of the missing uncertainty data by utilizing experimental uncertainties in integral measurements of thermal cross-section and resonance integrals. Where covariance data are missing for certain energy regions of the ENDF evaluations, the TSUNAMI codes can substitute user-defined uncertainties for the missing data.

7. NEWT Uses SCALE Generalized Geometry Package

The geometry input format for the NEWT (**N**ew **E**SC-based **W**eighting **T**ransport code) flexible mesh discrete ordinates code has been redesigned in SCALE 5.1, based on the SCALE Generalized Geometry Package (SGGP) combinatorial input format employed by KENO-VI. The use of a common input format reduces the learning curve in model development for SCALE users. Although limited to two dimensions, the use of the SGGP input format provides virtually all the geometric flexibility of Monte Carlo for a deterministic solution. It also allows a means for direct comparison of Monte Carlo vs deterministic methods. Using the same cross-section data and virtually identical geometric configurations, differences in results can be attributed to differences in the two transport techniques.

NEWT's automated grid-generation scheme, based on the placement of simple bodies within a problem domain, allows rapid development of a model without the need to manually input a complex and irregular grid structure. Figure 4 shows the computational grid generated by NEWT for a VVER fuel assembly. Note that this model contains no curved surfaces but instead consists of arbitrary polygons computed by NEWT in which volumes are conserved.

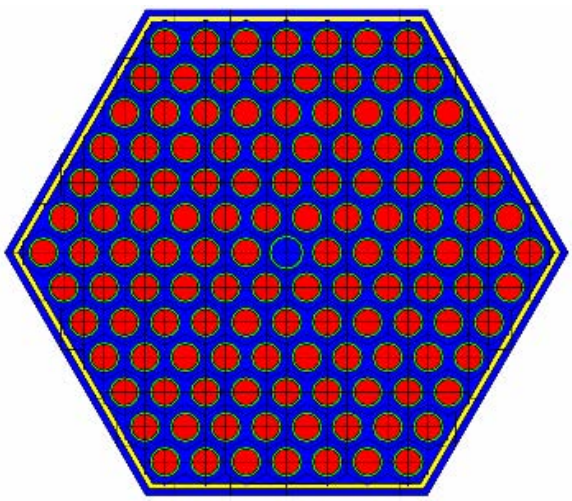

Figure 4. NEWT two-dimensional (2-D) VVER fuel assembly model.

8. Monte Carlo Depletion in TRITON

The TRITON control module in SCALE 5.1 is able to perform three-dimensional (3-D) depletion calculations using the KENO V.a or KENO-VI Monte Carlo transport codes. TRITON couples these neutron transport codes with ORIGEN-S in a method similar to that used in 2-D depletion calculations with NEWT in SCALE 5.0. This capability allows the user to perform detailed calculations such as track the isotopic depletion by individual fuel rods, axial portions of a fuel rod (in 3-D), or concentric rings in a rod loaded with burnable poison.

9. Javapeño

Javapeño (**Java** **P**lots, **E**specially **N**ice **O**utput) is an interactive 2-D and 3-D plotting package that is written in Java and operates on numerous computing platforms. Javapeño enables the plotting of data from TSUNAMI sensitivity data files, KENO V.a and KENO-VI data files generated with KMART and KMART6, XSDRNPM data files, and SMORES data files. New for SCALE 5.1, Javapeño includes a 3-D plotting engine and can plot data directly from binary AMPX master and working formatted cross-section data libraries and from binary COVERX formatted cross-section-covariance data libraries. A sample plot of ^{239}Pu fission covariance data from the 44GROUPV6REC is shown in Fig. 5. Javapeño executes on any system with a Java Virtual Machine (JVM) version 1.5 or newer installed. Java3D components for 3-D plotting, and Java Advanced Imaging components for image exporting must be downloaded separately from the Java website.

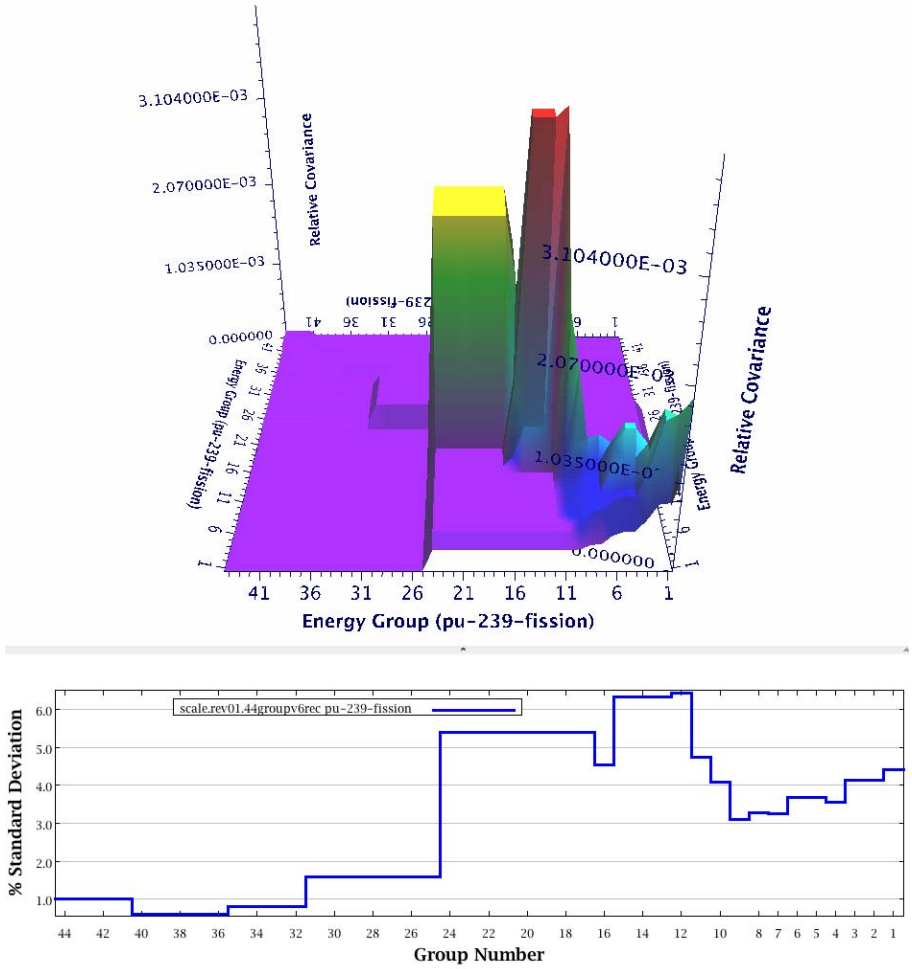

Figure 5. Javapeño 3-D plot of ^{239}Pu fission covariance data.

10. Current Development for SCALE 6

Continuous-energy (CE) capability has been integrated into KENO V.a and KENO-VI and will be released in SCALE 6. The primary objective in the development of these new versions of KENO is to create CE codes completely independent of other CE Monte Carlo codes and compatible with SCALE. This effort also includes new cross-section data that are processed independently of data used in other CE codes. The independence of the CE data has been ensured by developing a set of modules using the AMPX series of cross-section data processing codes [3] to produce the required CE cross-section libraries.

The geometry handling, random walk techniques, and most data management used in the KENO codes remains unchanged. The majority of the changes center on cross-section data storage, manipulation, and use. The object was to provide users with new versions of KENO V.a and KENO-VI that can run existing cases in either CE or multigroup mode by simply changing the cross-section library name in the input.

A new CE cross-section library has been developed using AMPX and based on ENDF/B-VI Release 7. Some CE radiation transport codes have the ENDF laws and procedures programmed in the code. As changes are made to the ENDF formats, the radiation transport code and associated cross-section processing code system must be updated to process the new ENDF laws and procedures. Because AMPX processes the raw ENDF/B data into a CE library, the burden of treating the ENDF formats lies solely on the AMPX cross-section generation code, and not on the KENO transport codes.

Because CE-KENO uses CE cross-section data, no preprocessing is required. The data in the CE library are stored as discrete points, typically with a tolerance of 0.1%, with the exception of the unresolved resonance data. Because of the statistical nature of the unresolved parameters used to describe the unresolved resonance region, probability tables are used to provide cross-section probability distribution functions for energy ranges at specific temperatures within the unresolved region [4].

Testing of the new codes and data is currently under way, and a significant number of critical experiment benchmarks will be used to validate the CE capability [5] in KENO V.a and KENO-VI prior to their release in SCALE 6.

11. Availability of SCALE 5.1

SCALE 5.1 has been implemented and tested on Linux, Unix, and Windows computing platforms. It is available from

- Radiation Safety Information Computational Center (RSICC) in the USA,
- Organization for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA) Data Bank in Europe, and
- Research Organization for Information Science and Technology (RIST) in Japan.

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