Oak Ridge National Laboratory

SCALE Newsletter

Number 41 Winter/Spring 2010

Special Points of Interest:

SCALE Workshops
March 2010 at ORNL

Inside This Issue:

New Captain at the Helm

The SCALE development team is pleased to announce that Brad Rearden is now serving as SCALE Project Leader, replacing Steve Bowman in August 2009. Brad received his PhD in Nuclear Engineering from Texas A&M University and has been a member of the SCALE development team for 12 years, serving primarily as the TSUNAMI code manager. Steve has assumed the role of Group Leader for Reactor Physics within the Nuclear Science and technology Division, and his group will continue to provide maintenance and development support to SCALE in the areas of cross-section physics and reactor physics.

Brad Rearden, left, and Steve Bowman

Some Parting Words from Steve Bowman

I am grateful for the opportunity to have served as the SCALE Project Leader for the past 14 years. It has been my pleasure to work with an outstanding team of professionals who are not only smart but also fun to work with. The success of SCALE over its 30-year history is due to their dedicated efforts and the faithful support of our sponsors at the NRC and DOE. I also want to thank our users for their support. Providing quality training and technical support to our users was a primary objective during my tenure, and it has been a privilege to meet and interact with many users over the years. I hope that I will continue to see or hear from many of you.

Message from Brad Rearden, SCALE Project Leader

It is my great honor to serve as SCALE Project Leader, continuing the role previously held by Steve Bowman and Cecil Parks before him. Steve and I have worked closely together to provide a smooth transition for our users, sponsors, and developers. I am appreciative to our users and sponsors, and I'm proud of our strong development team and the capabilities they have produced.

"Captain" Rearden and family

SCALE 6.0 provides a powerful and unique toolbox for nuclear safety analysis and design, and we have even more capabilities in the final phases of development for SCALE 6.1, some of which are highlighted in this newsletter.

My initial goal as SCALE Project Leader is to provide an improved user experience with SCALE. We will accomplish this goal by providing state-of-the-art capabilities that are reliable, robust and easy to use. Recently, the SCALE team identified some deficiencies in SCALE 6.0 and issued several updates to the website, which are documented in this newsletter. The SCALE team's goal is to make SCALE 6.1 the most robust and reliable version of SCALE ever released.

We have an extensive training schedule for the spring of 2010, and I hope to see you in one of our sessions in the near future. If you have any questions or comments about SCALE, please contact me at scalehelp@ornl.gov.

New TRITON Code Manager

Mark DeHart has served as the primary developer and code manager for the TRITON reactor analysis capabilities of SCALE since their inception and first release with SCALE 5.0. Mark is well recognized in the international community for his development of TRITON, especially in the area of lattice physics analysis with the NEWT 2-D lattice physics code. Mark's innovation and creativity in the development of TRITON have dramatically advanced the reactor analysis capabilities in SCALE and have led to the use of SCALE by many in the reactor physics community. Many of you may recall that prior to TRITON, SCALE's reactor analysis capabilities were limited to those available in the SAS2 1-D depletion sequence. Since August 2009, Mark has focused his development efforts on algorithms in NEWT and has taken on new responsibilities in spent fuel characterization studies.

To allow Mark to focus on his new responsibilities, Matthew Jessee has assumed the role of TRITON Code Manager for SCALE. Matt joined ORNL in 2008 after receiving his PhD in Nuclear Engineering from North Carolina State University. As part of his doctoral research in BWR lattice depletion, Matt developed an initial implementation of sensitivity and uncertainty analysis capabilities within TRITON. Recently, Matt has transitioned his research into production capabilities for SCALE 6.1, a topic that is described later in this newsletter. Matt has a strong background in reactor physics and has collaborated with Mark in the development of recent enhancements to TRITON that will be released in SCALE 6.1.

Mark DeHart

Matthew Jessee

Preview of SCALE 6.1

The SCALE development team is finalizing a number of enhancements for SCALE 6.1, which will be released in 2010 and will introduce several new tools and important enhancements and improved reliability for the powerful capabilities of SCALE 6.0. The SCALE team is dedicated to providing a robust and reliable software suite for use in nuclear analysis and licensing environments. Several SCALE 6.1 updates are listed here, and detailed explanations of updates to TRITON, MAVRIC, and GeeWiz are provided in subsequent articles in this newsletter.

CENTRM/PMC are improved to provide faster solutions, especially for TRITON depletion calculations.

GeeWiz provides full support for TRITON and STARBUCS as well as all other enhancements to previously supported sequences (e.g., CSAS, MAVRIC, TSUNAMI).

Javapeño provides the ability to plot continuous-energy KENO data and contour plots of NEWT results.

KENO codes provide enhanced output, error messages, and user guidance.

MAVRIC has improved response and source specifications, improved tallies, and improved automation in criticality accident alarm system (CAAS) analysis.

NEWT is improved with parallel capabilities and numerous other enhancements.

ORIGEN provides the use of problem-dependent spectral data in a fine-group structure (e.g., 44, 200, or 238 groups), ENDF/B-VII nuclear data with improved branching fractions and neutron decay modes, improved gamma data, and energy-dependent fission yield libraries.

TRITON is improved with a 1-D depletion sequence option, parallel branching capabilities, and numerous other enhancements.

TSUNAMI is enhanced with a 2D eigenvalue sensitivity analysis capability using TRITON/NEWT named TSUNAMI-2D; 1D and 2D generalized perturbation theory (GPT) capability for reactor physics calculations; 1D fixed-source sensitivity capability; and, for TSUNAMI-3D, improved mesh volume calculations, improved mesh tracking, and updated HTML output.

Continuous energy cross-section data for ENDF/B-VI.8 and ENDF/B-VII.0 are enhanced with improved probability table treatments for the unresolved resonance energy range.

Multigroup cross-section libraries for ENDF/B-VI.8 and ENDF/B-VII.0 are updated with an improved weighting spectrum for improved performance in high-temperature reactor analysis.

The release date for SCALE 6.1 will be set after adequate testing has been performed on all codes and data.

Overview of New TRITON Capabilities for SCALE 6.1

Several new capabilities and methods improvements have been implemented into TRITON for SCALE 6.1. These improvements include the following:

• The new TSUNAMI-2D sequence has been developed for sensitivity and uncertainty analysis using the NEWT transport module for two-dimensional geometries. TSUNAMI-2D performs two eigenvalue transport calculations—one in forward mode and one in adjoint mode – before invoking the SAMS module for sensitivity and uncertainty analysis. Introduced in SCALE 5.0 for the TSUNAMI-1D and -3D sequences, the SAMS module computes sensitivity coefficients of k_{eff} with respect to the nuclear data used in the model, as well as the uncertainty in k_{eff} due to nuclear data uncertainties provided in the SCALE covariance library. With the completion of the TSUNAMI-2D sequence, SCALE now supports a sensitivity and uncertainty analysis capability for each of its multi-group eigenvalue transport modules.

• Although TSUNAMI-2D can be used for criticality safety validation applications similar to TSUNAMI-1D and TSUNAMI-3D, the new sequence was developed to support uncertainty quantification for reactor physics parameters such as reaction rate ratios. To quantify the uncertainty in parameters other than k_{eff}, TSUNAMI-2D employs generalized perturbation theory (GPT) to compute the sensitivity of a system response with respect to nuclear data. Using GPT, TSUNAMI-2D performs additional adjoint transport calculations that include an external adjoint source derived for each user-defined system response. The new input options to define system responses will be provided in the SCALE 6.1 TRITON User's Manual. The new GPT capability is also supported in the TSUNAMI-1D sequence, and has also been applied to generate results for the OECD Uncertainty Analysis Modeling Benchmark.

• A new sequence (T-DEPL-1D) has been developed for 1-D depletion analysis using the XSDRNPM transport module, restoring a pin-cell depletion capability once available with SAS2H. The T-DEPL-1D sequence was designed to offer the same functionality as the T-DEPL sequence, which uses the 2-D NEWT transport module. T-DEPL-1D supports several features of the T-DEPL sequence, including ALIAS block definitions and branch calculations as well as all available geometry configurations in XSDRNPM (slab, cylindrical, and spherical). T-DEPL-1D also supports depletion of doubly heterogeneous fuel designs, and has been tested against other codes for pebble-bed-type fuels.

• TRITON now supports two new parallel computing capabilities. The NEWT transport module can optionally employ multi-threading to decrease the run time of the transport calculation in T-NEWT and T-DEPL sequences. The number of computing threads is defined by the user and has been shown to improve run time by a factor of 1.6 using two cores and more that 2.5 times on four cores for a pressurized-water-reactor assembly calculation. In addition to this multi-threading option, branch calculations can be run simultaneously for the T-DEPL and T-DEPL-1D sequences on Linux and Unix platforms. In the Linux and Unix distribution of SCALE 6.1, an auxiliary program called RUNNER is provided. RUNNER is invoked by TRITON to manage and send branch calculations to available computing nodes specified by user input.

• Several other enhancements to TRITON have been implemented. All depletion sequences have been integrated with the new multigroup ORIGEN-S libraries described in the July 2009 Newsletter. The use of the new multigroup ORIGEN-S libraries allows for the use of problem-dependent detailed flux spectra to prepare ORIGEN-S cross sections as opposed to the use of pretabulated three-group ORIGEN-S libraries in earlier versions of SCALE. In NEWT, hexagonal-based geometry modeling has been significantly improved with the implementation of a new coarse-mesh finite-difference acceleration algorithm to decrease run time and provide support for reflective and periodic boundary conditions on nonrectangular global boundaries.

Improvements for MAVRIC in SCALE 6.1

For SCALE 6.1, enhancements in MAVRIC provide the user more-flexible input and several new source specification capabilities. All these items will help make MAVRIC easier to use for more-complex problems.

Responses – Users will be able to define responses as binned histograms or as value/function pairs, use interaction cross sections directly from the cross-section library, and generate response plots for easy input verification.

Source Specification – Enhanced capabilities include multiple source specification, with biased sampling available; user-defined distributions that can be used for space, energy, and angle distributions; distributions defined as binned histograms or as value/function pairs; special distributions including Watt, axial fuel profiles, and data from an ORIGEN-S calculation; generation of distribution plots for easy input checking; and generation of mesh-based versions of each source for easy input checking.

Tallies – Users will be able to include scalar multipliers for each tally or all tallies (for unit conversions, etc.); limit the sampling of point detectors, based on weight windows; view six statistical checks on each tally, including the behavior of the mean, the relative variance, and the relative uncertainty of the variance; specify sampling parameters to improve point detector tallies; and specify a material limiter in mesh tallies (for reaction rate calculations).

Criticality Accident Alarm Systems (CAAS) – Enhancements include more automation and improved fission photon accounting.

Other improvements include more keywords for easier grid geometry specification, generation of geometry/mesh files for easy input checking, an ability to create 2-D geometry *.png files using a "READ PLOT" block like KENO, keywords to optionally reduce the file sizes of mesh-based sources and mesh tallies, and default weight windows if none are specified.

The "macromaterial" feature will create a homogenized material for each voxel in the Denovo S_N calculation. This will provide more accurate importance map, which will give better figures of merit in the Monte Carlo calculation.

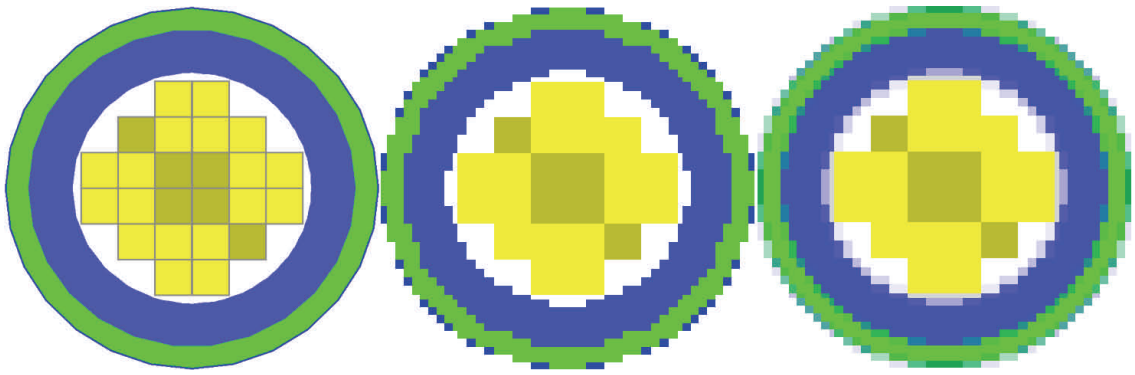
Changes have been made to the MeshFileViewer to show the macromaterials used by the Denovo S_N code.

Users can easily use a coarse-group library for the importance calculations and a fine-group library for final forward Monaco calculation in one input file.

Changes to the forward weighting capability make it easier to use and optimize different responses in one simulation.

SCALE 6.1 will also include a new set of Monaco/MAVRIC-related utility programs for convenient processing of data files.

The SCALE 6.1 sample problems for Monaco, MAVRIC have been updated to demonstrate the new features. These improvements were funded by the Office of Nuclear Material Safety and Safeguards, Division of Spent Fuel Storage and Transportation of the U.S. Nuclear Regulatory Commission (NRC).



Geometric representation of a spent fuel cask: (a) Monte Carlo geometry, (b) Denovo geometry using cell-center testing, and (c) Denovo geometry using the new macromaterial feature.

GeeWiz Enhancements for SCALE 6.1

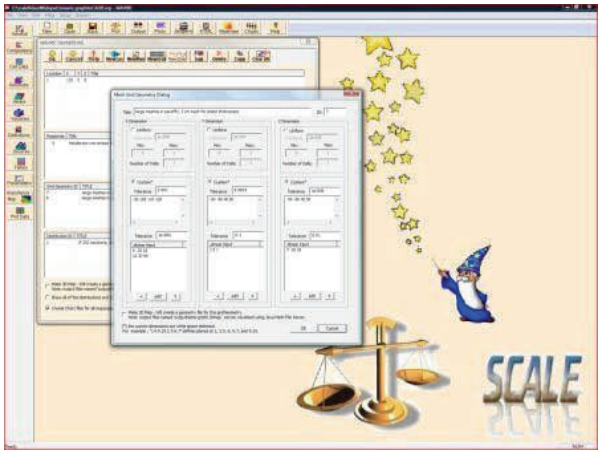
GeeWiz allows SCALE users to create, edit, and execute a SCALE input file for most of the SCALE sequences including CSAS, MAVRIC, and TSUNAMI. Active development is leading to a more complete SCALE user experience. Thanks to the feedback of users from around the world, GeeWiz will provide a more stable and intuitive interface.

Noticeable enhancements include the following:

- Full support for TRITON, including 2-D depletion with NEWT.
- Updated MAVRIC sequence support allowing:
  1. Response functions using cross sections from libraries
  2. Simplified grid-geometry input methods
  3. Support for distributions
  4. Referencing distributions from defined sources
  5. Mesh source saver functionality, allowing for source visualization
  6. 2-D geometry plot capability
  7. Unit multipliers for tallies
  8. Ability to limit a mesh tally by unit, region, or material
  9. Support for forward-weighting the adjoint sourcee
- 2D sensitivity analysis using the new TSUNAMI-2D and TSUNAMI-2DC sequences
- Full support for burnup credit using the STARBUCS sequence
- Support for generalized perturbation theory calculations with TSUNAMI-1D and –2D.

The following sequences, listed by functional area, are supported by GeeWiz in SCALE 6.1:

- 1D transport: CSAS1, SAS1, T-XSDRN
- 2D transport: T-NEWT
- 3D eigenvalue Monte Carlo with KENO-V.a: CSAS5, CSAS5S
- 3D eigenvalue Monte Carlo with KENO-VI: CSAS6
- 3D fixed-source Monte Carlo with Monaco: MAVRIC
- ID sensitivity analysis: TSUNAMI-1D, TSUNAMI-1DC
- 2D sensitivity analysis: TSUNAMI-2D, TSUNAMI-2DC
- 3D sensitivity analysis: TSUNAMI-3D-K5, TSUNAMI-3D-K6
- Depletion: T-DEPL, T5-DEPL, T6-DEPL, T-DEPL-1D
- Burnup credit: STARBUCS
- Cross-section processing: CSASI, CSAS-MG, T-XSEC
- Material optimization: SMORES

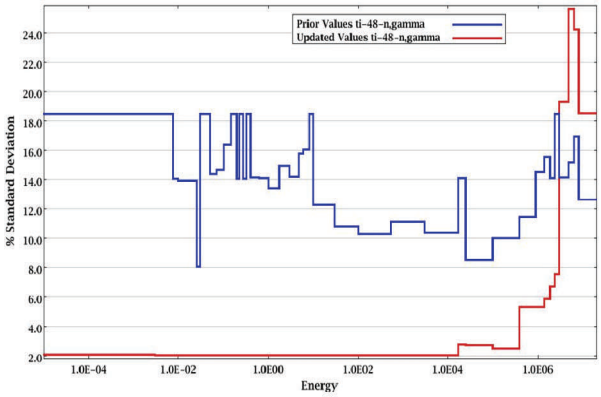


GeeWiz for SCALE 6.1 with new MAVRIC definitions and grid geometry input

SCALE 6.0 Updates Available for Download

Several important updates were recently posted to the SCALE Download page at: http://www.ornl.gov/sci/scale/scale6_updates.htm Please visit the website to review and install the enhancements to SCALE.

Covariance Library Update for ^{48}Ti



Standard deviation in ^{48}Ti n,gamma.

The covariance data for ^{48}Ti distributed with SCALE 6.0 were based on the best-available prerelease ENDF/B-VII data. Since this release, new data have become available that offer improvements to the previous version. This update of the SCALE 44GROUPCOV library includes improved evaluation for ^{48}Ti for the following reactions: total; n,n'; n,2n; n,gamma; n,p; and n,alpha. New data are now available for the following reactions: elastic scattering; n,n'alpha; and n,n'p. Additionally, cross-reaction covariance data are available for elastic to total; elastic to n,n'; elastic to n,2n; elastic to n,n'alpha; elastic to n,n'p; elastic to n,gamma; elastic to n,p; elastic to n,alpha; and n,gamma to total.

For the updated covariance data, the uncertainties are generally reduced relative to the previously reported values. The standard deviation in the group-wise values for ^{48}Ti n,gamma for the prerelease and updated libraries is shown in the accompanying figure. Note that the uncertainties at thermal energies have decreased from approximately 18% to approximately 2%. After installing this update, TSUNAMI calculations with ^{48}Ti will reflect more-accurate uncertainty values. In an sample system, the uncertainty in k_{eff} due to ^{48}Ti n,gamma was reduced from 2.66% Δk/k to 0.68% Δk/k.

Coupled Library Update for Ambient Dose Equivalent Rates

In addition to the dose functions for neutrons and gammas, the three shielding libraries (200n47g for ENDF/B-VI.8 and ENDF/B-VII.0 and 27n19g for ENDF/B-VII.0) also contain coupled dose functions that combine the neutron and gamma doses into one MT value for ease of use. Two of these combined dose functions (MT=9734 and MT=9735) were coupled incorrectly in the libraries distributed with SCALE 6.0. This update corrects the coupling. Calculations using the component of "ambient dose equivalent (ICRU-57)" rates (using MT=9734 or 9735) will change. For rates calculated with MT=9734, the photon component will be about a factor of 100 smaller. For rates calculated with MT=9735, the photon component will be about a factor of 100 higher. The impact on the total dose equivalent rate will depend on the relative contributions of the neutron and photon components in the calculation.

KMART5 / KMART6 (TRITON/KENO Depletion)

A error was identified in the KMART5 and KMART6 modules that impacts the **TRITON/KENO T5-DEPL** and **T6-DEPL** calculations. The error involved processing cross sections used to determine mixture powers for the depletion calculation. In general, if a mixture is used only in a single region of the KENO model, the results are correct. However, if the mixture is used in more than one region, the results are unpredictable. The impact of the error is problem dependent, so T5-DEPL and T6-DEPL calculations should be reevaluated using the updated versions of KMART5 and KMART6. This error has also been identified in the SCALE 5.0 and SCALE 5.1 versions of TRITON, but this patch applies only to SCALE 6.0. It is recommended that SCALE 5 users upgrade to SCALE 6.0.

TRITON

An error was found in the TRITON control module when writing the NEWT material block in the input file for the NEWT functional module using the new advanced material format. With this update, problems that previously failed to run will now work correctly.

Continued on page 8

SCALE 6.0 Updates Available for Download (Cont.)

TSURFER
TSURFER was updated to support features of the Intel Fortran Compiler (rev 11.1) on Mac computers. An error occurred with formatted write statements in the file outpt.f90. These write statements have been updated so that the TSURFER compiles correctly using the new compiler. This update includes other minor revisions to additional files to limit line lengths to 132 columns. Previous calculations are not affected by this update.

GeeWiz
Several updates were made to the GeeWiz Windows interface to improve functionality and reliability. Most significantly, GeeWiz now provides full support for the TRITON sequences **T-XSEC**, **T-DEPL**, and **T-NEWT** in addition to its previous support for T5-DEPL and T6-DEPL.

ORIGENARP GUI, USLSTATS, and VIBE
Each of these codes was updated for improved functionality and reliability.

SCALE Resource File
A file used to set user preferences for HTML output (*.scalerc)* was inadvertently omitted from the SCALE 6.0 distribution. This file is installed with this update. Users can edit the file to set preferences for colors and other aspects of the HTML output. In future SCALE releases, this file may offer users other setting options for the computational modules of SCALE. This file is installed in *scale6/data/.scalerc*.

Windows .Bat Files
On some Windows Vista systems, users have reported problems launching the Java applications Javapeño, USLSTATS, and VIBE. The .bat files used to launch these applications have been modified to provide improved performance.

KENO3D
This update provides several important functionality improvements and "bug fixes" and is recommended for all users of KENO3D. The improvements include recognition of SCALE 6.0 sequence names and their respective geometry types, a more-descriptive message for zero-volume units, and proper treatment of the TSUNAMI "center" keyword input.

Enhancements and Corrections to SCALE 6

Click here to see a summary of code and data modifications that have been made to the configuration-controlled version of SCALE at ORNL since the previous issue of the *SCALE Newsletter*. These will be included in the SCALE 6.1 release.

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Words to the Wise . . . TRITON User Notice

TRITON provides powerful depletion capabilities by coupling ORIGEN-S with NEWT or KENO for lattice physics or Monte Carlo depletion calculations. With the rapid evolution of these methods and a growing user base with a diverse set of applications, several deficiencies have been identified that affect a subset of the overall capabilities of TRITON. Some issues are resolved with updates available on the SCALE website, while others will be corrected in future releases or updates.

Guidelines on T5-DEPL and T6-DEPL Modeling in TRITON/KENO Depletion

Certain KENO data blocks (PLOT, VOLUME, START) do not function or function incorrectly for TRITON depletion problems. Plot files can be generated for the model geometry by using the CSAS5 and CSAS6 sequences. Without access to the VOLUME block for T6-DEPL calculations, the ***vol=*** keyword should be used to specify volumes as part of the media definition record in the GEOMETRY block. These volumes can be determined by KENO3D (*SCALE Newsletter*, January 2006, p. 4) or from the output of a CSAS6 calculation. Because the START block does not function, TRITON always uses a default uniform neutron distribution for the KENO calculation.

Certain keywords have limited functionality in T5-DEPL and T6-DEPL. In the KENO PARAMETER block, the ***npg=*** keyword should be less than 100,000 histories per generation. In the COMPOSITION and CELLDATA blocks, all mixture numbers should be less than 512. In the KENO BOUNDS block, albedo boundary conditions do not function properly. KENO models should be modified to include albedo materials in the problem geometry, and vacuum boundary conditions should be utilized.

An error was identified in the KMART5 and KMART6 modules, impacting T5-DEPL and T6-DEPL calculations, and a patch for SCALE 6.0 has been posted to the SCALE Download web page. The error involved processing cross sections used to determine mixture powers for the depletion calculation. The impact of the error is problem dependent, so T5-DEPL and T6-DEPL calculations should be reevaluated using the updated versions of KMART5 and KMART6. The cross-section processing error has also been identified in the SCALE 5.1 and SCALE 5.0 versions of TRITON. SCALE 5 users should upgrade to SCALE 6.0 and use the module updates available on the SCALE website.

Other TRITON and NEWT Issues

An error was identified in processing the ALIAS block in TRITON. If the ALIAS block is used, all blocks of data used in the input should be terminated with a lowercase ***end*** keyword. If the ALIAS block is not used, the ***end*** keyword is case insensitive (i.e., *end, End*, *END*, etc., are acceptable). In SCALE 6.1, all ***end*** keywords are case insensitive, regardless of whether the ALIAS block is used.

A problem was identified in cross-section processing calculations for all TRITON depletion sequences. At the beginning of each transport calculation, TRITON calls a SCALE Material Input Processor LIBrary (MIPLIB) subroutine to calculate Dancoff factors and other parameters used in the cross-section processing calculations. For some lattice configurations, TRITON passes data incorrectly to the MIPLIB subroutine, which leads to incorrect Dancoff factors and other resonance self-shielding parameters. The error impacts only certain configurations, mostly those involving annular cells. All slab configurations and most standard non annular lattice configurations are not affected.

Periodic boundary conditions in TRITON/NEWT are not implemented and will produce the same results as vacuum boundary conditions.

Finally, a few output edits in TRITON and NEWT present misleading information. For the delayed neutron group edit in NEWT, the column headings for *Decay Constant* and *Beta Fraction* are reversed. The numeric values in the *Decay Constant* column are actually the delayed neutron fractions. Likewise, the numeric values in the *Beta Fraction* column are the decay constant values. For the homogenized few-group cross-section edit—both in the NEWT output and in the xfile016 cross-section database, users should be aware of issues involving the few-group homogenized cross sections. The homogenized few-group diffusion coefficients and the transport cross sections are computed using the so-called inscatter approximation method. As documented in the NEWT manual, groupwise diffusion coefficients can be negative for light elements in some problems. Additionally, there is a minor error in the calculation of collapsed nu-bar and fission cross-section values. The errors in these cross sections were on the order of 1% for a light-water-reactor assembly and less than 1% for a high-temperature gass-cooled reactor prismatic assembly. It is important to note that the "nu times fission" cross section is calculated correctly.

All these issues will be corrected in SCALE 6.1, and as many as possible have been or will be corrected in pending updates on the SCALE website.

Words to the Wise . . . Considerations for Criticality Searches with CSAS5S

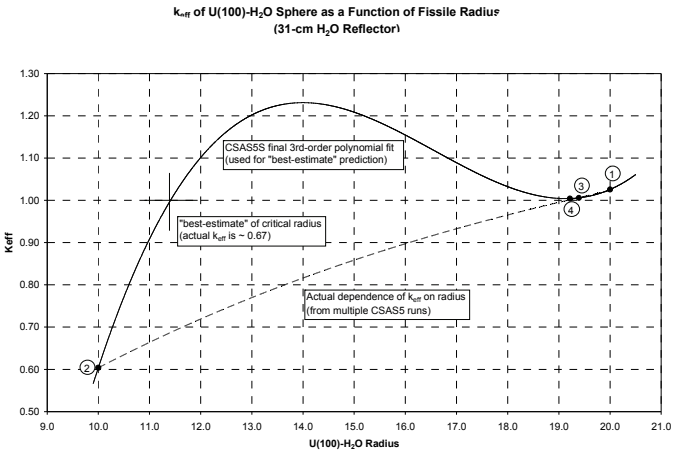
A SCALE user recently sent an inquiry to SCALE Help scalehelp@ornl.gov regarding an unexpected result from a CSAS5S critical search case. The intent was to determine the critical radius for a water-reflected sphere of an idealized homogeneous mixture of ^{235}U and H_2O.

As shown in an edited excerpt from the output below, convergence occurred on the fourth pass through CSAS5S/KENO-V.a. A fissile radius of 19.216 cm was found to have a computed k_{eff} value (1.00425) that was within the tolerance factor (EPS=0.005) of the desired k_{eff} value (1.000). However, CSAS5S provided a much-different "best-estimate" prediction for the critical fissile radius (11.413 cm). The best-estimate prediction has a computed k_{eff} value of ~0.67.

```
**********************************************************************************
 convergence was achieved on pass  4  the parameter was  -3.92153E-02
 the equation used in the search was:
 k-eff = +1.02569E+00 +1.04669E+00*p +1.38002E+01*p**2 +2.67883E+01*p**3

 k-effective=  1.00425E+00 + or -  1.83701E-03   the corresponding geometry follows:

    ******************  global  ******************
          -----  unit    1  -----
    1 sphere        1  1  radius =  19.216
    2 sphere        2  1  radius =  50.216
**********************************************************************************************
 based on the preceding data, the best estimate of the parameter is   -4.29355E-01
the geometry corresponding to this parameter follows:

    ******************  global  ******************
          -----  unit    1  -----
    1 sphere        1  1  radius =  11.413
    2 sphere        2  1  radius =  42.413
**********************************************************************************
```

This poor prediction results from a combination of factors, including the initial radius guess, the search limits, and use of default CSAS5S parameters such as EPS, GEN, and NPG. When these factors combine such that convergence occurs on the fourth pass, and the uncertainties for the k_{eff} values for each pass are comparable to the k_{eff} difference between the third and fourth passes, a poor best-estimate prediction can result.

The figure below illustrates how this occurred. Point 1 (number inside a circle)



illustrates the k_{eff} result for the first CSAS5 pass (initial radius guess), Point 2 represents the lower parameter limit (lower limit for radius), and Points 3 and 4 are close to the "correct" critical radius for passes 3 and 4. Also, the k_{eff} results for Points 3 and 4 are very close. The variability of computed k_{eff} values for Points 3 and 4 leads to a third-order polynomial fit that differs significantly from the actual relationship of k_{eff} to the radius. Hence, the "best-estimate" root is for dimensions significantly different than for the final CSAS5 pass.

This example highlights an important note for all users performing criticality searches using CSAS5S:

> ***Always verify that the best-estimate prediction and the configuration used by the final CSAS5 pass are consistent.***

This problem can usually be resolved by reexecuting the CSAS5S case with increased values for GEN and/or NPG, a reduced value of EPS, or both.

Further explanation of the above example is provided on page 36 of the SCALE 6 Notebook. Also included is guidance for CSAS5S problems where no root is found (although there is a valid root), and problems involving multiple valid roots.

Words to the Wise … MULTIREGION Unit Cell Calculations

One of the unit cell types available in SCALE is MULTIREGION, which is used to define a unit cell to be used in resonance self-shielding calculations by BONAMI, NITAWL, and CENTRM/PMC. A MULTIREGION cell is usually used when the cell type does not meet the requirements for LATTICECELL, INFHOMMEDIUM, or DOUBLEHET. Although not common, occasionally one may want to break a region in the problem into many smaller subregions to obtain better tallies or, in the case of sensitivity/uncertainty calculations, to obtain better sensitivities as a function of radial distance. SCALE calculates the Dancoff factors describing the geometric interaction probabilities for each region based on the dimensions of the region, the nuclides in that region, and the nuclides in the other region(s) of the cell for use in BONAMI and NITAWL. The algorithm implemented in SCALE for Dancoff factor calculations assumes that a given nuclide will not appear in more than one cell. If a region is subdivided into subregions of the same material, the calculated Dancoff factors will most likely not be accurate, depending on the nuclides, corresponding nuclide densities, and region and subregion dimensions. If the actual problem contains adjacent absorber (fission is also an absorption event) regions that are not the same mixtures (e.g., highly enriched uranium next to low-enriched uranium or mixed oxide) and the MULTIREGION cell is used for resonance self-shielding correction, the Dancoff factors may be in error. The latest SCALE multigroup cross-section libraries contain full-range Bondarenko factors that are modified by BONAMI based on the problem-dependent materials and Dancoff factors. For ENDF/B-VI and ENDF/B-VII calculations, CENTRM/PMC provides resonance self-shielded cross sections through most of the multigroup cross-section energy range, reducing the dependence on the Dancoff factors used by BONAMI in the unresolved resonance energy range. On rare occasions, the energy groups treated with BONAMI may contain cross sections processed with inaccurate Dancoff factors that may result in error in calculated k_{eff} values. For sensitivity calculations, the implicit effects may be incorrect, which can cause the sensitivities to be inaccurate. There is no absolute rule about what type of systems may be affected.

SCALE 6.0 does not allow users to override the internally calculated Dancoff factors when CENTRM is used for resonance self-shielding. The purpose of this restriction is to protect users from inadvertently obtaining erroneous results by using pre–SCALE 5 input files with SCALE 5 and above. Before SCALE 5, one could explicitly define only one unit cell. All other mixtures had to be resonance self-shielded using MORE DATA entries RES and DAN, where RES defines the mixture number, geometry type, and dimension while DAN defines the Dancoff factor. Because these entries are ignored when CENTRM is used with SCALE 5 and later, a restriction was implemented to alert users to update the input. In SCALE 6.1 this restriction will be relaxed to allow users to precompute Dancoff factors for multiregion unit cells that use similar materials in multiple zones and enter them with the DAN keyword for use in BONAMI. Note that the RES keyword will continue to trigger an error, preventing the use of pre-SCALE 5 input.

If the objective is to obtain more-detailed flux distributions, there is no need to subdivide the cell regions in the unit cell definitions. One may simply subdivide the actual problem geometry in the transport code (KENO, NEWT, or XSDRN) and use the same mixture number. The transport code will compute the region-wise fluxes (if requested). Likewise, region-wise nuclide sensitivities may be obtained without subdividing the regions in the multiregion unit cells. The self-shielding calculations may not be as accurate as those from subdivided region calculations for thick absorber regions surrounded by moderators (rim effect). However, the effect on calculated region-wise sensitivities should be reasonably small.

Following are some guidelines for users who wish to subdivide their MULTIREGION unit cell regions for more-detailed tallies or sensitivities, or if their MULTIREGION cell definition contains adjacent regions with different absorber mixtures.

Continued on page 12

Words to the Wise … MULTIREGION Unit Cell Calculations (Cont.)

For SCALE 6.0:

1. If some cell regions are subdivided, run the original problem and the subdivided problem in the multigroup mode using a reasonable number of total histories (i.e., no need to obtain very small standard deviations). If the k_{eff} values agree, stop and proceed with the subdivided model.

2. Run the original problem in the continuous energy mode to establish the expected k_{eff} value. If some cell regions are subdivided and if the calculated k_{eff} from the subdivided multigroup mode case agrees with the continuous energy mode k_{eff}, stop and proceed with the new subdivided model. If the cell definition contains adjacent absorber regions and the calculated k_{eff} from the multigroup mode case agrees with the continuous energy mode k_{eff}, stop and proceed with the original model.

3. If some cell regions are subdivided and results of steps 1 or 2 are inconsistent, do not use subdivided regions in the MULTIREGION cell definition.

4. If the cell definition contains adjacent absorber regions and the k_{eff} values from multigroup and continuous energy calculations do not agree, contact scalehelp@ornl.gov.

For SCALE 6.1 (to be released later in 2010):

1. Run the original problem and the subdivided problem in the multigroup mode using a reasonable number of total histories (i.e., no need to obtain very small standard deviations). If the k_{eff} values agree, stop and proceed with the subdivided model.

2. Run the original problem in the continuous energy mode to establish the expected k_{eff} value. In the MORE DATA section (multigroup calculation) for that cell, enter DAN(X)=1 for each mixture X in the cell and calculate the k_{eff}. If the calculated k_{eff} agrees with the original multigroup k_{eff} or the continuous energy mode k_{eff}, stop and proceed with the new subdivided model.

3. Calculate the Dancoff factors using the definitions in the SCALE manual, Section M7.2.5.4, and redo the multigroup calculation in step 2 with these calculated Dancoff factors. If the calculated k_{eff} agrees with the original multigroup k_{eff} or the continuous energy mode k_{eff}, stop and proceed with the new subdivided model.

4. If agreement cannot be achieved, contact scalehelp@ornl.gov.

Spring 2010 SCALE Training Courses

Date	Title	Location	Registration Fee
March 8-12, 2010	SCALE Criticality Safety and Shielding Course (KENO-VI/MAVRIC)	ORNL Oak Ridge, TN USA	$2000*
March 15-19, 2010	SCALE Lattice Physics and Depletion Course (ORIGEN-ARP/TRITON)	ORNL Oak Ridge, TN USA	$2000*
March 22-26, 2010	SCALE Sensitivity/Uncertainty Tools Course (TSUNAMI) (Experienced KENO users only)	ORNL Oak Ridge, TN USA	$2000*
April 29-30, 2010	Advanced Sensitivity and Uncertainty Analysis Techniques for Criticality Code Validation	OECD/NEA Data Bank Issy-les-Moulineaux (Paris), France	€1000
May 3-7, 2010	SCALE Criticality Safety and Shielding Course	OECD/NEA Data Bank Issy-les-Moulineaux (Paris), France	€1000

*A discount of $200 for each additional week of training will be applied for registration in multiple courses.

Foreign National Visitors: You MUST register at least 40 days in advance to obtain security clearance, and payment MUST be received at least one week prior to training course.

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For more information and online registration, please visit
http://www.ornl.gov/sci/scale/training.htm

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