Oak Ridge National Laboratory

SCALE Newsletter

Number 31 January 2005

Special points of interest:

- SCALE 5.1 scheduled for 2005
- SCALE workshops in March/April at ORNL; $300 discount until February 28.

Inside this Issue:

Advances in SCALE Development

Significant development efforts continue to be made in the SCALE software system since the release of Version 5 in June 2004. This article highlights some of the advances that are being made in SCALE. There will be a special session on this topic at the American Nuclear Society (ANS) meeting in San Diego, June 5-9, 2005.

Version 5.1

Several improvements that have recently been completed as part of ORNL's ongoing development activities will be included in Version 5.1 of SCALE, which is scheduled for release in 2005.

ENDF/B-VI Data

ENDF/B-VI cross-section libraries, both multigroup and continuous energy, have been developed and tested and will appear in SCALE for the first time in Version 5.1. A 238-group library, corresponding to the SCALE 238-group ENDF/B-V energy-group structure, and continuous-energy cross sections for the CENTRM one-dimensional (1-D) discrete-ordinates resonance-processing code will be included.

HTML Output

An advanced HTML-formatted output interface has been developed for the Monte Carlo code KENO V.a. In addition to easily navigated and color-coded tables of data, interactive plotting capabilities are available. A version of the SCALE 5 data plotting code Javapeno has been developed that executes within the web browser as a Java applet. Javapeno compatible data files are created by KENO V.a. so that the user may view data in colorful, interactive, and

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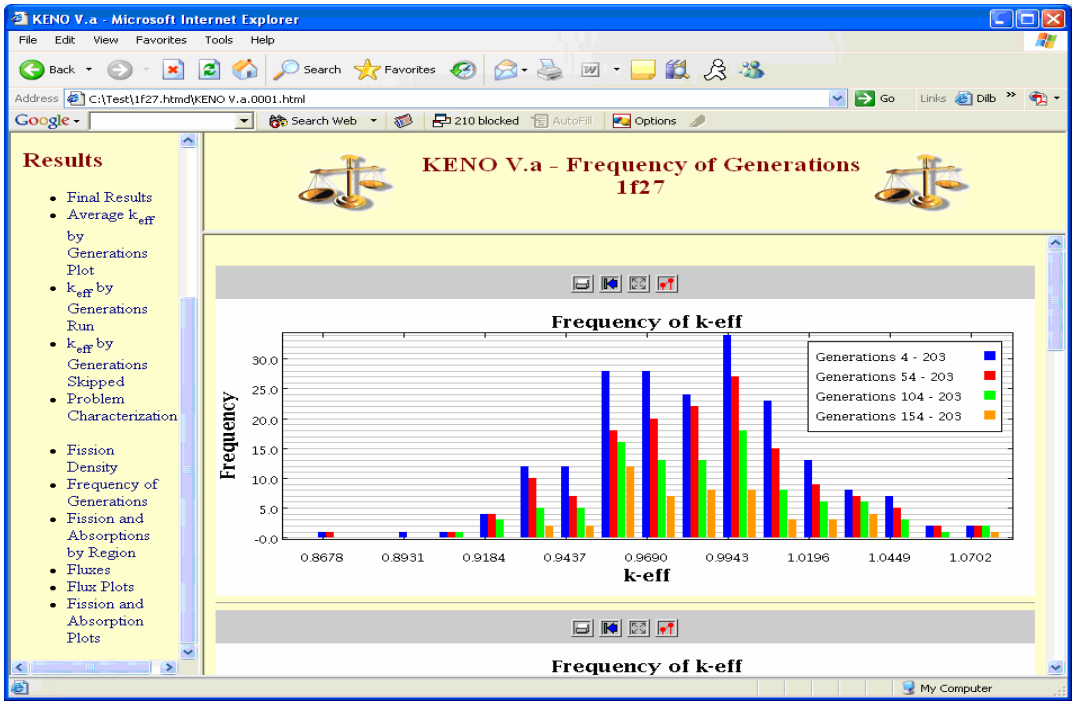

Fig. 1 KENO Frequency of K-eff plot in HTML output.

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customizable plots (Fig. 1).

CENTRM
- New two-region approximation allows faster self-shielding computations for many problems.

- Unit cell calculations for doubly heterogeneous fuel lumps.

CENTRM

The introduction of ENDF/B-VI data in SCALE 5.1 will rely heavily on using continuous-energy CENTRM transport calculations instead of NITAWL for resonance self-shielding. (The CPU time required by NITAWL with ENDF/B-VI data is excessively long.) Several important improvements are being made to the CENTRM/PMC codes and the SCALE calculational sequences. The enhancements include improved physics approximations and numerical procedures; more accurate techniques to treat nonuniform arrays and doubly heterogeneous fuel lumps; and a new two-region approximation that allows faster self-shielding computations for many conventional types of problems.

TRITON

The TRITON fuel depletion module in SCALE 5 has received major upgrades, including the capability to perform three-dimensional (3-D) depletion calculations using the KENO V.a or KENO-VI Monte Carlo codes. In addition, the geometry input for NEWT, the discrete-ordinates code used by TRITON for 2-D depletion, has been replaced with the more versatile SCALE Generalized Geometry Package (SGGP) in KENO-VI. This upgrade improves the portability of input between NEWT and KENO, makes NEWT input for arrays easier, and reduces the input learning requirements for users. (See TRITON article on page 4.)

MONACO
A new general-purpose 3-D Monte Carlo radiation shielding code. Benchmark comparisons vs. MCNP show good agreement and faster execution.

TSUNAMI

New and enhanced TSUNAMI (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation) capabilities for criticality safety in SCALE 5.1 provide a number of advantages over the SCALE 5 implementation. The improved capabilities include

1. analysis of models with more than 50 nuclides with resolved-resonance data;

2. assessment of uncertainty with an improved cross-section covariance data library;

3. processing of ENDF/B-V and -VI data with the new sensitivity version of CENTRM known as CENTRMST; and

4. estimation of biases and uncertainties with TSURFER [Tool for Sensitivity/Uncertainty (S/U) Analysis of Response Functionals using Experimental Results], a generalized linear least-squares computational tool that combines computed and measured benchmark results and provides an estimate for the computational bias and uncertainty.

Beyond SCALE 5.1

Other important development activities under way will not be completed before the release of SCALE 5.1 but are expected to be available in the subsequent version of SCALE.

Continuous Energy KENO

Continuous-energy versions of KENO V.a and KENO-VI have been developed and successfully tested with prototype cross-section data. Additional work remains to improve the efficiency of these codes in both CPU time and memory requirements. Also, the KENO continuous-energy cross-section data are currently limited to only 50 nuclides, each at only one temperature. These data need to be tested thoroughly prior to creating a complete KENO continuous-energy ENDF/B-VI library of all nuclides at multiple temperatures.

MONACO

A new general-purpose 3-D Monte Carlo radiation shielding code named MONACO is currently under development. Notable improvements have recently been made in the particle tracking efficiency. Testing and validation of MONACO have been performed using benchmark problem comparisons with MCNP. Good agreement has been achieved between the two codes. In addition to comparing the neutron fluxes calculated by MCNP and MONACO, the CPU times were compared. In this series of benchmarks, for the same number of histories in each code, the CPU time used by MONACO was notably less than that for MCNP. Additional work remains to be done to implement a 3-D automated variance-reduction scheme that has been previously demonstrated with MCNP.

GEMI-NEWTRN

Another development is focused on eliminating approximations used in current resonance treatments by developing continuous-energy multidimensional transport methods for problem-dependent self-shielding calculations. A new code is being developed that utilizes

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the continuous-energy resonance treatment in CENTRM and the two-dimensional (2-D) discrete-ordinates solver NEWT. This new code, GEMI-NEWTRN (Group and Energy-Pointwise Methodology Implemented in NEWT for Resonance Neutronics), performs continuous-energy, multidimensional resonance self-shielding calculations. Preliminary application to an advanced heterogeneous boiling-water-reactor lattice indicates that the problem-specific 2-D resonance self-shielding calculation may have an impact on the prediction of the lattice spectrum.

STARBUCS

The STARBUCS burnup credit sequence in SCALE 5 is being enhanced by the development of an automated search sequence that will perform iterative STARBUCS calculations to generate a burnup/ enrichment loading curve for loading spent fuel in casks or storage pools.

DORT/TORT

DORT and TORT are 2-D and 3-D, respectively, discrete-ordinates radiation transport codes that were developed at ORNL and are used nationally and internationally, primarily for radiation protection and shielding analyses. Despite their recognized capabilities and numerous organizations' reliance on these codes for bulk shielding analyses, DORT and TORT have not been actively developed or improved in many years. As a result, the codes are in need of modernization and enhancement, particularly in terms of their user-friendliness. Therefore, efforts have been initiated to address these needs. DORT and TORT have been converted from FORTRAN 77 to FORTRAN 90, and additional related programming modernization is under way. Because the capability exists in SCALE 5 to generate problem-dependent cross sections for use by DORT and TORT, the next planned step is to develop a user-friendly SCALE sequence based on TORT.

Improved BONAMIST and NITAWLST Codes for TSUNAMI

TSUNAMI
Limit of 50 resonance nuclides removed from NITAWLST in SCALE 5.1.

One obstacle occasionally encountered in TSUNAMI sensitivity/uncertainty analyses is the limit of 50 nuclides with resolved-resonance data in a system model. This limit is imposed by the NITAWLST code, which produces resonance self-shielded cross sections and their sensitivities to input data, a.k.a. "implicit sensitivities." The 50-nuclide limit was partially imposed by limitations in the GRESS software used for automatic differentiation in NITAWLST. An updated version of GRESS has been developed that increases the previous number of allowed independent parameters from 200 to 10,000. Additionally, the updated version of GRESS provides automatic differentiation of a subset of Fortran 90 source code, whereas the implementation of GRESS used with SCALE 5 would process only Fortran 77. An updated NITAWLST code developed with the new version of GRESS has no limit on the number of nuclides in the system model. Additionally, an updated BONAMIST code, used for producing resonance self-shielded cross sections and their sensitivities to input data for the unresolved-resonance region, has been developed with the new version of GRESS. Although less restrictive than NITAWLST, the SCALE 5 version of BONAMIST limited analyses to a sum of nuclides and mixtures not exceeding 200. The updated BONAMIST increases this limit to a sum of nuclides and mixtures in a single unit cell not exceeding 10,000. The improved versions of BONAMIST and NITAWLST will be available with SCALE 5.1.

New 3-D and Improved 2-D Depletion with TRITON

TRITON/KENO
3-D Monte Carlo depletion option available in SCALE 5.1.

NEWT
- More versatile SGGP geometry package.

- Computational efficiency substantially improved.

Increasing complexity in reactor designs is beginning to require robust geometric modeling capabilities to represent neutron transport in complex configurations. Monte Carlo transport methods offer the flexibility needed for such applications. Two new TRITON automated depletion sequences have been developed to perform Monte Carlo-based depletion using KENO V.a and KENO-VI and are planned for release in SCALE 5.1.

The SCALE utility codes KMART and KMART6, originally developed to post-process KENO calculations, have been adapted to provide collapsed cross sections and fluxes required by TRITON for setting up ORIGEN-S depletion calculations. The KENO restart capability is used to provide an improved starting source for each depletion step, thus further improving calculation times. Ongoing work seeks to study and implement methods using variance reduction techniques to improve the efficacy of iterative depletion based on Monte Carlo transport solutions. Error propagation from the results of Monte Carlo simulations is planned as a key part of the system.

Benchmark calculations have been performed using pressurized water reactor fuel assembly data provided in validation reports of the 1-D SAS2 depletion sequence in SCALE. Benchmark models of the spent fuel assemblies have been developed with both TRITON/KENO V.a (TRITON-K5) and TRITON6/KENO-VI (TRITON-K6). The calculated results compare well with the measured radiochemical spent fuel assay data and previously calculated SAS2 and TRITON/NEWT (TRITON-2D) results. The validation cases are standard benchmarks to ensure that the Monte Carlo codes have been properly incorporated into the TRITON depletion methodology. Further validation is planned using cases that specifically require 3-D representation to obtain accurate results.

NEWT remains a key element of TRITON. NEWT has continued to evolve as a 2-D deterministic transport solver, and has been demonstrated to be valuable in light water reactor fuel assembly depletion analysis and in generating time-dependent lattice physics parameters for nodal code reactor simulator calculations. NEWT's geometry processing capabilities have been significantly enhanced, providing improved stability in grid generation over the initial release. Input for the new geometry package is a 2-D version of the SCALE Generalized Geometry Package (SGGP) that is used by KENO-VI. NEWT input will be easily generated by users familiar with KENO-VI geometry specifications. The former geometry package will be supported in this update to SCALE but will eventually be phased out.

Another significant improvement in NEWT is a coarse-mesh finite-difference (CMFD) accelerator implemented in the iterative solution. Use of this option considerably increases convergence; speedups of a factor of 10 or more have been measured for lattice calculations with large adjacent reflectors. With CMFD and other optimizations added to NEWT, speedups of a factor of two or more are commonly observed. Multiple enhancements have been made relative to generation of lattice physics parameters. Numerous modifications have been made to help overcome convergence issues for certain classes of problems. Periodic boundary conditions have been added to NEWT, and support has been added for a "white" non-absorbing medium to apply a white boundary condition to non-rectangular problem boundaries.

A paper on the TRITON-K5 and TRITON-K6 sequences will be presented at the Monte Carlo 2005 Topical Meeting in Chattanooga, Tennessee, on April 17–21, 2005. A paper on lattice physics calculations coupling TRITON and the advanced reactor core simulator code PARCS for MOX core-follow calculations will be presented at the ANS Annual Meeting in San Diego, California, June 5–9, 2005.

Important ORIGEN-S Updates *(revised March 7, 2005)*

The following updates for ORIGEN-S in SCALE 5 have been posted on the SCALE website.

The Lahey Fortran compiler options used to generate the ORIGEN-S code executable for the PC were changed to prevent round-off errors from occurring. The problem could cause the code to halt during execution because of a negative time step. A new version of the executable, generated with revised compiler flags, is available from the SCALE download page.

An updated version of the Master Photon Library (line energy yields) used by ORIGEN-S is included in both download files. The Master Photon data library, MPDKXGAM, containing discrete and continuous energy gamma lines and intensity data was revised to correct double accounting of some photons associated with decay transitions to or from a metastable nuclide. The problem occurred because some nuclear data evaluations included the gamma emission data with the parent nuclide of the transition, while other evaluations included the data with the metastable daughter product. The library was regenerated ensuring that the source of the evaluation for both parent and daughter nuclides were consistent. The updated library now yields photon release energies (MeV/s) calculated from the gamma spectra that agree with the decay gamma heating values (based on Q values) to well under 1%. The changes have no impact on previous calculations at most practical decay times of interest (days to years). For very short decay times (less than one day) the correction is on the order of 1%. For decay times less than 5 minutes the correction is about 5%, with the original SCALE 5 library giving a slightly larger (more conservative) photon energy yield.

In addition, the library size was reduced by removing the photon emission data for nuclides that were not in the ORIGEN-S decay library. This change resulted in a revised library of 1132 nuclides with explicit photon emission data.

ORIGEN-S

- Updated PC executable.

- Updated Master Photon Library corrects gamma energy release rates.

SAMS Update

The SAMS (Sensitivity Analysis Module for SCALE) module, which computes sensitivity data with TSUNAMI-1D and TSUNAMI-3D, has been modified to correct the calculation of the statistical uncertainty in the sensitivity coefficients when the mesh flux option in KENO V.a is used. The version released in SCALE 5 underestimated the uncertainty.

Memory usage for TSUNAMI-3D calculations has been greatly reduced. In many cases, the SCALE 5 version of SAMS would require more resources than the associated KENO V.a calculations and could cause jobs to fail for lack of system resources after completing the Monte Carlo simulations. The memory requirements for SAMS are now typically less than those of the associated KENO V.a calculations.

The reduction in memory requirements forced the removal of the option to print the forward and adjoint flux solutions. The "PRTFLX" option of SAMS has been disabled. If PRTFLX is encountered in an input file, it will be ignored. Options for printing flux solutions from KENO V.a (PFX and PMF in the parameter data) are still available.

Optional screen output data have been added to certain sections of the code. This real-time screen output can be accessed using the "scale5" command or the "batch5" command with the "-m" option. Output of the calculation time has also been added to the end of the text output and to the screen output.

The process for opening the cross-section-covariance data has been modified to prevent a runtime error on some systems. Systems that did not encounter this error are unaffected by the change.

TSUNAMI

Error in calculation statistical uncertainty in the sensitivity coefficients corrected.

Words to the Wise

Changes in SCALE 5 Version of ORIGEN-S

ORIGEN users should be aware of updates in SCALE 5 that may require modification of older input files.

Many important code and nuclear data library enhancements have been made in the SCALE 5 version of ORIGEN-S. In order to support some of these developments, changes were required in the input requirements and formats. Other input changes were made in order to make the input more consistent and logical. As a result of these changes, some minor modification of older input files run previously under SCALE 4 may be required to run with equivalent results under SCALE 5. The changes most commonly causing problems for users are

1. The definition of the card-image three-group cross sections has been modified. The resonance and fast group cross sections now represent group-averaged values. The definitions of the weighting constants RES and FAST (4* array) have therefore also been changed. The factors are now defined as the ratio of the resonance flux to thermal flux, and fast flux to thermal flux, respectively. Therefore, any old cases using the card-image library need to use revised values of RES and FAST to produce equivalent results.

2. The upper thermal energy group boundary has been increased from 0.5 eV to 0.625 eV, a boundary value that is available in most transport cross-section libraries.

3. The default value of NGRP (3$ array) used to specify the neutron energy group structure is zero. Thus, a neutron source calculation is now performed only if specifically requested by the user, whereas it was always generated previously. The default value of NG (3$ array) used to specify the gamma group structure is also zero (unchanged).

4. The fixed 12- and 18-energy-group gamma source spectra are no longer printed. Gamma source spectra are now requested by using NG (3$ array) and defining the gamma energy group structure in the 83* array. Spectra are now always generated directly from the discrete photon line-energy data library (Master Photon Library). Note that by setting NG=12 or NG=18, the previous fixed-group structure is requested without the need for the user to enter the structure in the 83* array.

5. The extra title cards (IA records) previously required when performing gamma spectra calculations using the Master Photon Library are no longer required or allowed. These titles, one line for each time period where a gamma source spectrum was requested (by input in the 82$ array), were previously required after the Data Block 6 terminator. Old input files must delete these extra title lines to prevent errors.

Infinite Homogeneous Medium Calculation in CENTRM

CENTRM users should be aware of different options for performing infinite homogeneous cross-section processing.

When using CENTRM (by specifying PARM=CENTRM), the default cross section processing method for any material that is not included in the READ CELLDATA data block is an infinite homogeneous medium calculation. The default calculation uses a zonewise homogeneous calculation with a fixed source of 1 for every energy group and point.

If the user specifies an infinite homogeneous medium calculation in READ CELLDATA (i.e., "infhommedium *mixture_number* end"), then a different set of defaults is used. A fission source is assumed and a complete 1-D Sn transport calculation is performed for every energy group and point. Reflecting boundary conditions are assumed. This second method yields similar results but requires much more CPU time.

We recommend using the zonewise homogeneous calculation for all processes. If users need to specify an infinite homogenous calculation to utilize other options (e.g., specifying a fission source), they should be aware of the differences.

Spring 2005 SCALE Training Courses at ORNL

Date	Title	Registration Fee*
Mar. 28 – Apr. 1, 2005	**KENO VI Criticality Safety Course**	$1800
Apr. 4 – 8, 2005	**SCALE Source Terms and Shielding Course**	$1800
Apr. 11 – 13, 2005	**TRITON**	$1200
Apr. 25 – 28, 2005 (Week after Monte Carlo 2005 Conference)	**TSUNAMI Sensitivity/Uncertainty Tools** (Experienced KENO users only)	$1500

*A late fee of $300 will be applied after February 28, 2005.
A discount of $600 per each additional week will be applied for registration to multiple courses.
Foreign nationals must register at least two months in advance to obtain security clearance.
Register for these courses.

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

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