Oak Ridge National Laboratory

SCALE Newsletter

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Special Points of Interest:

SCALE workshops October and November 2009 at ORNL; $300 discount until September 19, 2009

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Updates to SCALE 6

SCALE 6 was released in February. Recently three updates to version 6 have been posted on the SCALE Download web page for users to install.

SCALE 6 Multigroup Libraries Update

The SCALE modules assume that the multigroup cross-section data contain no upscatter data above the first thermal energy group. The ENDF/B-VI and –VII multigroup libraries distributed in SCALE 6 contained upscatter data above the first thermal group for the following nuclides: ^{242m}Am, ^{197}Au, W, ^{182}W, ^{184}W, ^{186}W, ^{155}Gd, and ^{209}Bi in the ENDF/B-VI multigroup libraries; and ^{101m}Ag, ^{242m}Am, ^{244m}Am, ^{115m}Cd, ^{58m}Co, ^{156}Eu, ^{199}Hg, ^{201}Hf, ^{166m}Ho, ^{148m}Pm, ^{124}Sb, ^{127m}Te, ^{129m}Te, ^{182}W, ^{184}W, and ^{186}W in the ENDF/B-VII multigroup libraries. The presence of the upscatter data caused a cross-section library collapse within a TRITON case to fail. Note that this phenomenon is not conventional upscattering caused by molecular motion, but it is the unusual case of scattering from a nucleus in an excited state (i.e., metastable nuclide), where the outgoing neutron gains energy from the nuclear excitation energy.

New multigroup libraries without upscatter data above the first thermal group have been created for the 238-neutron-group libraries for ENDF/B-VI and -VII as well as the coupled shielding libraries. Based on benchmark testing with a suite of 272 benchmark cases, results with the updated libraries are consistent with those obtained with the original SCALE 6.0 libraries. Moreover, the testing demonstrates acceptable results for the benchmark problems. The new libraries are recommended for all SCALE 6 users.

Sensitivity/Uncertainty Update to TSUNAMI/BONAMIST

An update was made to correctly index the implicit sensitivity of Dancoff factors used in BONAMIST. This corrects a discrepancy that caused incorrect propagation of implicit sensitivities due to the calculation of the Dancoff factor for clad, gap, and moderator materials in TSUNAMI models where multiple LATTICECELL models are defined in the same calculation. It is recommended that users install this update and rerun any SCALE 6 TSUNAMI cases that contain multiple LATTICECELLs.

A model of a partially flooded critical experiment with a low-enriched uranium fuel and aluminum clad lattice was computed with TSUNAMI-3D-K5. Before the update, the sensitivity of k_{eff} to the aluminum above the moderator was computed by TSUNAMI to have a value of -0.012, indicating that doubling the density of aluminum in the cladding above the active fuel would decrease k_{eff} by 1.2%. Direct perturbation showed that the impact of the cladding on k_{eff} should be negligible. After the update to BONAMIST, of the sensitivity was properly calculated to be 0.00015.

Because this correction occurred in a group of subroutines shared by all sensitivity/uncertainty modules in SCALE, the following modules are updated by this change.

BONAMIST	SAMS6	TSUNAMI-3D_K6
NITAWLST	TSUNAMI-1D	TSUNAMI-IP
SAMS5	TSUNAMI-3D_K5	TSURFER

(Continued on page 2)

Updates to SCALE 6 (Cont.)

(Continued from page 1)

Lattice Physics Update to NEWT/TRITON

NEWT was updated to address the following problems:

(1) I/O efficiency has been significantly improved in processing nuclide scattering data when creating macroscopic cross sections. Execution time for a very large problem was decreased by a factor of 5.

(2) Fixed-field widths for cross-section ID numbers were increased to allow large mixture numbers without field overflow.

(3) The code was modified to correct a fatal error that occurs when reading and mixing scattering cross sections if no scattering data are available.

(4) Errors have been corrected in the NEWT calculation of few-group homogenized cross sections.

(5) The geometry edit has been updated to remove the printing of asterisks (***) for some output fields.

Because TRITON and TRITON6 depend on NEWT, new executables were generated for both of these modules.

Changes in ORIGEN Nuclear Data Libraries in SCALE 6.1

Significant improvements to the ORIGEN nuclear data and methods to support advanced reactor analysis are being implemented in preparation for the SCALE 6.1 release in 2010. Nuclear decay data have been upgraded to ENDF/B-VII data. Decay transitions have been expanded to include double beta (b^-b^-), neutron emission (n) has been added for ^{5}He decay, and beta-alpha ($b^-\alpha$) decay has been added to represent ^{11}Be decay. Re-evaluation of the decay library resulted in an increase in the number of tracked nuclides by 281, including 904 activation products, 174 actinides, and 1149 fission products.

The procedures and data used to generate the base ORIGEN cross sections have been significantly extended in preparation for SCALE 6.1. The base three-group cross-section library, used previously to supply cross sections for nuclides not updated with ENDF/B data from a SCALE transport calculation, has been replaced by fine-group cross-section evaluations from the Joint Evaluated Fission and Fusion File special purpose activation files JEFF-3.0/A, which were developed from the European Activation File EAF-2003. The JEFF data can still be updated using ENDF/B-based cross sections from a SCALE transport calculation as performed previously. The JEFF activation files contain neutron data for 774 target nuclei, including ground and metastable isomeric states, and 12,617 neutron-induced reactions below 20 MeV. The following neutron reaction types are now included in the ORIGEN transition matrix: (n,n′), (n,2n), (n,3n), (n,f), (n,n′α), (n,2nα), (n,3nα), (n,n′p), (n,n2α), (n,n′d), (n,n′t), (n,n′h), (n,4n), (n,2np), (n,γ), (n,p), (n,d), (n,t), (n,h), (n,α), (n,2α), (n,2p), and (n,pα).

AMPX multigroup libraries based on the JEFF data are being generated for the following transport library group structures available in SCALE:

- 238-group neutron (thermal applications)
- 200-group neutron (fast applications and shielding)
- 44-group neutron (collapsed version of 238 groups)

The use of the JEFF-3.0/A cross sections and AMPX multigroup libraries has a number of technical advantages:

- The number of available reaction types simulated in ORIGEN increases from 6 to 28.
- All reaction cross sections are available in a fine-energy-group representation.
- The reactions to ground and isomeric states are stored as separate MTs, allowing energy-dependent branching between reaction product levels to be a free variable that is calculated dynamically when the cross sections are collapsed.
- The average fission energy is calculated for each fissionable nuclide based on the neutron spectrum and fission spectrum and used to obtain energy-dependent fission product yields.

Fission product yields are included for 30 actinides with neutron-induced fission yields in ENDF/B–VII, including ^{227,228,232}Th, ^{231}Pa, $^{232\text{-}238}$U, ^{237,238}Np, $^{238\text{-}242}$Pu, ^{241,242m,243}Am, $^{242\text{-}246,248}$Cm, ^{249,252}Cf, and ^{254}Es. An ORIGEN fission yield library has been implemented with yields for all tabulated incident neutron energies: thermal, fast, and high-energy (14 MeV). The average neutron energy causing fission is calculated automatically from the multigroup fission cross-section data and flux spectrum for each actinide, and the fission yields are interpolated using the average fission energy and applied automatically in the transition matrix.

Tips from the SCALE 6 Notebook

Included below are several useful entries from the SCALE 6 Notebook. Users are encouraged to consult the notebook for answers to frequently asked questions.

Using ORIGEN ABTR Fast Library in TRITON

An ORIGEN binary fast reactor library for the Advanced Burner Test Reactor (ABTR) was included in SCALE 6 to provide TRITON users with the capability to perform fast reactor analyses. The ABTR library provides fast cross sections for isotopes not updated from the transport calculation and also supplies fast fission yields. This library can be used as the base ORIGEN library instead of the default pressurized water reactor (PWR) library when performing TRITON calculations. However, the SCALE 6 Manual failed to document how to use this library with TRITON. The method for attaching an alternate library was previously documented in Sects. M6 and T1, but changes prior to the release omitted this information. The ORIGEN library name and unit number associations are listed in a file named **origen_filenames** located in the SCALE data directory. The file contains the ORIGEN reference unit number in the first column, the base filename in the second column, and the I/O unit number used by SCALE to open the file in the third column.

21	pwr33gwd	21
22	abtrx	22
23	maphnobr	23
24	maphh2ob	24
26	maphuo2b	26
27	end6dec	27
28	pwrlib	28
81	xn238v7	88
82	xn27g19v7	88
83	xn44	88
84	xn238	88
85	xn238v6	88
86	xg18	88
87	xn200g19v7	88
88	xn27g19v7	88

The fast library is automatically used in ORIGEN stand-alone calculations if read on unit 22. For TRITON cases, the starting base library is always read on unit 21. To use the fast library in place of pwr33gwd, you can update the origen_filenames and swap unit numbers 21 and 22, so that unit 21 is associated with the abtrx library.

Note that you can also use the abtrx library with an input file generated using the OrigenArp Windows user interface by editing the input file to remove the =ARP section of input (interpolation is not needed) and replacing the library unit (first entry in 3$ input record) with 22, and setting the third entry to 1 for all occurrences of the 3$ input record.

Information for Foreign Language Windows Users

Subroutines GETMTM in \scale6\src\scalelib and GETMTM_ALL in the QAUPDATE program (\scale6 \src\misc\qaupdate) perform searches for keywords contained in the output from the DOS "dir" command. If a SCALE job fails with an error in subroutine GETMTM, the default date format does not match that expected by SCALE. The problem can be corrected by selecting the proper date format in Windows.

Click on Start => Control Panel => Regional and Language Options

In Windows Vista: on the Formats tab, under "Current format" select English (United States).

In Windows XP: on the Regional Options tab, select English (United States).

If SCALE runs correctly but the message "This is not a scale configuration controlled code" is shown in the Program Verification Information table in the SCALE output, please note the information in the Getting Started file (Sect. 5) about the language.dat file.

RAID Card Improves Performance on Windows Dual Quad Core PC

We received this information from Mark Scott, a SCALE user at Los Alamos National Laboratory.

"I recently purchased a new computer with the goal of being able to run SCALE while at the same time using the computer as my main desktop (usually I have 4–6 other programs open at all times). I purchased a Dell T7400 with dual quad core XEON 3.2GHz CPUs and 4 GB of memory running on Windows XP. When I ran my TRITON cases, my computer would slow to a crawl but my memory and CPU usage were quite low. I quickly realized it was my hard drive. I had two 1TB 7200RPM SATA drives. I then installed a 3ware 9650SE RAID card with 4 SSDs in a RAID0 configuration. After the new drives were installed, the computational time was cut by more than half and now my computer shows no sign of slowing down when I run my TRITON cases. I was expecting a small boost in computational time and better multitasking ability, but a 100% improvement was unexpected."

SCALE 6.0 Sensitivity/Uncertainty (TSUNAMI) User Notice

Some deficiencies have recently been identified by ORNL staff in the TSUNAMI sensitivity analysis codes released in SCALE 6.0. SCALE code managers are working to address these deficiencies and to release updates in the near future.

Implicit Sensitivity Calculation with Multiple LATTICECELL Models

An error was identified in TSUNAMI calculations where multiple LATTICECELL models are defined in the same calculation. TSUNAMI-1D, TSUNAMI-3D-K5, and TSUNAMI-3D-K6 incorrectly propagate the implicit sensitivity for clad, gap, and moderator materials due to the calculation of the Dancoff factor. Please see article on page 1 for details.

TSUNAMI Mesh Issues

With SCALE 6.0, a more dynamic mesh flux accumulator capability was added to KENO V.a for use with TSUNAMI-3D-K5, and sensitivity capabilities for KENO-VI were introduced with TSUNAMI-3D-K6, using the same meshing algorithms. The volumes of each region of the model within each mesh interval are computed stochastically by randomly sampling the geometry model volume and accumulating points within each mesh. This process is repeated over many generations of points to determine the average volume and standard deviation of each mesh interval for each region. With TSUNAMI-3D-K6, the number of points per generation and the number of generations for volume calculations have default values that can be overridden by the user with the *READ VOLUME* input block. However, this input capability was not added to TSUNAMI-3D-K5. KENO V.a has never had a *READ VOLUME* input block, because KENO V.a always calculates the volumes analytically.

TSUNAMI-3D-K5 calculations are performed with default volume sampling values, which produce reliable results for most cases. However, the user has no control over how many points are sampled, and the final mesh volumes are not printed in the output. Furthermore, uncertainties in the mesh volumes are not propagated to uncertainties in the sensitivity coefficients, so it may not be immediately obvious when a particular mesh volume is inadequately sampled.

The potential impact is that some mesh volumes may be undersampled, producing inaccurate sensitivity coefficients. Of the hundreds of models ORNL has analyzed with TSUNAMI-3D-K5 in SCALE 6.0, only a few have been identified that yielded inaccurate results as a result of inadequate volume sampling. These models typically have a large overall volume and relatively small internal parts with a significant sensitivity contribution. As always, users are encouraged to verify TSUNAMI sensitivity results by comparison with direct perturbation calculations.

Additionally, users will occasionally encounter a crash in KENO V.a or KENO-VI when running TSUNAMI-3D-K5 or TSUNAMI-3D-K6 with the error message "lost in grid" followed by some additional details. This error most often occurs at the boundary of the global unit, where the dimensions of the mesh and the actual geometry have a slight discrepancy due to round-off errors. This situation can be corrected by manually entering mesh boundaries that exceed the outermost geometry boundaries using the *READ GRID* input block in KENO V.a or KENO-VI.

In TSUNAMI-3D-K5, if the outermost boundary of the global unit is not a cuboid, the mesh volume is sampled within a cuboid enclosing the global unit. In these cases, message *k5-077* is printed each time a mesh volume point is sampled within the enclosing mesh cuboid but outside the global unit. A single output file can potentially contain thousands of these messages, which can be ignored. To avoid these messages in your output, it is recommend that the global unit geometry include a cuboid of void as the outermost region surrounding the model geometry.

Software modifications to address these issues will be included in SCALE 6.1.

Use of CELLMIX Cross Sections with TSUNAMI

The use of cell-averaged cross sections via the "CELLMIX=" keyword in TSUNAMI calculations has been allowed but discouraged due to the implicit sensitivity effects introduced in the XSDRNPM calculations that are not represented in the final sensitivity coefficients. The resulting sensitivity coefficients may be representative of the true sensitivities but will likely be in error up to several percent. However, results of this type may be useful for scoping calculations. In SCALE 6.0 the CELLMIX functionality was disabled in TSUNAMI-3D-K5 and TSUNAMI-3D-K6. For models that use CELLMIX, the calculation begins in SCALE 6.0 but terminates with no information provided. An appropriate modification to address this issue will be included in SCALE 6.1.

KENO-VI Fails to Start Particles in a Rotated Outer Boundary

The default method for initially starting particles in KENO-VI is to select points uniformly distributed within the outer boundary of the global unit. The starting types available in KENO-VI mimic those in KENO-V.a, but are more restricted because of the additional geometric complexities. A requirement for using the outer boundary of the problem is that it not be rotated. If the outer boundary is rotated, then START data must be specified for the problem. A simple fix is to specify the bounds of a cuboid that contain the fissionable materials in the START data. The cuboid can be larger than the outer boundary, but this will lead to a less efficient selection of the starting points. The code in SCALE 6.0 does not recognize that the outer boundary is a rotated boundary, so it will try to use the boundary as if it were not rotated. This discrepancy can lead to a long time attempting to generate the starting guess without finding any fissionable material. Prior to the release of SCALE 6.1, the code will be updated to terminate with an error message if the outer boundary is rotated or to correctly start particles in a rotated body.

New SCALE 6 Shielding V&V Report

A new SCALE verification and validation (V&V) report has been published that documents benchmark testing of the SCALE 6 MAVRIC shielding sequence and new shielding libraries. Two coupled neutron-gamma shielding libraries have been generated based on the Evaluated Nuclear Data File/B Version VI (ENDF/B-VI) Release 8 (ENDF/B-VI.8) and ENDF/B-VII Release 0 (ENDF/B-VII.0) cross-section evaluations. Both libraries were generated using 200 neutron and 47 gamma groups. The neutron group structure is identical to the 199-group VITAMIN-B6 structure, except that an additional neutron group has been added to extend the top energy boundary to 20 MeV. In addition to these fine-group libraries, a broad-group ENDF/B-VII.0 library has been generated using a 27-neutron and 19-gamma group structure. This report documents the cross-section library development and the benchmark testing of the new libraries with the new SCALE 6 MAVRIC shielding sequence.

This report provides detailed computational results using the new shielding libraries and radiation transport capabilities of MAVRIC. The report is available on the SCALE website at http://www.ornl.gov/sci/scale/pubs/nureg-cr6990.pdf.

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.

Fall 2009 SCALE Training Courses at ORNL

Date	Title	Registration Fee*
October 19–23, 2009	SCALE Criticality Safety and Shielding Course (KENO-VI/MAVRIC)	$2000
October 26–30, 2009	SCALE Lattice Physics and Depletion Course (ORIGEN-ARP/TRITON)	$2000
November 2–6, 2009	SCALE Sensitivity/Uncertainty Tools Course (TSUNAMI) (Experienced KENO users only)	$2000
November 9–13, 2009	SCALE Criticality Safety Course (KENO V.a)	$2000

*After September 19, 2009, the registration fee will increase to $2300. A discount of $200 for each additional week of training will be applied for registration in multiple courses.

Please note: Foreign nationals must register at least 40 days in advance to obtain security clearance.

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

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