Oak Ridge National Laboratory

SCALE Newsletter

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Special point of interest:

- SCALE workshops in October 2007 at ORNL; $300 discount until September 14th

SCALE 5.1 MIPLIB Update for Dancoff Factor Correction

The following updates have been made to the Material Information Processor Library (MIPLIB) in SCALE and posted on the SCALE website for users to download at http://www.ornl.gov/sci/scale/miplib_update.htm.

(1) An error in the calculation of Dancoff factors for clad regions was introduced in SCALE 5.0. This error affects only calculations that use LATTICECELL cell types and the NITAWL resonance-processing module. Approximately 180 critical benchmarks for LWR and MOX fuel were run with and without the correction. On average, the difference in the calculated k_{eff} values was 0.01%, with a maximum of 0.18%, indicating that

the effect on previous calculations is negligible (within statistical uncertainty).
(2) The calculation of zone volumes, as well as periodic boundary conditions and nonzero left boundary locations for slabs, was also corrected. These errors also had negligible impact on calculated k_{eff} values.

Note that this download is recommended for all SCALE 5.1 users. It contains updates previously posted on the SCALE website for BONAMIST and TRITON/NEWT/PMC/MIPLIB as well as the updates discussed above. This download includes updates for BONAMIST, CSAS, CSAS6, MODIFY, NEWT, PMC, STARBUCS, TRITON, TRITON6, TSUNAMI-1D, and TSUNAMI-3D.

Java 1.6 Update Impacts Javapeño

The default installation of Javapeño does not work correctly with the Java 1.6 update. Javapeño starts, allows the user to read a data file, but then ignores the user's requests to plot data.

The problem is caused by the fact that the new version creates a completely new directory, so that the Java Advanced Imaging and Java3D extensions from Sun that Javapeño needs are not accessible anymore. They have to be reinstalled in the new Java directory structure. Javapeño itself functions correctly; it just needs these two add-ins from Sun:
https://jai.dev.java.net/binary-builds.html
and
https://java3d.dev.java.net/binary-builds.html

A user who is running Windows Vista or XP on an Intel-based machine should use the following downloads:

http://download.java.net/media/jai/builds/release/1_1_3/jai-1_1_3-lib-windows-i586-jdk.exe
and
http://download.java.net/media/java3d/builds/release/1.5.1/java3d-1_5_1-windows-i586.exe

Other users should select their appropriate operating system and processors. Mac users are not affected by this update, because the JAI and Java3D extensions are installed by default with each Java update. However, Apple has not yet released a Java 1.6 update.

SCALE 5.1 for Windows Vista

The initial release of SCALE 5.1 for Windows was developed for Windows XP and is not fully compatible with the new Windows Vista operating system. An updated installation package for Windows Vista will be available from RSICC in August. If you are a registered SCALE 5.1 user

and need the Vista installation package, please contact RSICC at rsic@ornl.gov to obtain a free DVD. All compatibility problems are related to the Vista operating system; therefore, WindowsXP, Linux, and Unix users need not obtain this release.

TSUNAMI Code Manager Wins ANS Award

Brad Rearden, the SCALE TSUNAMI Code Manager, is the recipient of the American Nuclear Society (ANS) Landis Young Member Engineering Achievement Award for 2007. Brad is nationally and internationally recognized for his expertise and significant contributions in the implementation of sensitivity and uncertainty methods into Monte Carlo nuclear analysis codes. The prestigious ANS Landis Young Member Engineering Achievement Award recognizes "outstanding achievement in which engineering knowledge has been effectively applied to yield an engineering concept, design, safety improvement, method of analysis or product utilized in nuclear power research and development or commercial application." The award was presented to Brad at the ANS Annual Meeting in June, by Jack Ohanian, ANS Honors and Awards Chair.

ANS Landis Young Member Engineering Achievement Award Winner

Brad Rearden, left, receiving the ANS Landis Young Member Engineering Achievement Award presented by Jack Ohanian, ANS Honors and Awards Chair

Tips for NEWT Users

NEWT has an option that allows users to cease code execution in an orderly manner after the current iteration is completed so that a user can terminate a calculation early and still get useful results. The user can manually stop execution by placing a file named "stopnewt" in the temporary working directory where the SCALE job is executing. There are no requirements for the content of the stopnewt file.

Similarly, NEWT can generate flux plot files "on the fly" by the creation of a file named "plotnewt" in the SCALE temporary directory. If the file is found to be present at the end of an outer iteration, NEWT will create the postscript file "cleo.ps," which contains flux plots for each energy group based on the current iteration flux. This can be useful in debugging a problem that does not seem to converge. However, this file is not automatically copied back to the user's home directory. It must be copied manually or by using an "=shell" command in the input file.

Note that the final converged fluxes can be plotted by adding "prtflux=yes" to the parameter data block within NEWT.
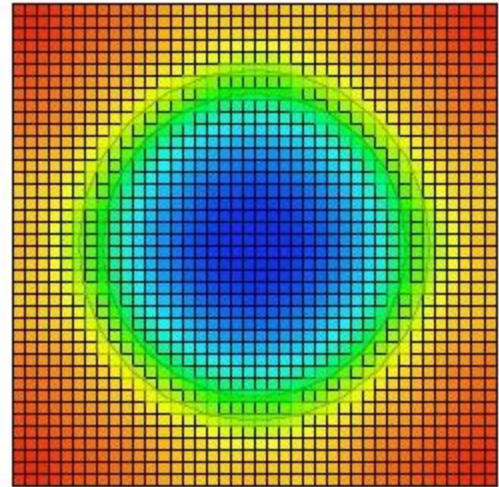
> Files named "stopnewt" and "plotnewt" can stop execution or generate debug flux plots.

Fig. 1. Flux plot (energy group 34 of 44) of mixed oxide pin cell

Explicit INFHOMMEDIUM Unit Cell Data May Reduce CENTRM Memory Requirements

As noted in the January 2007 article "Reducing CENTRM Memory Requirements," SCALE cases with large numbers of nuclides that use CENTRM/PMC may encounter memory limits, particularly in the Windows version of SCALE 5.1. The stated work-around is to use an individual INFHOMMEDIUM unit cell data for each mixture not defined in a unit cell.

When several mixtures are not explicitly specified in any unit cell, they are put into a single unit cell with individual zones for each mixture. Before CENTRM performs its zone-wise infinite homogeneous medium calculation, it unionizes the

cross sections into a common energy mesh. As a result, the CENTRM calculation for this unit cell containing multiple mixtures must store pointwise fluxes, cross sections, and scattering sources on the union mesh for all materials simultaneously, whereas only data for a single mixture must be stored if each nuclide is treated in a separate INFHOMMEDIUM unit cell. Both methods produce the same resonance self-shielded cross sections. However, users should be aware that calculated k_{eff} values from KENO may differ for these two cases because the random sampling is altered due to round-off differences in generating the cross sections.

Words to the Wise …

SCALE 5.1 ORIGEN Library Needs to Be Updated

Several updates were made to the ORIGEN card-image decay library, origen.rev03.end6dec.data, to make the half-lives for several activation products consistent with more up-to-date ENSDF values for isotopes that also occur as fission products. The changes, restricted to activation products only, were included in origen.rev04.end6dec.data, which was released in SCALE 5.1. The data changes are listed in the table below.

The binary ORIGEN library, pwr33gwd, was inadvertently not remade after the last update to the decay library, and the version origen.rev02.pwr33gwd distributed in SCALE 5.1 contains the older data and is identical to the library distributed in SCALE 5.0. In some cases, users who have performed decay calculations for activation products have found differences in the activities calculated using the different libraries,

resulting from differences in the decay constants (see page 95 of the ORIGEN-ARP Notebook).

Windows users can download and install the updated origen.rev03.pwr33gwd file. Unix/Linux users can update the library by performing the following steps.

1. Edit the scale5.1/work/origen_xslibs.input file and change the revision number from "rev02" to "rev03" in the data library name near the end of the input file.

2. Execute the updated origen_xslibs.input file using the following command (all on one line).

 env FORT_CONVERT15=BIG_ENDIAN batch5 origen_xslibs &

Table 1. Changes in decay half-life data in SCALE 5.1

Nuclide	Decay Mode	Activation Product Half-Life		
		Rev. 03	Rev. 04	Difference (%)
Se-79	β⁻	1.041E+13 s	2.947E+05 y	11.94
Rh-102	β⁻	9.152E+07 s	2.072E+02 d	411.23
Ru-106	β⁻	3.211E+07 s	1.017E+00 y	0.05
Ag-106	EC	1.440E+03 s	2.396E+01 m	0.16
Ba-131	EC	1.020E+06 s	1.150E+01 d	2.66
Ce-142	Stable	3.311E+18 s	0.000E+00 y	-
Sm-149	Stable	3.154E+23 s	0.000E+00 y	-
Gd-155m	IT	3.100E-02 s	3.197E-02 s	3.03

More Words to the Wise …

Anomaly in TSUNAMI Sensitivity Profiles with CENTRMST/ PMCST

An ORNL staff member recently identified a discrepancy in Javapeño sensitivity profile plot results for a TSUNAMI case that used CENTRMST/PMCST. As shown in Fig. 2, the ^{16}O scattering sensitivity obtained with ENDF/B-VI data and CENTRMST/PMCST (green line) shows an unusual behavior between 0.001 and 0.2 eV when compared with results obtained with ENDF/B-V data and NITAWLST (red line).

Although the plot shows a non-physical behavior in the low-energy range, the impact of the discrepancy on the calculated results is negligible in this case. It occurs only in the scattering sensitivity over a very narrow energy range. The impact on the calculated k_{eff} value is statistically insignificant, and the impact on sensitivity/uncertainty analysis is very small, particularly if the experiments and applications used the same CENTRM options. This irregularity does not occur in the CENTRM flux spectrum, but only in the CENTRMST/ PMCST implicit sensitivity data. This anomaly may be caused by the evaluation of flux derivatives in CENTRMST or PMCST within the thermal range where the pointwise (PW) and multigroup (MG) solutions join, and the derivatives are discontinuous. NITAWLST entirely ignores implicit effects at low energy, so the anomaly is not seen. The SCALE staff is investigating the cause of the discrepancy.

If a user encounters such an anomaly in their plots, two different workarounds may be used. One option is for the user to increase the PW cut-off energy (input parameter DEMIN) in CENTRMST from 0.001 eV to 0.2 eV. This option is essentially equivalent to the treatment in NITAWLST, as demonstrated by the blue line in Fig. 2. To implement this work-around, the following input should be inserted after each unit cell specified in the "READ CELLDATA" data block.

CENTRM DATA DEMIN=0.2 END CENTRM

Another option is to increase the number of outer iterations (input parameter IUP). When the number of upscatter iterations is increased from 3 to 15 in CENTRMST, the observed differences are reduced significantly, as shown by the yellow line in Fig. 2. Note that convergence was not obtained with IUP=15. It is expected that increasing IUP further to obtain a converged solution would produce results that agree with the DEMIN=0.2 line.

For the current sensitivity work under discussion, setting DEMIN=0.2 for the CENTRMST PW solution appears to be the best solution, because it runs faster and produces physically realistic results that are nearly identical to NITAWLST without increasing the runtime.
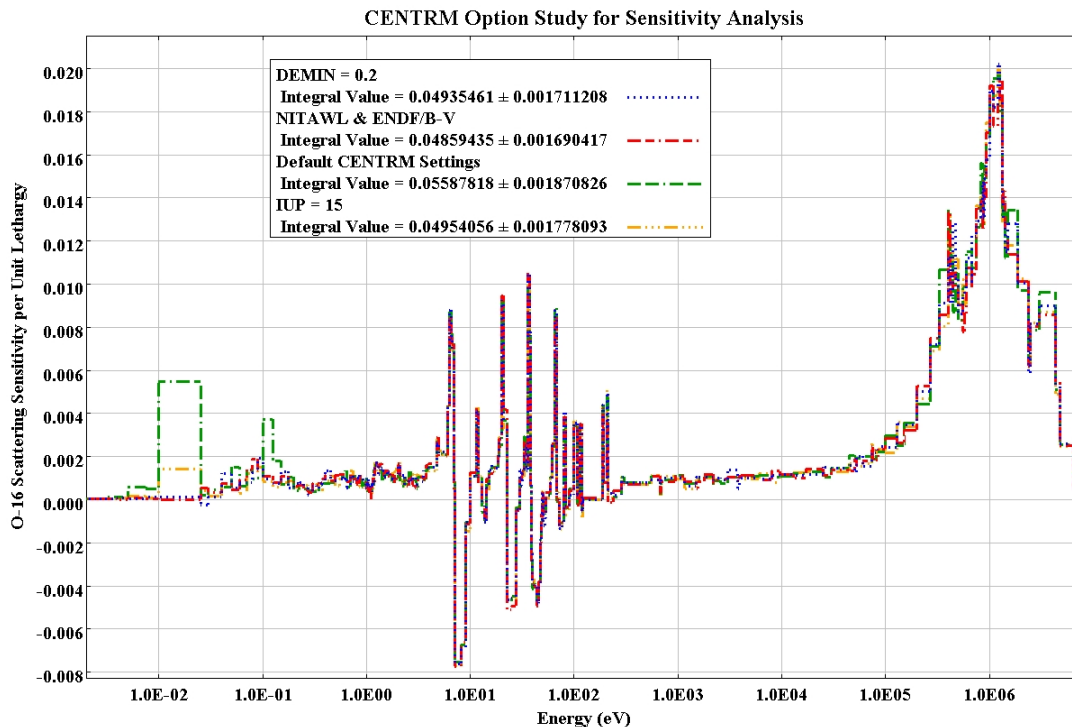

Fig. 2. ^{16}O scattering sensitivity profile plot comparing CENTRMST and NITAWLST results

Recent SCALE Publications and Presentations

You can find recent SCALE-related publications and presentations on the SCALE website. Look for the link near the bottom of the home page. Below are the 2007 files that are currently available. Publications from the ICNC 2007 meeting will be added soon.

M. D. DeHart, TRITON Workshop, a workshop presented at the *American Nuclear Society Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C+SNA 2007),* April 15–19, 2007, Monterey, California.

M. D. DeHart, S. Goluoglu, and M. E. Dunn, "KENO Continuous Energy Calculations for a Suite of Computational Benchmarks for the Doppler Reactivity Defect," mcsna01087full.pdf in *Proc. of Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C+SNA 2007),* April 15–19, 2007, Monterey, California, on CD-ROM, American Nuclear Society, LaGrange Park, Illinois (2007).

M. D. DeHart, I. C. Gauld, and M. L. Williams, "High-Fidelity Lattice Physics Capabilities of the SCALE Code System Using TRITON," mcsna05008full.1.pdf in *Proc. of Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C+SNA 2007),* April 15–19, 2007, Monterey, California, on CD-ROM, American Nuclear Society, LaGrange Park, Illinois (2007).

M. D. DeHart, "Simplification of Multi-Group Cross-Section Processing for Large Depletion Calculations in TRITON," mcsna01086full.pdf in *Proc. of Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C+SNA 2007),* April 15–19, 2007, Monterey, California, on CD-ROM, American Nuclear Society, LaGrange Park, Illinois (2007).

B. T. Rearden and J. E. Horwedel, "Automatic Differentiation with Code Coupling and Applications to SCALE Modules," mcsna01317full.pdf in *Proc. of Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C+SNA 2007),* April 15–19, 2007, Monterey, California, on CD-ROM, American Nuclear Society, LaGrange Park, Illinois (2007).

C. V. Parks, J. C. Wagner, D. E. Mueller, and I. C. Gauld, "Full Burnup Credit in Transport and Storage Casks: Benefits and Implementation," *RadWaste Solutions,* 14 (2), 32–41 (March/April 2007).

> Look for the "Recent SCALE Publications and Presentations" link near the bottom of the SCALE home page.

Corrections and Updates to SCALE 5

The attached file provides a summary of code and data modifications that have been made to the configuration-controlled version of SCALE at ORNL since the SCALE 5.1 release in November 2006.

Fall 2007 SCALE Training Courses at ORNL

Date	Title	Registration Fee*
October 15–19, 2008	**ORIGEN-ARP/TRITON Reactor Physics**	$1800
October 22–26, 2008	**KENO V.a Criticality Safety**	$1800
October 29–November 2, 2008	**TSUNAMI Sensitivity/Uncertainty Tools (Experienced KENO users only)**	$1800

*A late fee of $300 will be applied after September 14, 2007. A discount of $300 for each additional course 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.