Oak Ridge National Laboratory

SCALE Newsletter

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Special Point of Interest:

- SCALE workshops in March-April, 2008 at ORNL; $300 discount until February 29th

Inside This Issue:

New Shielding Module with Automated Variance Reduction to Be Available in SCALE 6

BACKGROUND

The primary radiation shielding modules in SCALE have been the MORSE Monte Carlo code and the SAS3 and SAS4 shielding analysis sequences. Several years ago, an effort was initiated to create updated shielding analysis tools in SCALE to regain state-of-the-art capabilities in this technical area. The result is the new shielding module **Monaco** that will be released in SCALE 6. Monaco is a fixed-source, 3-D generalized geometry, multigroup Monte Carlo radiation transport code. Monaco is based on the same physics as MORSE but uses the SCALE Standard Composition Library and the SCALE Generalized Geometry Package (SGGP) that is used by KENO-VI. For difficult shielding problems, the **MAVRIC** (Monaco with Automated Variance Reduction using Importance Calculations) sequence has been developed to provide automated 3-D variance reduction by automatically creating space/energy importance maps and biased source distributions for Monaco. A new ENDF/B-VII 200 neutron group and 47 gamma group library will be included in SCALE 6.

MONACO

Monaco is the result of a modernization effort combining the multigroup neutron and photon physics of MORSE with the flexibility of the second-order surface SGGP. Major efforts have been made in bringing the coding style up to modern Fortran 95 standards so that future development can be more easily continued.

Monaco is much more flexible than MORSE. Users can construct a source by specifying the separate spatial, energy, and directional distributions. Available tallies in Monaco include point detectors, region-based flux tallies and mesh tallies (a set of region tallies defined on a mesh that overlays the physical geometry). Any Monaco tally can be convolved with a response function, either user-defined or from a standard list available with each SCALE cross-section library. Mesh tally values and uncertainties can be viewed with a special Java viewer that works on Windows, Unix, Linux, and Mac platforms (Fig.1).

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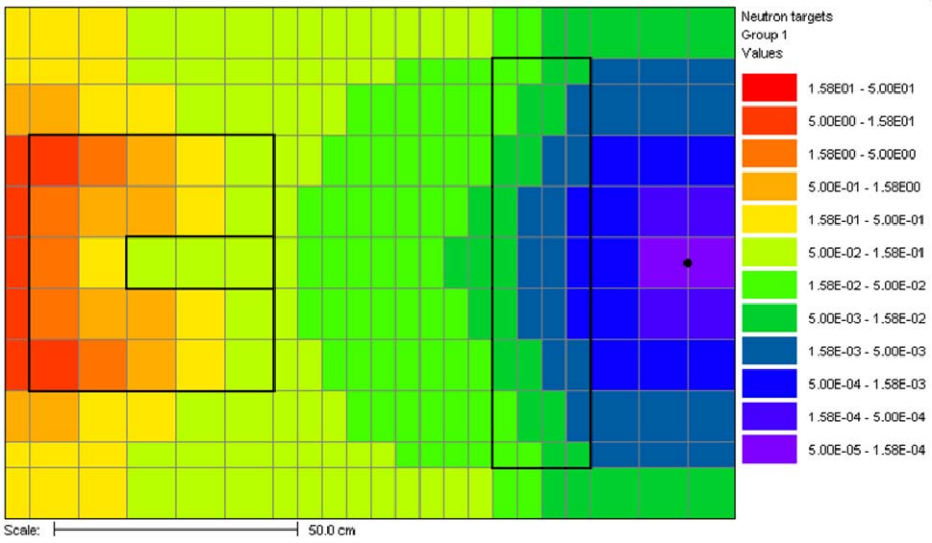

Fig. 1. Target weight window values for group 1 neutrons calculated by MAVRIC (shown in the Java Mesh File Viewer) for a simple shielding problem consisting of a Cf-252 source in a paraffin block on the left, a 20 cm thick shield on the right, and a point detector at the far right. Each energy group has a different importance map.

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MAVRIC

The MAVRIC sequence is based on the CADIS (Consistent Adjoint Driven Importance Sampling) methodology. For a given tally in a Monte Carlo calculation that a user wants to optimize, the CADIS method uses the result of an adjoint calculation from a 3-D deterministic code to create both an importance map for weight windows and a biased source distribution. MAVRIC is completely automated — from a single user input file, it creates the cross sections (forward and adjoint); calculates the first collision source for the discrete ordinates (where applicable); computes the adjoint fluxes; creates the importance map and biased source; and executes Monaco.

New ENDF/B-VII shielding library with 200 neutron groups and 47 gamma groups will be released with MAVRIC/Monaco.

Users can start and stop the calculation at various points so that progress can be monitored and importance maps can be reused for similar problems. The discrete ordinates calculation is based on the Monte Carlo input of sources and responses – so the only extra input required by the user is the listing of mesh planes that will be used to create a mesh geometry model. This same mesh is used for the importance map and the biased source. Results for some simple shielding problems show speed-up factors of 50. For dose-rate calculations from spent fuel casks, speed-up factors of several hundred were achieved using MAVRIC compared to analog Monaco. Figure 2 shows a comparison of results between analog Monaco and MAVRIC for a three-legged duct.

For simple problems that do not require advanced variance reduction, the MAVRIC sequence is an easy way to compute problem-dependent cross sections and execute Monaco with a single user input file. Standard region-based weight windows for particle splitting and roulette are available when the CADIS-based importance maps are not being used.

MULTIPLE TALLY OPTIMIZATION

With advances in computational resources, Monte Carlo methods are being used to compute fluxes or doses over large areas using mesh tallies. For problems that demand that the uncertainty in each mesh cell be less than a set maximum, computation time is controlled by the cell with the largest uncertainty. This issue becomes quite troublesome in deep-penetration problems, and advanced variance reduction techniques are required to obtain reasonable uncertainties over large areas.

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MAVRIC provides state-of-the-art 3-D variance reduction techniques.

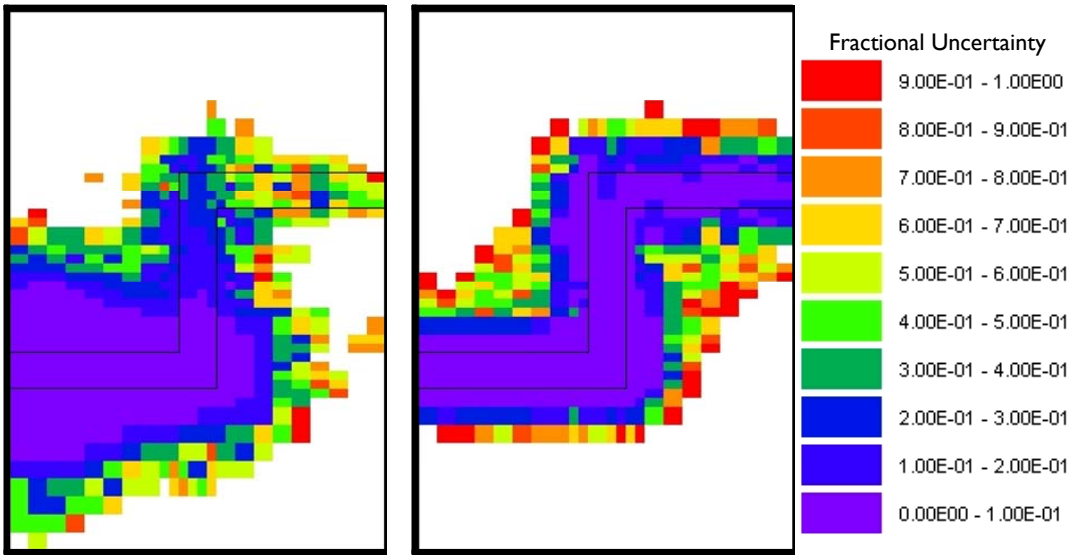

Fig. 2. Comparison of dose rate uncertainties for analog Monaco and MAVRIC using the CADIS methodology for a three-legged duct problem (source at lower left). Both were 90 minute calculations on a Dec Alpha. Analog Monaco has reasonable uncertainties in the first leg but has trouble in the second and third legs. The MAVRIC calculation does not spend time transporting particles deep into the block material and has uncertainties below 10% all the way to the duct exit (upper right).

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To optimize several tallies at once (i.e., calculate the tallies with similar relative uncertainties) or optimize the calculation of a mesh tally, an extension of the CADIS method has been implemented into the MAVRIC sequence. First, a forward discrete ordinates calculation over a coarse geometry mesh is performed to estimate the tally responses. Then, the adjoint problem is created with an adjoint source for each tally to be optimized, weighted inversely by its expected result. Like standard CADIS, the result of the adjoint calculation is used to create a set of target weight windows and a biased source distribution that are then used by Monaco. This forward-weighted CADIS (FW-CADIS) approach should be quite useful in many problems.

GRAPHICAL USER INTERFACE

The GeeWiz (Graphically Enhanced Editing Wizard) user interface for many of the SCALE sequences has been expanded in SCALE 6 to include the MAVRIC sequence. This allows users to create, edit, and view the geometry using the highly interactive KENO3D visualization tool, easily define the physical materials, set all of the calculational parameters, and set up the mesh planes for the discrete ordinates adjoint calculation.

CAAS CAPABILITY

Also planned for the SCALE 6 release is a new capability to perform criticality accident alarm systems (CAAS) safety analyses. Users will be able to model a critical assembly using KENO-VI and save the final distribution of fission sites as a mesh source. Then MAVRIC can use the mesh source and calculate fluxes and dose rates throughout the facility. Rigorous testing and verification will be a part of the development of all new features.

For more detailed information on Monaco and MAVRIC, click to see a list of relevant publications.

Capability to analyze CAAS with KENO-VI and Monaco is being developed for SCALE 6.

Errors in MALOCS and PMC Impact TRITON Procedure for Cross-Section Library Collapse

The TRITON sequence in SCALE 5.1 provides an option "PARM=WEIGHT" to collapse a multigroup master cross-section library to a broader energy group structure (Sect. T1.4.3 of the SCALE Manual). The procedure uses the problem-dependent flux spectrum computed by NEWT to generate a weighted master broad-group library. The purpose is to allow users to create a problem-dependent master broad-group library from a fine-group library, such as the 238-group libraries in SCALE.

Recently it was found that the collapsed ENDF/B-VI broad-group cross-section data did not reproduce the original fine-group eigenvalue results for some broad-group structures. The differences have been attributed to three sources: (1) an error in collapsing partial fission channel data in the MALOCS module; (2) Bondarenko factor ranges that begin and/or end in the middle of broad groups are not collapsed consistently in MALOCS; and (3) treatment of the broad-group resonance interface between the resolved and unresolved resonance regions in the PMC module. Because ENDF/B-V contains no partial fission spectra nuclides, libraries collapsed from the 238-group ENDF/B-V library (e.g., the SCALE 44-group library) are not affected by the first MALOCS error. It is unknown whether it is affected by the Bondarenko problem, but the unresolved ranges for important nuclides occur at energies where any discrepancy will be small.

The MALOCS and PMC errors have been corrected and will be available in SCALE 6. The PMC error also was shown to have a small impact on results obtained with the distributed SCALE ENDF/B-V 44-group ENDF/B-V library. The largest impact observed from the PMC error on the calculated k_{eff} was 0.4% for one case. The corrections tend to improve agreement with 238-group library results.

Users should refrain from using the "PARM=WEIGHT" option in TRITON until SCALE 6 is available. If users have collapsed an ENDF/B-VI fine-group library (e.g., the V6-238 library) to a broad structure and used the collapsed library for important calculations, they should compare results with those from using the fine group library.

TRITON option "PARM=WEIGHT" in SCALE 5.1 should not be used.

Words to the Wise …

SCALE 5.1 ORIGEN-S Libraries Update

This update contains changes in the ORIGEN card-image cross-section library to correct cross-section values obtained from the FENDL-2.0 evaluated nuclear data library. Only FENDL data were updated. The updated library, origen.rev03.pwrlib.data, replaces the previous version origen.rev02.pwrlib.data. As a result of these changes to the card-image library, the binary library PWR33GWD was updated to origen.rev04.pwr33gwd. This update supersedes the previous update to origen.rev03.pwr33gwd posted on August 7, 2007 (see July 2007 newsletter article, "SCALE 5.1 ORIGEN Library Needs to Be Updated"). The impact of this update is that results for some activation product (i.e., light element) nuclides are corrected. Actinide and fission product inventories are largely unchanged.

Large differences were reported in comparisons of the calculated isotopic activities obtained using the card-image library (with typical values of the flux weighted factors) and activities calculated using one of the new ORIGEN-ARP binary cross-section libraries. Evaluation of the discrepancies revealed that differences were caused by incorrect FENDL-2.0 based cross sections.

A systematic error occurred during processing of the FENDL data due to a nonstandard format used to represent reaction transitions to metastable product states. The FENDL library contains partial cross sections for each reaction channel to different product states. For example, capture reactions to the ground state are stored as MT=102, to the first metastable state as MT=402, and second metastable state as MT=702. Only the MT=102 transitions to ground state levels were recognized and included in the total capture cross section during processing. Therefore, cross sections for isotopes with a significant branching fraction leading to metastable states were systematically underestimated.

The FENDL data discrepancies in the card-image library do not apply to the binary libraries for most isotopes because problem-dependent data from ENDF/B-V evaluations are used to update the card-image data. However, some FENDL data are retained when ENDF/B-V cross sections are not available.

It was also observed that several high-energy threshold reaction cross sections changed for transitions that do not have metastable product states. Further analysis found the cause to be associated with temperature broadening of the pointwise FENDL data by an AMPX routine that incorrectly shifted the cross-section data by one energy grid point. For threshold reactions with relative coarse energy grid points and peak reaction rates occurring near the threshold energy, this shift caused significant changes in the group cross-section values. The updated data were generated without temperature broadening.

Changes were made to the library data processing routines to include all branching transitions in calculating the cross sections required by ORIGEN, and the library was regenerated. The number of cross-section changes is extensive. A summary of all cross-section values that changed by more than 1% is listed in a separate file www.ornl.gov/sci/scale/downloads/origen-libraries-update-details.txt. These changes will result in minor changes (typically less than 1%) in some of the SCALE sample problems that depend on ORIGEN-S or ORIGEN-S data (e.g., ORIGEN-S, OPUS, TRITON, SAS1, SAS2).

More Words to the Wise …

Am-241 and Am-243 Update for ENDF/B-VI 238-Group Library

The Am-241 and Am-243 fission data in the ENDF/B-VI 238-group library (i.e., V6-238) were corrected and posted under SCALE 5.1 Updates, on the SCALE Download web page in August 2007.

Critical mass calculations for Am-241 and Am-243 revealed errors in the multigroup fission data for these nuclides due to an error in AMPX module Y12, which incorrectly processed the Madland-Nix fission spectrum such that neutron energy transfers were only allowed down in exit energy from the incident energy. The error has been corrected, and the data for these nuclides have been regenerated. The impact is significant only for criticality mass calculations involving these nuclides alone, where the calculated k_{eff} values were more than 75% lower. In particular, the impact is negligible on spent nuclear fuel and mixed oxide (MOX) fuel cases. For fast critical Pu benchmark systems that contain Am, an increase of 0.1 to 0.3% in the calculated k_{eff} value was observed.

Table 1 compares calculated k_{inf} values of some actinides using various library and code options. The Monte Carlo uncertainties are less than 0.0001 for all cases. The first column of calculated values is based on SCALE 5.1 with the update for Am-241 and Am-243. Note that the continuous energy (CE) SCALE/KENO results are based on a prereleased version of SCALE 6 and are considered preliminary. The MCNP and KENO CE results for ENDF/B-VI.8 agree well, except for Cm-245, Cm-246, and Pu-244, which are within 5%. Further data testing and validation are planned before the SCALE 6 release.

Table 1. Infinite system eigenvalue calculations for various minor actinides and U-238

	SCALE/KENO			MCNP
	Multigroup (MG)	Continuous Energy (CE)		CE
Nuclide	ENDF/B-VI.7 (V6-238)	ENDF/B-VI.7	ENDF/B-VI.8	ENDF/B-VI.8
Am-241	1.98892[a]	1.99042	1.99042	1.99359
Am-243	1.67868[a]	1.67907	1.67878	1.68339
Cm-244	2.64497	2.65208	2.65208	2.64163
Cm-245	3.51176	3.51131	3.51131	3.68778
Cm-246	2.47498	2.46826	2.46826	2.39581
Np-237	1.70622	1.69346	1.69346	1.70136
Pu-236	2.87376	2.87444	2.8746	2.8736
Pu-237	3.05102	3.05734	3.05734	3.05118
Pu-238	2.76152	2.76246	2.76246	2.76108
Pu-239	2.98078	2.98276	2.98305	2.98584
Pu-240	2.26748	2.27231	2.27185	2.26199
Pu-244	1.57976	1.61728	1.61704	1.57321
U-234	1.52667	1.52904	1.5291	1.52025
U-235	2.27339	2.27777	2.27161	2.27585
U-236	0.73695	0.73903	0.73907	0.73056
U-238	0.34632	0.34478	0.34465	0.33961

[a] Updated Am-241 and Am-243 cross sections

Recent SCALE Publications and Presentations

Presentations from the ANS Special Session on SCALE are accessible from the SCALE website.

Recent SCALE-related publications and presentations are available on the SCALE website. The link is near the bottom of the home page. Below are publications from the second half of 2007.

S. M. Bowman, "Overview of the SCALE Code System," *The American Nuclear Society and the European Nuclear Society 2007 International Conference on Making the Renaissance Real,* November 11–15, 2007, Washington, D.C., *Trans. Am. Nucl. Soc.* **97**, 589–591 (2007).

M. L. Williams, S. M. Bowman, and C. V. Parks, "Plans for Future SCALE Development Beyond Version 6.0," *The American Nuclear Society and the European Nuclear Society 2007 International Conference on Making the Renaissance Real,* November 11–15, 2007, Washington, D.C., *Trans. Am. Nucl. Soc.* **97**, 606–607 (2007).

S. Goluoglu, S. M. Bowman, and M. E. Dunn, "KENO Monte Carlo Code Capabilities," *The American Nuclear Society and the European Nuclear Society 2007 International Conference on Making the Renaissance Real,* November 11–15, 2007, Washington, D.C., *Trans. Am. Nucl. Soc.* **97**, 592–594 (2007).

Germina Ilas, Brian D. Murphy, and Ian C. Gauld, "Overview of ORIGEN-ARP and Its Applications to VVER RBMK," *The American Nuclear Society and the European Nuclear Society 2007 International Conference on Making the Renaissance Real,* November 11–15, 2007, Washington, D.C., *Trans. Am. Nucl. Soc.* **97**, 601–603 (2007).

Douglas E. Peplow, Edward D. Blakeman, and John C. Wagner, "Advanced Variance Reduction Strategies for Optimizing Mesh Tallies in MAVRIC," *The American Nuclear Society and the European Nuclear Society 2007 International Conference on Making the Renaissance Real,* November 11–15, 2007, Washington, D.C., *Trans. Am. Nucl. Soc.* **97**, 595–597 (2007).

J. C. Wagner, E. D. Blakeman, and D. E. Peplow, "Forward-Weighted CADIS Method for Global Variance Reduction," *The American Nuclear Society and the European Nuclear Society 2007 International Conference on Making the Renaissance Real,* November 11–15, 2007, Washington, D.C., *Trans. Am. Nucl. Soc.* **97**, 630–633 (2007).

Bradley T. Rearden, "TSUNAMI Sensitivity and Uncertainty Analysis Capabilities in SCALE 5.1," *The American Nuclear Society and the European Nuclear Society 2007 International Conference on Making the Renaissance Real,* November 11–15, 2007, Washington, D.C., *Trans. Am. Nucl. Soc.* **97**, 604–605 (2007).

Mark D. DeHart, "High-Fidelity Lattice Physics Capabilities of the SCALE Code System Using TRITON," *The American Nuclear Society and the European Nuclear Society 2007 International Conference on Making the Renaissance Real,* November 11–15, 2007, Washington, D.C., *Trans. Am. Nucl. Soc.* **97**, 598–600 (2007).

G. Ilas and I. C. Gauld, "SCALE Analysis of CLAB Decay Heat Measurements for LWR Spent Fuel Assemblies," *Annals of Nuclear Energy,* **35**, 37-48 (January 2008).

Corrections and Updates to SCALE 5

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.*

Spring 2008 SCALE Training Courses at ORNL

Date	Title	Registration Fee*
March 31 – April 4, 2008	**ORIGEN-ARP/TRITON Course**	$1800
April 7–11, 2008	**KENO-VI Criticality Safety Course**	$1800

*After February 29, 2008, the registration fee will increase to $2100. A discount of $300 for each additional week 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.

OAK RIDGE National Laboratory

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