Oak Ridge National Laboratory

SCALE Newsletter

Number 32 July 2005

Special points of interest:

- SCALE 5.1 scheduled for late 2005
- SCALE workshops in Oct./Nov. at ORNL; $300 discount until September 17

Inside This Issue:

Coming Attractions: SCALE 5.1 and ORIGEN-ARP 5.1

The release of SCALE 5.1 is rapidly approaching. ORIGEN-ARP 5.1 will be included as a separate smaller package within SCALE 5.1 for users who want to upgrade from ORIGEN2 but do not want the entire SCALE package. Including the ORIGEN-ARP package within SCALE assures ORIGEN users that they are using the same state-of-the-art software as SCALE users and provides them with the possibility to upgrade their installation to the full SCALE package at no additional cost.

SCALE 5.1 will include the following important enhancements:

- ENDF/B-VI cross-section libraries (both multigroup and continuous energy)
- 3-D Monte Carlo–based depletion with KENO V.a or KENO-VI coupled to ORIGEN-S in TRITON
- New 2-D geometry in TRITON/NEWT based on the KENO-VI format
- Improved resonance and thermal treatments in CENTRM
- Target irradiation capability in ORIGEN-ARP
- New ARP libraries and a more rigorous interpolation scheme in ARP for ORIGEN-ARP depletion
- HTML output in KENO V.a
- Enhanced sensitivity/uncertainty tools in TSUNAMI

For more detailed information on these topics, refer to the January 2005 issue of the *SCALE Newsletter.*

Currently the SCALE staff is working to complete software testing, configuration control, and documentation. The SCALE 5.1 package is expected to be available from the Radiation Safety Information Computational Center (RSICC) before the end of the year. Users are encouraged to join the SCALE News E-mail List. These users will be notified the day that SCALE 5.1 is available.

Notice to International Users

Due to delays in the signing of the Organization of Economic Cooperation and Development / Nuclear Energy Agency (OECD/NEA) agreement, SCALE 5(and soon SCALE 5.1) is not available from the OECD/NEA Data Bank. However, the latest version of SCALE is available to all international users on an individual license basis from the RSICC at Oak Ridge National Laboratory (ORNL). Contact RSICC to request a copy of SCALE.

SCALE 5.1 Tutorials at NCSD Topical Meeting

Two tutorials on new capabilities in SCALE 5.1 are being conducted at the American Nuclear Society (ANS) Nuclear Criticality Safety Division (NCSD) Topical Meeting in Knoxville, Tennessee. The tutorials are scheduled for the afternoon of Sept. 22 and the morning of Sept. 23 and are free to conference registrants who preregister. Note that seating is limited. The topics and brief descriptions follow.

3-D Monte Carlo Depletion with KENO in SCALE 5.1

Advanced reactor designs, evolutionary concepts, and non-reactor applications such as safeguards, security, and nonproliferation, require robust geometrical modeling capabilities to accurately model neutron transport for complex configurations. Monte Carlo transport methods offer the type of flexibility needed for such applications but present other difficulties not encountered in deterministic transport

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SCALE 5.1 Tutorials at NCSD Topical Meeting

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methods. Code sequences have been developed (using the KENO V.a and KENO-VI Monte Carlo transport codes in SCALE) to perform Monte Carlo–based depletion coupled with ORIGEN-S in TRITON. Use of these new code sequences will be discussed in detail.

Enhanced Resonance Self-Shielding in SCALE 5.1

SCALE resonance processing capabilities have recently been expanded. Systems that employ doublyheterogeneous fuel types can now be modeled within the user-friendly sequences CSAS, CSAS6, and TRITON. In addition, an inverse Dancoff calculation method has been implemented. This method allows calculation of a pitch for a uniform lattice given the Dancoff factor of a nonuniform lattice. The inverse Dancoff feature is useful in determining the pitch to be used in nonuniform lattice cell calculations in CENTRM that preserves the Dancoff factor. Theory and use of these new features will be discussed.

New Validation Reports on CENTRM and KENO-VI

CENTRM and KENO-VI validations include more than 160 benchmarks from theICSBEP Handbook.

Validation of CENTRM and KENO-VI using ENDF/B-V nuclear data were recently documented in ORNL/TM-2004/66 and ORNL/TM-2004/60, respectively. These reports are available on the SCALE Criticality Safety Validation web page: http://www.ornl.gov/sci/scale/criticality_safety.htm.

The objective of these reports is to document the validation for the use of the CENTRM/PMC resonance processing codes and the KENO-VI Monte Carlo code over a wide range of applications using SCALE 5. Both validations consist of 164 critical configurations from 17 experiments. The CENTRM/PMC validation report also includes a set of 30 OECD/NEA calculational benchmarks. All but one of the experiments and the critical configurations are listed in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook. The one critical configuration not listed in the ICSBEP Handbook is from a set of mixed-oxide (MOX) experiments with gadolinium poison that was performed at Pacific Northwest National Laboratory (PNNL). The calculational benchmarks consist of a set of MOX pellets in a uranyl nitrate solution at various uranium enrichments and concentrations.

The experiments are divided into seven chapters based on the type of fuel: high-enriched uranium fuel, intermediate-enriched uranium fuel, low-enriched uranium fuel, mixed plutonium/uranium fuel, plutonium metal fuel, ^{233}U fuel, and OECD calculational benchmarks. The calculational benchmarks use XSDRNPM instead of KENO-VI to calculate the system criticality. Each experiment is briefly described in a separate section in its appropriate chapter. At the end of each chapter, a separate section analyzes all the experiments in the chapter and examines any trends in the data. All results are compared with the benchmark k-eff and uncertainty in the ICSBEP Handbook, except for the OECD/NEA calculational benchmarks, which are compared with MCNP results. The SCALE 5 results compare well with the results listed in the ICSBEP handbook and the MCNP results.

Updates Available to Download

This update could potentially affect any TSUNAMI-3D problem that uses the mesh flux option.

CENTRM and KENO-VI validation input files are available. Updated versions of LWR critical experiments from NUREG/CR-6361 can also be downloaded.

TSUNAMI

This update corrects several minor errors identified in TSUNAMI-1D and TSUNAMI-3D. Affected modules include BONAMIST, NITAWLST, and KENO V.a. This update also includes the SAMS update that was previously posted in February on the SCALE Download web page.

The updated versions of BONAMIST and NITAWLST (with associated SENLIB update) allow certain problems to run on Windows that previously failed due to hard-coded storage parameters. Problems that would previously run are not affected by these updates.

KENO V.a has been modified to correct errors in the mesh flux tallies used for sensitivity coefficient generation with TSUNAMI-3D. Errors were identified that particularly affect models where the size of the mesh interval is smaller than a mean free path and where a mesh interval is closely, but not exactly, aligned with a geometry boundary. This update could potentially affect any TSUNAMI-3D problem that uses the mesh flux option. Other KENO V.a calculations, such as CSAS25, that do not use the mesh flux option are not affected by this update. This update to KENO V.a does contain the correction for the HOLE error that was posted earlier.

CENTRM/KENO-VI Validation Input Files

The input files used for the CENTRM and KENO-VI validation calculations (see "New Validation Reports on CENTRM and KENO-VI" article) are provided on the SCALE Download web page for user convenience. These cases demonstrate the validity of the codes and data used. Users should perform their own validation studies using benchmark cases that are relevant to their particular applications.

The benchmark cases from these two reports are identical, except for the resonance self-shielding of the cross sections. The CENTRM validation cases use the "PARM=CENTRM" option to invoke CENTRM and PMC to process the resonance data, while the KENO-VI validation cases use NITAWL for resonance processing. Note that some of these cases may require 6 or more hours of CPU time. The entire benchmark set for each code took over 200 CPU hours on late-model Unix workstations at ORNL. Users can expect that each set (CENTRM and KENO-VI) will require approximately 1 to 2 weeks of CPU time on most modern computers.

LWR Benchmark Cases

NUREG/CR-6361, *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*, Appendix A, contains SCALE input files for 180 benchmark cases. The original input files were posted on the SCALE website in 1997. Two input files from the original posting were updated in 2000. The calculated k-eff values for the corrected files were not statistically different from those published in NUREG-6361.

All files have now been updated for compatibility with SCALE 5 by using GeeWiz to convert them. Some of the files required manual modifications.

Most of these were minor adjustments for nuclide distributions that did not sum to 100%. Special thanks to Maik Hennebach of WTI GmbH and Franz Hilbert of Nuclear Cargo + Service GmbH for their contributions to these adjustments.

Origen-Arp

Version 5.01 of the OrigenArp user interface for Windows contains minor corrections. In particular, the lowercase "f" keyboard character did not work in Version 5.0. That bug has been fixed.

Words to the Wise . . . KENO V.a HOLE Error

A corrected version of KENO V.a for SCALE can be downloaded from the SCALE

A bug was discovered in KENO V.a that under very specific conditions will cause a neutron to skip a HOLE. This may cause a case to run and produce an incorrect calculated k-eff value with no warning. The condition arises when the end face of a HOLE whose outer boundary is a cylinder or hemicylinder shares a common boundary with another HOLE, region, or unit.

We sincerely regret the impact that this error has had on many users and apologize for the inconvenience caused. Although a number of users have had to rerun many validation cases, no one has reported any significant impact on previous results.

This error occurs due to numerical round-off. The HOLE passes the geometry-checking portion of KENO. However, when a particle tries to cross inward to the HOLE, the boundary of the HOLE is rounded off such that the initial point of the current track is already inside the HOLE. Because the point is already inside the HOLE, it does not cross into it. This occurs only when another region and the cylindrical HOLE share a top or bottom boundary and the machine causes a round-off error that makes the HOLE appear to be at or outside the other region in one check and then inside the HOLE later. A particle will still correctly pass through the side of the cylinder, regardless of the condition at the top or bottom. The same model will experience different round-off on different machines and with different compilers, so the performance is unpredictable. However, we believe this problem very rarely causes erroneous results. These same checking and crossing procedures have been in place in KENO V.a for about 20 years, and this is the first time the problem has been detected.

The error was corrected, and an updated version of KENO V.a for SCALE 5 was posted on the SCALE website. Subscribers to the SCALE News E-mail Notification List were notified of this error in March, and a notice was also posted on the website.

User Notebooks Provide Online Technical Assistance

Electronic user notebooks are provided on the SCALE and RSICC websites to provide users with a forum where they can post questions, discuss items of technical interest, and find answers to frequently asked questions (FAQs). The five SCALE-related user notebooks are listed below.

Click on any of these links to view the notebooks.

SCALE 5 User Notebook
SCALE 4 User Notebook
KENO3D User Notebook
ORIGEN-ARP User Notebook
TRITON User Notebook

Special Session on SCALE at American Nuclear Society (ANS) Meeting

A special session titled "SCALE State-of-the-Art Analysis Tools" was conducted at the annual ANS meeting in San Diego, California, on June 6–9, 2005. The session was organized by the SCALE Project Leader Steve Bowman and featured eight papers by ORNL staff and students. More than 50 participants attended the session. The following topics were included:

- Overview of Advances in SCALE Development
- Continuous-Energy Version of the SCALE Control Modules for Use with Continuous-Energy KENO V.a and KENO-VI
- Recent Enhancements to the SCALE 5 Resonance Self-Shielding Methodology
- Continuous-Energy Multidimensional Sn Transport for Problem-Dependent Resonance Self-Shielding Calculations
- ENDF/B-VI Library Generation and Testing for the SCALE Code System
- Advances in the TSUNAMI Sensitivity and Uncertainty Analysis Codes Beyond SCALE 5
- Assessment of TRITON and PARCS for Full-Core MOX Fuel Calculations
- GeeWiz: Integrated User Interface for SCALE

Click on any title to view the presentation slides.

Fall 2005 SCALE Training Courses at ORNL

Date	Title	Registration Fee*
Oct. 17–21, 2005	**SCALE Source Terms and Shielding Course**	$1800
Oct. 24–28, 2005	**KENO V.a Criticality Safety Course**	$1800
Oct. 31–Nov. 3, 2005	**TSUNAMI Sensitivity/Uncertainty Tools (Experienced KENO users only)**	$1500

*A late fee of $300 will be applied after September 17, 2005.
A discount of $600 for each additional week will be applied for registration to multiple courses.
Foreign nationals must register at least 40 days 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.

NSTD The Nuclear Science and Technology Division

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