Oak Ridge National Laboratory

SCALE Newsletter

Number 38 **July 2008**

Special Points of Interest:

- SCALE workshops in October, 2008 at ORNL; $300 discount until September 13, 2008.
- SCALE 6 to be released in December.

Inside This Issue:

Continuous Energy Capability in KENO for SCALE 6

The capability to use continuous energy nuclear data has been implemented and thoroughly tested in the KENO-V.a and KENO-VI Monte Carlo criticality codes for release in SCALE 6. (The expected release date of SCALE 6 from RSICC is December 2008.) Both KENO codes can perform the neutron transport calculations in either multigroup (MG) or continuous energy (CE) mode. The energy treatment mode is automatically selected based on the cross-section library name when KENO is invoked by the CSAS (Criticality Safety Analysis Sequence) control module CSAS5 or CSAS6.

A crucial aspect of this new KENO capability is the CE nuclear data libraries generated by the AMPX code system, which provides processed nuclear data libraries that are completely independent from the widely used NJOY system. Hence the CE capability and data in KENO provide a truly independent CE capability.

New Features in CE Mode

Current SCALE 5.1 versions of KENO use the MG cross-section treatment in the transport simulation, which allows these codes to execute and calculate the desired parameters much faster than codes that use the CE treatment. When MG cross sections are generated using proper weighting functions, the results are typically very accurate. However, for certain problem types where appropriate MG cross sections may not be available or the suitability of the MG cross sections is questionable, it is highly desirable to have the CE capability for routine and/or reference calculations.

The CE capability in KENO uses AMPX-generated CE cross-section data specifically designed for KENO. Changes to the input structure have been minimized to enable SCALE users to easily modify their existing KENO input models. The SCALE user simply replaces the MG cross-section library name with the CE cross-section library name in the CSAS input file.

In CE mode, KENO automatically calculates the (n,2n) and (n,3n) reactions in addition to fissions, absorptions, and leakage. By default, the code samples from the prompt and delayed fission spectra. A new input parameter has been added to allow sampling using the prompt fission spectrum only.

In addition, a new parameter has been added to the KENO parameter data to allow easy binning of integral values such as fluxes and absorptions in one of the existing SCALE MG energy-group structures. Users may also specify their own energy-group structure to be used for binning calculated results.

CE Data in SCALE 6

CE cross-section libraries based on ENDF/B-VI Release 8 and ENDF/B-VII Release 0 evaluations have been prepared using the AMPX code system. Both sets of cross sections have been generated to an energy tolerance of 0.1% for multiple temperatures: 293, 600, 900, 1200, and 2400 K. A plot of the ENDF/B-VII.0 ^{238}U capture cross-section data at 293 K is provided in Figure 1. In addition, cross sections for nuclides with thermal scattering data have been generated at the temperatures that are provided in the corresponding ENDF/B evaluation files. Although temperature interpolation of cross sections is not yet available in the CE mode of KENO, the availability of multiple temperature cross sections allows analysis of high-temperature systems.

(Continued on page 2)

Continuous Energy Capability in KENO for SCALE 6

(Continued from page 1)

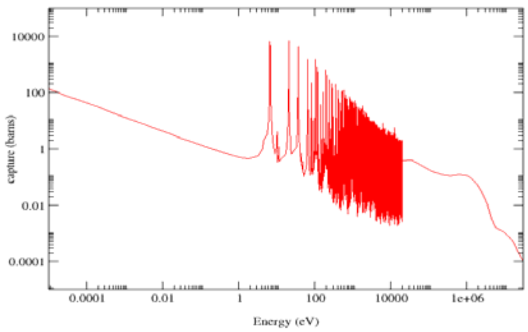

Figure 1. Continuous Energy ENDF/B-VII.0 ^{238}U capture at 293 K

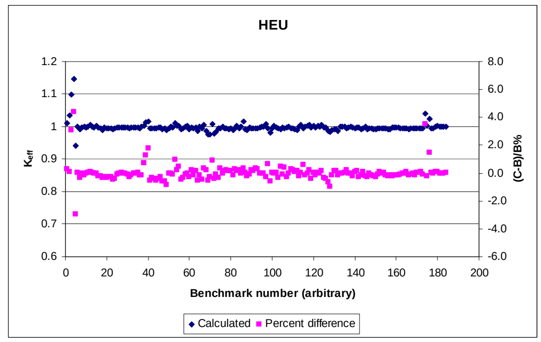

Figure 2. Continuous Energy validation results for highly enriched uranium (HEU) benchmarks.

Validation of KENO CE Methods and Data

Critical benchmark experiments that include a wide variety of fissile systems in various moderator and reflector configurations have been used to validate the KENO CE methodology and data. More than 500 benchmark problems in six categories (HEU, LEU, IEU, MOX, Pu, ^{233}U) have been modeled and analyzed.

Plots of the ENDF/B-VII validation results for the HEU and LEU experiments are shown in Figures 2 and 3, respectively, as examples. Results for the other benchmark categories are similar. The dark blue points are the calculated k_{eff} values and are aligned with the left Y-axis, showing that most cases are near k_{eff} = 1.0. The bright pink points are the percent difference between calculated and benchmark k_{eff} values and are aligned with the right Y-axis, showing that most values are near 0.0.

Although there are some benchmark cases in these groups that calculate poorly, calculations reported by the evaluators of these benchmarks using other code and data sets show similar poor agreement. Oak Ridge National Laboratory (ORNL) staff will continue to investigate anomalous results and make corrections to the data where needed prior to the release of SCALE 6.

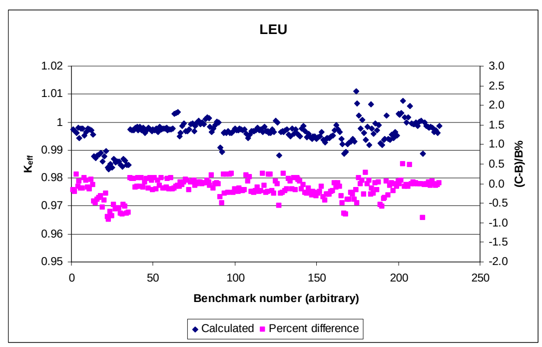

Figure 3. Continuous Energy validation results for low enriched uranium (LEU) benchmarks.

Use of TSUNAMI-3D with Large Models

TSUNAMI-3D has been successfully applied to very large and complex models, such as pin-by-pin models of full-core power reactors with distributed burnup. For example, the model in Figure 1 modeled each pin explicitly with 18 axial zones and calculated sensitivity coefficients for approximately 47,000 nuclides results in approximately 420,000 sensitivity profiles in 238 energy groups. Successful completion of these calculations requires that the computer system on which they are run be appropriately configured. Because CENTRMST and KENO V.a can require large amounts of random access memory (RAM) and temporary disk space for intermediate files, the Linux cluster at ORNL has been configured as follows.

Each node has multiple 64-bit AMD processors with 16 or 32 GB of RAM and 500 MB of hard disk space dedicated to the temporary directory (/var/tmp). Additionally, the system limitations for sizes were essentially removed to allow any single job to access as many resources as possible. The "ulimit -a" command on one node returns the following information, which will be valuable to a system administrator.

core file size	(blocks, -c) 0
data seg size	(kbytes, -d) unlimited
file size	(blocks, -f) unlimited
pending signals	(-i) 1024
max locked memory	(kbytes, -l) unlimited
max memory size	(kbytes, -m) unlimited
open files	(-n) 1024
pipe size	(512 bytes, -p) 8
POSIX message queues	(bytes, -q) 819200
stack size	(kbytes, -s) unlimited
cpu time	(seconds, -t) unlimited
max user processes	(-u) 268288
virtual memory	(kbytes, -v) unlimited
file locks	(-x) unlimited

Once the machine is appropriately configured, SCALE must be built in 64-bit mode. The Linux binaries distributed with SCALE 5.1 are 32-bit and cannot address more than 4 GB of RAM. Please consult your compiler documentation for information on compiling the Fortran and C source files in 64-bit.

For spent fuel models, CENTRMST typically requires 6 to 8 GB of RAM to compute pointwise fluxes and the sensitivities to every nuclide in the model. These CENTRMST cases can run for 2 hours or more for each pin cell. For large geometries with fine spatial meshes, KENO V.a can require 5 to 10 GB of RAM. For these types of models, the following input parameter data are recommended to ensure adequate sampling and convergence of the forward

gen=10000	sample for up to 10,000 generations
npg=100000	sample 100,000 particles per generation for the forward calculation; note that 300,000 particles per generation will be sampled for the adjoint calculation
nsk=50	skip 50 generations for the forward case before accumulating fluxes; note that 150 generations will be skipped for the adjoint calculation
sig=0.0005	stop the forward calculation when the calculated k_{eff} value is converged to a standard deviation of 0.0005
asg=0.001	stop the adjoint calculation when the calculated k_{eff} value is converged to a standard deviation of 0.001

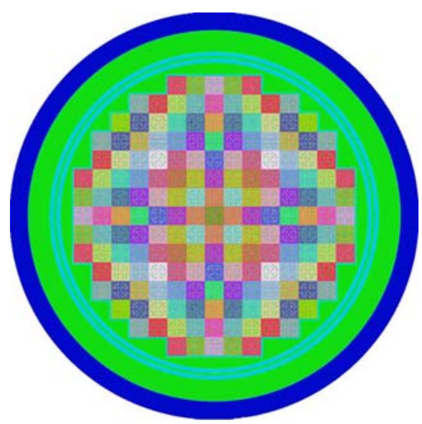

Figure 1. Full core PWR model.

(Reference**:** G. Radulescu, D. E. Mueller, and J. C. Wagner, *Sensitivity and Uncertainty Analysis of Commercial Reactor Criticals for Burnup Credit*, NUREG/CR-6951 (ORNL/TM-2006/87), prepared for the Nuclear Regulatory Commission by Oak Ridge National Laboratory, Oak Ridge, TN, December 2007.)

SCALE TSUNAMI Training Course in Budapest, Hungary

The Organisation for Economic Co-operation and Development (OECD)/Nuclear Energy (NEA) Data Bank is hosting a training course from **13 to 17 October 2008** on sensitivity and uncertainty analysis using the SCALE TSUNAMI sequence at the Hungarian Academy of Sciences KFKI Atomic Energy Research Institute. The course is open to participants in the Expert Group on Uncertainty Analysis in Modeling (UAM) and others from the OECD/NEA member countries who wish to get training in this important area of application. The course is being held in support of the first phase of the UAM activity concerned with neutronics in reactor cores and various other activities, including multi-scale / multi-physics uncertainty analysis, radiation shielding, and criticality margin assessments.

The course will provide hands-on training with the TSUNAMI code sequence. More information may be found in the online Syllabus and Registration Form.

The course is organized by the OECD NEA Data Bank and the SCALE project team with the support of the Radiation Safety Information Computational Center (RSICC). It will be taught by SCALE team members from Oak Ridge National Laboratory.

The deadline for registration is **31 August 2008**. The number of participants is limited to about 20. Registered participants will receive further information on request or after the registration deadline.

Recent SCALE Publications and Presentations

Recent SCALE-related publications and presentations are available on the SCALE Web site. The link is near the bottom of the home page. Below are publications from the first half of 2008.

D. E. Peplow, T. M. Evans, and J. C. Wagner, "Simultaneous Optimization of Tallies in Difficult Shielding Problems," presented at ICRS-11/RPSD-2008, Pine Mountain, GA, April 13–18, 2008.

A.M. Fleckenstein and B. T. Rearden, "Extensible SCALE Intelligent Text Editor - ExSITE," *Trans. Am. Nucl. Soc.* **98**, 223–226 (2008).

J. C. Wagner, D. E. Peplow, and T. M. Evans, "Automated Variance Reduction Applied to Nuclear Well-Logging Problems," presented at ICRS-11/RPSD-2008, Pine Mountain, GA, April 13–18. 2008.

Updates for 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.*

Fall 2008 SCALE Training Courses at ORNL

Date	Title	Registration Fee*
October 13–17, 2008	KENO V.a Course	$1800
October 20–24, 2008	ORIGEN-ARP/TRITON Course	$1800
October 27–31, 2008	KENO-VI/MAVRIC Course	$1800
November 3–7, 2008	TSUNAMI Sensitivity/Uncertainty Tools Course (Experienced KENO users only.)	$1800

*After September 13, 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.

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