SCALE Newsletter

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In This Issue

High-Fidelity Reactor Modeling with KENO

Andrew T. Godfrey

Recent advances in SCALE's continuous-energy Monte Carlo capabilities have enabled high-fidelity reference solutions for reactor modeling within the Consortium for Advanced Simulation of Light Water Reactors (CASL), a US DOE Energy Innovation Hub that is focused on advanced modeling and simulation of commercial pressurized water reactors (PWRs). Currently in its fourth year, CASL has steadily demonstrated progress towards completing a high-fidelity, multi-physics, largely parallel reactor core simulation capability, recently completing an analysis of the initial startup physics testing of Tennessee Valley Authority's (TVA) Watts Bar Nuclear Unit 1 (WBN1). From the beginning of the consortium, which is led by Oak Ridge National Laboratory (ORNL), CASL has depended on SCALE developers and software components for its success and in return has significantly contributed to the latest SCALE capabilities, testing, and validation bases.

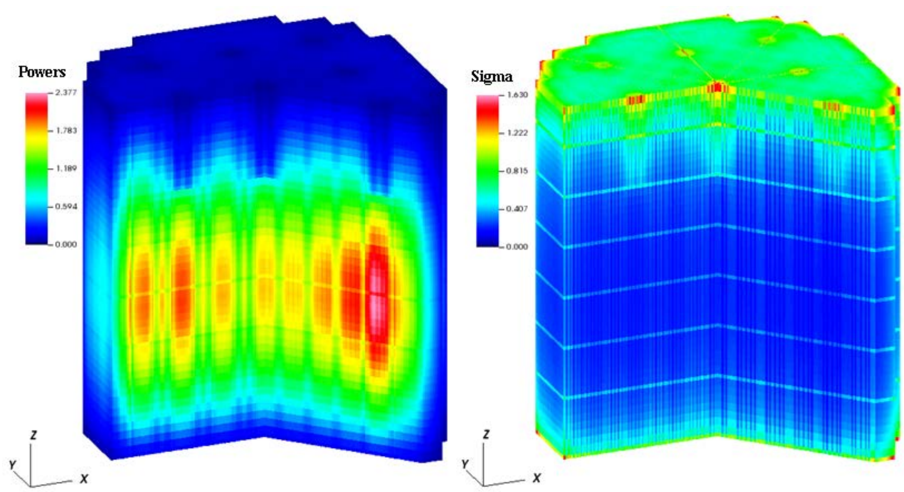

Figure 1. KENO-VI 3D normalized fission rates and uncertainties for initial WBN1 criticality

In beta testing the latest capabilities in SCALE 6.2 (including parallel calculations with KENO, greatly reduced memory footprint, improved accuracy, and problem-dependent temperature corrections), CASL has generated over 120 continuous-energy Monte Carlo neutronics reference solutions for PWR fuel geometries ranging from single pin-cells up to 3D quarter-core reactor models. Results from these high-fidelity models include eigenvalues and pin-by-pin fission rate distributions. These results are based on publicly available data, including comparisons to measured plant data when available, and have been released by CASL. For example, the 3D pin-by-pin normalized power for WBN1 initial criticality is shown in Figure 1. (continued on next page)

High-Fidelity Reactor Modeling with KENO (cont.)

CASL has benchmarked the SCALE 6.2 Beta CSAS6 sequence, utilizing the improved continuous-energy ENDF/B-VII.0 data and KENO-VI, against the initial startup physics tests of WBN1. These include measurements at isothermal zero power conditions of reactor criticality, control bank reactivity worths, differential boron worth, and the moderator temperature coefficient. For criticality, 10 conditions were selected for simulation, including the initial configuration, all-rods-out, and insertions of each of eight control banks. For the bank worths, the KENO-VI calculations were performed consistently with methodology originally employed for rod swap, including recalculation of the "shadow factors" for inferring the measured worths.

The KENO input for these models was generated by a pre-processor developed by CASL, which created a unique unit for every region in the core where a fission rate tally was needed (a mesh tally option has recently been added to KENO for this purpose). The model includes significant detail, including fuel rod plenums and end gaps, spacer grids, inserted annular Pyrex burnable absorbers and solid AIC/B_4C hybrid control rods, radial structures such as the core baffle, barrel, neutron pad, and vessel, and homogenized assembly nozzles and lower and upper core plates, all with cold dimensions. The input contained over 800,000 units and over 14,000 arrays for nearly 9.5 million total lines of input. Additionally, CASL developed a post-processor that converted the fission rate tallies and uncertainties by unit to a normalized power distribution for comparison with results from other neutronics methods. A graphic depicting the WBN1 model is shown in Figure 2, produced mainly by the PLOT block in the KENO input.

The majority of the KENO-VI cases were executed on Idaho National Laboratory's Fission supercomputer using 300 parallel computing cores, each with access to approximately 4 GB of memory. A total of 7.5 billion particles were used, with 5 million per generation, skipping 500 generations. These runs required about 44 hours each and resulted in an estimated eigenvalue uncertainty of <1.2 pcm. However, an even higher-fidelity result was desired as a reference for the power distribution.

One calculation was executed on Fission to better resolve the 3D pin-by-pin fission rate distribution using 180 parallel computing cores, each with access to approximately 11 GB of memory. In this calculation, 100 billion particles were used, with 10 million per generation, skipping 500 generations. This run took about 29 days and resulted in an estimated eigenvalue uncertainty of 0.25 pcm and a maximum fission rate uncertainty over all fuel rod locations (with 49 axial levels) of 1.63%. The 3D fission rate distribution resulting from this calculation is used by CASL for 3D pin-by-pin power distribution verification and was previously shown in Figure 1.

The criticality benchmark results are provided in Table 1. Of the 10 critical conditions selected, the average difference between KENO-VI and the WBN1 measurements is -129 pcm, and the maximum difference is -177 pcm. All the results are negative, indicating that KENO-VI consistently under predicts the plant reactivity, a bias expected when modeling low-enriched uranium systems with ENDF/B-VII.0 cross-section data. Several manual corrections were applied, including a small correction to adjust for the thermal scattering at 565K (the data is at 550K) of ~-43 pcm, a correction for thermal expansion of ~-57 pcm, and a correction for rotational symmetry for the SC and SD rod banks only (i.e., assumption of quarter core reflective symmetry is wrong when only one of these banks is inserted) of ~-53 pcm.

The comparisons to control bank reactivity worths are provided in Table 2. The Bank D worth was measured directly through system dilution, and then the subsequent banks were measured by swapping against Bank D. The worth of the swapped banks was inferred from the critical Bank D position when the test bank was fully inserted, using pre-calculated "shadow" factors from the core design methods at that time. These factors have been recalculated with KENO-VI and the inferred worths modified accordingly. All of the bank worths were slightly over predicted except for Bank B, with an average error of 2.9% and a maximum error of 6.4%.

The differential soluble boron worth (DBW) was calculated directly with KENO-VI and compares well to the measured value with a 0.56 pcm/ppm difference, as shown in Table 3. The isothermal temperature coefficient (ITC) was more difficult to calculate due to the small temperature perturbation (4°F), the lack of interpolation of thermal scattering data on temperature (a feature in development for KENO at the time of this calculation), and the statistical variation in Monte Carlo eigenvalues from case to case. To accomplish this, three components of the ITC were calculated separately and combined (the Doppler fuel temperature coefficient, the moderator density coefficient, and a moderator temperature-only coefficient to isolate the effects of thermal scattering). For the first two, coefficients were determined by fitting the KENO-VI results for several temperatures. After processing the results of 16 cases, the final ITC was calculated to be -1.01 pcm/°F different from the measured value.

Following the success of CASL in simulating WBN1, Westinghouse decided to perform a similar analysis of the initial startup testing of its new AP1000® reactor design for the CASL first "Test Stand" release. A Test Stand is a delivery of CASL products to a potential end user for early applications. CASL again utilized CE KENO-VI to generate numerical reference solutions for the AP1000 comparisons, including over 67 more cases ranging from 2D fuel lattices up to a 3D quarter-core model of the AP1000. The results are documented in a publicly available report.

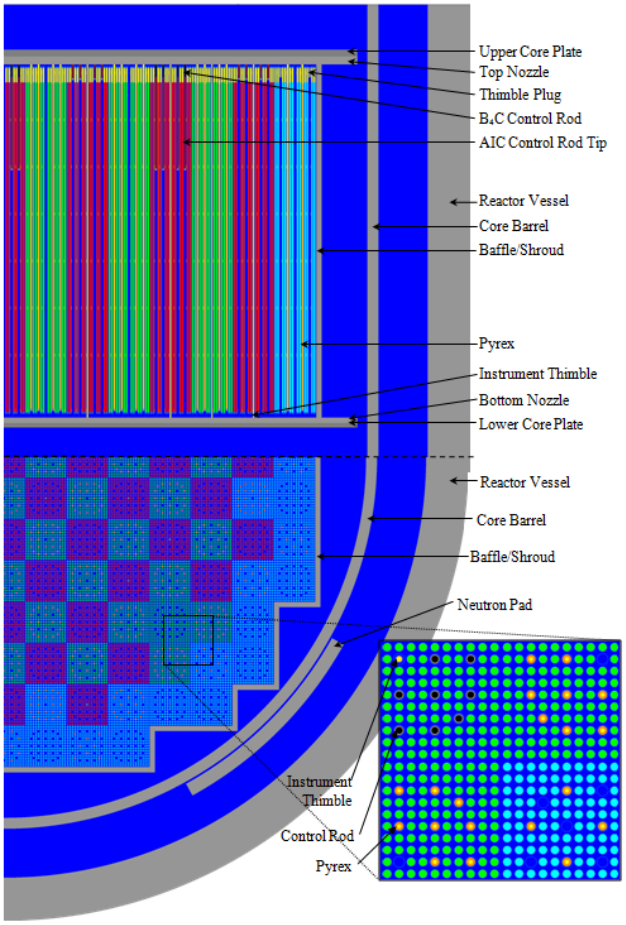

Figure 2. KENO-VI model of Watts Bar Unit 1 Cycle 1

For more information on these models and data as well as the CASL project, please see the following:

- www.casl.gov
- http://www.energy.gov/articles/five-years-building-next-generation-reactors-0
- J.C. Gehin et al., "Operational Reactor Model Demonstration with VERA: Watts Bar Unit 1 Cycle 1 Zero Power Physics Test," CASL-U-2013-0105-001, CASL, August 2013. http://www.casl.gov/docs/CASL-U-2013-0105-001_final.pdf
- http://www.ornl.gov/ornl/news/news-releases/2014/7233c6c8-55e6-4a77-9ff9-f6954e79c365
- F. Franceschini et al., "Westinghouse VERA Test Stand - Zero Power Physics Test Simulations for the AP1000 PWR," CASL-U-2014-0012-001, CASL, March 2014. http://www.casl.gov/docs/CASL-U-2014-0012-001.pdf

Table 1. KENO-VI Criticality Results for WBN1

Condition	Bank D Position (steps withdrawn)	k-effective*	Difference (pcm)
Initial	167	0.99933	-67 ± 1
ARO	230	0.99975	-25 ± 1
Bank D Inserted	18	0.99852	-148 ± 1
Bank C Inserted	119	0.99847	-153 ± 1
Bank B Inserted	113	0.99879	-121 ± 1
Bank A Inserted	97	0.99823	-177 ± 1
Bank SD Inserted	71	0.99841	-159 ± 1
Bank SC Inserted	71	0.99841	-159 ± 1
Bank SB Inserted	134	0.99876	-124 ± 1
Bank SA Inserted	69	0.99845	-155 ± 1
Average		**0.99871**	**-129 ± 1**

* standard deviation = 0.00001 for all cases

Table 2. KENO-VI Control Bank Worth Results for WBN1

Bank	Measured Worth (pcm)	Calculated Worth (pcm)	Difference (%)
D	1342	1386 ± 2	3.3 ± 0.1
C	951	984 ± 2	3.5 ± 0.2
B	879	875 ± 2	-0.5 ± 0.2
A	843	898 ± 2	6.4 ± 0.2
SD	480	499 ± 2	4.0 ± 0.4
SC	480	499 ± 2	3.9 ± 0.4
SB	1056	1066 ± 2	1.0 ± 0.2
SA	435	447 ± 2	2.6 ± 0.4
Total	**6466**	**6654 ± 5**	**2.9 ± 0.1**

Table 3. KENO-VI Reactivity Coefficient Results for WBN1

	Measured	Predicted	Difference
Differential Boron Worth (pcm/ppm)	-10.77	-10.21 ± 0.02	**0.56**
Isothermal Temperature Coefficient (pcm/°F)	-2.17	-3.18 ± 0.04	**-1.01**

USLSTATS – Upper Safety Limit Statistics Program Update

Donald E. Mueller

USLSTATS is a statistical program for computing upper subcritical limits for criticality safety validation. Although USLSTATS has been deployed with recent releases of SCALE, it was developed outside formal SCALE software quality assurance as a post-processing utility.

Recently, a programming error affecting the calculation of USL-2 data was discovered in the Java-based version of USLSTATS distributed with SCALE 6.0–6.1. An astute user who was independently qualifying this code for use in his work noticed that for one of his calculations the USL-2 limits became 1.7% Δk more restrictive when using the same input file in the current version of USLSTATS relative to the SCALE 5.1 version. Investigation by the SCALE development team identified a coding error that was introduced during the conversion of the Fortran source code to Java for SCALE 6.0. The error affects only a small subset of USL-2 calculations where data are skewed towards one end of the trending range. The USL-2 is consistently computed when the data are fairly evenly split above and below the middle of the range.

The example calculations shown in Figure 3 utilize a data set that is heavily represented on the low side of the independent variable and exhibit the USL-2 error. The plot shows both the erroneous and correct USL-2 results.

Note that the error did not affect the more important USL-1 calculations. Typically, USL-2 is not used as a safety limit in criticality analysis validation studies. A corrected version of USLSTATS is available for download at http://scale.ornl.gov/downloads.shtml.

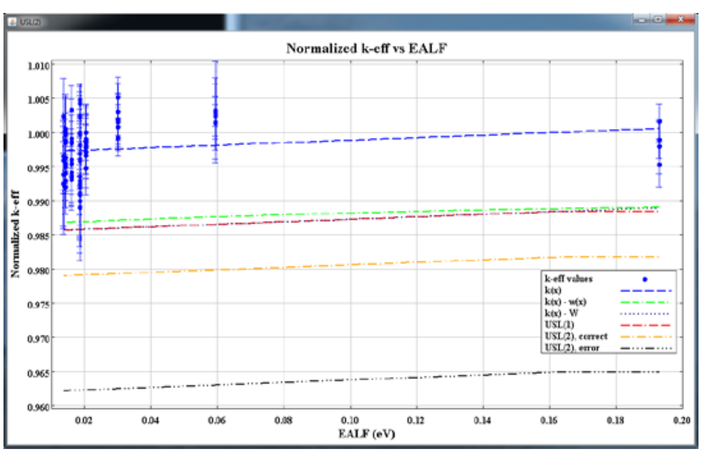

Figure 3. Example USLSTATS calculation with data skewed towards the lower end of the trending range

Resonance Absorber Control Rod Materials in TRITON

Brian J. Ade

The control rods in many PWR cores are composed of a mixture of three elements—silver, indium, and cadmium (AgInCd). Unlike B_4C, which is a common neutron poison with very few cross-section resonances, AgInCd contains many cross-section resonances. Because AgInCd is a resonance absorber, special self-shielding treatment is needed for this material when using multigroup physics in SCALE, such as those used in TRITON lattice physics calculations. It is recommended that the control rod be modeled using a "multiregion" unit cell specification that contains the control rod in the center, surrounded by a homogenized mixture of fuel, clad, and moderator, as shown in Figure 4. The resulting self-shielded mixtures should then be used in the construction of the 2D or 3D model. Proper self-shielding of the control rod material has an impact of ~2000 pcm for rodded calculations when compared to the default infinite homogeneous medium approximation for the AgInCd absorber.

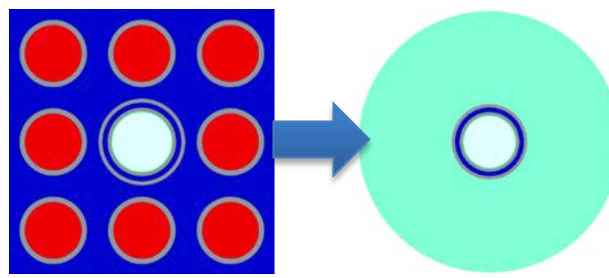

Figure 4. Generation of a multiregion model for the control rod

Modeling self-shielded control rods in SCALE/TRITON is counterintuitive for the user when branch calculations are being performed. For rodded branch calculations, a mixture exchange is performed in order to insert or remove control rod mixtures. SCALE/TRITON automatically swaps the mixture numbers in both the geometry portion of the input file ***and*** in the cross-section processing portion ("celldata" block) of the input file for rodded branches. Typically, the nominal or base branch corresponds to an unrodded condition. For the unrodded nominal depletion case, unrodded materials should be used in the celldata and the geometry blocks of the input file.

However, for unrodded histories, if the control rod mixtures are specified in the celldata section, the unrodded mixtures will be substituted for the rodded materials in the resonance self-shielding calculations for any rodded branches. The result of this treatment is that the control rod mixtures will not be self-shielded for rodded branches, leading to a bias of ~2000 pcm for rodded branches. The user must be cognizant of this issue when constructing a SCALE/TRITON model with any control rod mixtures that require self-shielding treatment. In short, the user should specify mixtures corresponding to unrodded conditions in the celldata section for unrodded histories and specify mixtures corresponding to rodded conditions for rodded histories. Examples of the incorrect and correct methods to input self-shielded control rod mixtures can be found below.

Incorrect:

```
=t-depl parm=(addnux=2, centrm)
...
read composition
  silver   1  den=10.16      0.85    581.34   end
  indium   1  den=10.16      0.15    581.34   end
  cadmium  1  den=10.16      0.05    581.34   end
  he-4     2  den=1.4485e-4 1.0     581.34   end
  ss304    3  den=7.8620     1.0     581.34   end

  h2o      4  den=0.65649    1.0000  581.34   end
  h2o      5  den=0.65649    1.0000  581.34   end
  h2o      6  den=0.65649    1.0000  581.34   end
...
end composition
read celldata
...
  multiregion cylindrical right_bdy=white end
      1    0.4000
      2    0.4400
      3    0.4900
    300    0.5600
    200    0.6000
    400    0.7109
    100    2.8490    end
end celldata
...
read branch
...
  define crin  1  2  3    end
  define crout 4  5  6    end
  cr=0 dm=0.65649 sb=0.0 tf=813.000 tm=581.34  end
  cr=1 dm=0.65649 sb=0.0 tf=813.000 tm=581.34  end
...
end branch
...
read model
...
unit 36
  com='guide tube'
  cylinder 10 0.4000
  cylinder 20 0.4400
  cylinder 30 0.4900
  cylinder 40 0.5600
  cylinder 50 0.6200
  cuboid 60 4p0.6300
  media 4    1 10
  media 5    1 20 -10
  media 6    1 30 -20
  media 311 1 40 -30
  media 211 1 50 -40
  media 311 1 60 -50
  boundary 60
...
end model
```

AIC control materials are **incorrectly** used in the celldata block for an unrodded "branch 0" condition

Branch 0 is unrodded

Water materials correctly fill guide tube for an unrodded "branch 0" condition

Correct:

```
=t-depl parm=(addnux=2, centrm)
...
read composition
  silver   1  den=10.16      0.85    581.34   end
  indium   1  den=10.16      0.15    581.34   end
  cadmium  1  den=10.16      0.05    581.34   end
  he-4     2  den=1.4485e-4 1.0     581.34   end
  ss304    3  den=7.8620     1.0     581.34   end

  h2o      4  den=0.65649    1.0000  581.34   end
  h2o      5  den=0.65649    1.0000  581.34   end
  h2o      6  den=0.65649    1.0000  581.34   end
...
end composition
read celldata
...
  multiregion cylindrical right_bdy=white end
      4    0.4000
      5    0.4400
      6    0.4900
    300    0.5600
    200    0.6000
    400    0.7109
    100    2.8490    end
end celldata
...
read branch
...
  define crin  1  2  3    end
  define crout 4  5  6    end
  cr=0 dm=0.65649 sb=0.0 tf=813.000 tm=581.34  end
  cr=1 dm=0.65649 sb=0.0 tf=813.000 tm=581.34  end
...
end branch
...
read model
...
unit 36
  com='guide tube'
  cylinder 10 0.4000
  cylinder 20 0.4400
  cylinder 30 0.4900
  cylinder 40 0.5600
  cylinder 50 0.6200
  cuboid 60 4p0.6300
  media 4    1 10
  media 5    1 20 -10
  media 6    1 30 -20
  media 311 1 40 -30
  media 211 1 50 -40
  media 311 1 60 -50
  boundary 60
...
end model
```

Water materials are **correctly** used in the celldata block for an unrodded "branch 0" condition

Branch 0 is unrodded

Water materials correctly fill guide tube for an unrodded "branch 0" condition

SCALE Publications

The SCALE Team provides numerous publications on development and application activities in peer-reviewed journals, technical reports, and conference publications. Often, publications are jointly created with users and developers throughout the community. A summary of some recent and pending publications is provided here.

Peer-Reviewed Journal Articles

M. Piro, K. Clarno et al., "Coupled thermochemical, isotopic evolution and heat transfer simulations in highly irradiated UO_2 nuclear fuel," *J. Nucl. Matls.*, **441**, 240–251 (2013).

C. McGraw and G. Ilas, "PWR ENDF/B-VII Cross-Section Libraries for ORIGEN-ARP," *Nucl. Technol.*, **183**, 436–445 (2013).

M. Williams, G. Ilas, M. A. Jessee, B. T. Rearden, D. Wiarda, W. Zwermann, L. Gallner, M. Klein, B. Krzykacz-Hausmann, and A. Pautz, "A Statistical Sampling Method for Uncertainty Analysis with SCALE and XSUSA," *Nucl. Technol.*, **183**, 515–526 (2013).

J. Peterson and J. Wagner, "Characteristics of Commercial Spent Nuclear Fuel: Distributed, Divers, and Changing with Time," *Radwaste Solutions,* **51**, 51–58 (2014).

G. Ilas, I. C. Gauld, and H. Liljenfeldt, "Validation of ORIGEN for LWR used fuel decay heat analysis with SCALE," *Nucl. Eng. Des.*, **273**, 58–67 (2014).

G. Radulescu, I. C. Gauld, G. Ilas, and J. C. Wagner, "Approach for Validating Actinide and Fission Product Compositions for Burnup Credit Criticality Safety Analyses," *Nucl. Technol.* (accepted).

S. Vaccaro, J. Hu, J. Svedkauskaite, A. Smejkal, P. Schwalbach, P. De Baere, and I. C. Gauld, "A New Approach to Fork Measurements Data Analysis by RADAR-CRISP and ORIGEN Integration," *Transactions on Nuclear Science* (accepted).

G. G. Davidson, T. M. Evans, J. J. Jarrell, S. P. Hamilton, T. M. Pandya, and R. N. Slaybaugh, "Massively Parallel, Three-Dimensional Transport Solutions for the k-Eigenvalue Problem," *Nucl. Sci. Eng.* (accepted).

Technical Reports

S. Palmtag et al., *Demonstration of Neutronics Coupled to Full-core Thermal-hydraulics for a Full-core Problem Using VERA*, CASL-U-2013-0196-000, December 2013.

J. Hu, I. C. Gauld, J. Banfield, and S. Skutnik, *Developing Spent Fuel Assembly Standards for Advanced NDA Instrument Calibration – NGSI Spent Fuel Project*, ORNL/TM-2013/576, UT-Battelle, LLC, Oak Ridge National Laboratory, February 2014.

EPRRSD - 13th Robotics & Remote Systems for Hazardous Environments – 11th Emergency Preparedness & Response, Knoxville, TN, USA (August 2011)

V. J. Jodoin, R. W. Lee, D. E. Peplow, and J. P. Lefebvre, "Application of the ORIGEN Fallout Analysis Tool and the DELFIC Fallout Planning Tool to National Technical Nuclear Forensics."

INMM 53rd Annual Meeting, Orlando, Florida, USA (July 2012)

M. Monterial, V. J. Jodoin, J. P. Lefebvre, D. E. Peplow, and D. A. Hooper, "Automating the Coupling of ORIGEN with GADRAS via the Fallout Analysis Tool for National Technical Nuclear Forensics."

Waste Management Conference WM 2013, Phoenix, AZ (February 2013)

R. T. Jubin, N. R. Soelberg, D. M. Strachan, and G. Ilas, **"**Impact of Storage Time on the Needed Capture Efficiency for Volatile Radionuclides."

Topical Meeting on Nuclear Criticality Safety, NCSD 2013, Wilmington, NC (September 2013)

B. T. Rearden, M. E. Dunn, D. Wiarda, C. Celik, K. Bekar, M. L. Williams, D. E. Peplow, C. M. Perfetti, I. C. Gauld, W. A. Wieselquist, J. P. Lefebvre, and R. A. Lefebvre, "Overview of SCALE 6.2."

W. A. Wieselquist, K. S. Kim, G. Ilas, and I. C. Gauld**,** "Comparison of Burnup Credit Uncertainty Quantification Methods."

W. J. Marshall, D. Wiarda, C. Celik, B. T. Rearden, and D. R. Wentz, "Validation of Criticality Safety Calculations with SCALE 6.2."

C. M. Perfetti and B. T. Rearden, "Use of SCALE Continuous-Energy Monte Carlo Tools for Eigenvalue Sensitivity Coefficient Calculations."

K. B. Bekar, C. Celik, D. Wiarda, D. E. Peplow, B. T. Rearden, and M. E. Dunn, "Enhancements in Continuous-Energy Monte Carlo Capabilities in SCALE."

W. J. Marshall and B. T. Rearden, "The SCALE Verified, Archived Library of Inputs and Data – VALID."

B. T. Rearden, K. J. Dugan, and F. Havlůj, "Quantification of Uncertainties and Correlations in Criticality Experiments in SCALE."

2013 Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo, Paris, France (October 2013)

C. M. Perfetti and B. T. Rearden, "Development of a SCALE Tool for Continuous-Energy Eigenvalue Sensitivity Coefficient Calculations."

B. T. Rearden, L. M. Petrie Jr., D. E. Peplow, K. B. Bekar, D. Wiarda, C. Celik, C. M. Perfetti, A. M. Ibrahim, S. W. D. Hart, and M. E. Dunn, "Monte Carlo Capabilities of the SCALE Code System."

American Nuclear Society, 2013 Winter Meeting, Washington, DC, USA (November 2013)

C. M. Perfetti and B. T. Rearden, "A New Method for Calculating Generalized Response Sensitivities in Continuous-Energy Monte Carlo Applications in SCALE."

B. T. Rearden, M. E. Dunn, D. Wiarda, C. Celik, K. Bekar, M. L. Williams, D. E. Peplow, C. M. Perfetti, J. P. Lefebvre, F. Havlůj, and K. J. Dugan, "SCALE and AMPX Advancements to Support NCS Applications."

I. Hill, J. Gulliford, J. B. Briggs, B. T. Rearden, and T. Ivanova, "Generation of 1800 New Sensitivity Data Files for ICSBEP Using SCALE 6.0."

International Workshop on Nuclear Data Covariances, Santa Fe, NM, USA (April 2014)

M. T. Pigni, M. W. Francis, and I. C. Gauld, "Investigation of Inconsistent ENDF/B-VII.1 Independent and Cumulative Fission Product Yields with Proposed Revisions."

M. L. Williams, D. Wiarda, G. Ilas, W. J. Marshall, and B. T. Rearden, "Covariance Applications in Criticality Safety, Light Water Reactor Analysis, and Spent Fuel Characterization."

G. Arbanas, M. L. Williams, L. C. Leal, M. E. Dunn, B. A. Khuwaileh, C. Wang, and H. Abdel-Khalik, "Advancing Inverse Sensitivity/Uncertainty Methods for Nuclear Fuel Cycle Applications."

G. Arbanas, L. C. Leal, G. I. Fann, M. L. Williams, and M. E. Dunn, "Covariance Matrix of Thermal Neutron Scattering Kernal."

G. Arbanas, B. A. Khuwaileh, M. L. Williams, L. C. Leal, M. E. Dunn, and H. Abdel-Khalik, "Integral Benchmark Experiments in Inverse Sensitivity/Uncertainty Computations."

I. C. Gauld and M. W. Francis, "^{235}U Fission Product Yield Covariance Data for the Thermal Neutron Range."

INMM Information Analysis Technologies, Techniques and Methods for Safeguards, Nonproliferation and Arms Control Verification Conference, Portland, OR, USA (May 2014)

S. Vaccaro, I. C. Gauld, J. Hu, P. Schwalbach, P. De Baere, and W. Koehne, "Enhanced Spent Fuel Verification by Analysis of Fork Measurements Data Based on Nuclear Modelling and Simulation."

18th Topical Meeting of the Radiation Protection and Shielding Division of the American Nuclear Society – RPSD 2014, Knoxville, TN (September 2014)

G. Radulescu, D. E. Peplow, and J. M. Scaglione, "Dose Rate Analysis of As-Loaded Spent Nuclear Fuel Casks."

D. E. Peplow, G. Radulescu, M. L. Williams, and R. A. Lefebvre, "SCALE Enhancements for Detailed Cask Dose Rate Analysis."

2014 International Conference on the Physics of Reactors, Kyoto, Japan (September 2014)

B. T. Rearden, R. A. Lefebvre, J. P. Lefebvre, K. T. Clarno, M. A. Williams, L. M. Petrie, and U. Mertyurek, "Modernization Enhancements in SCALE 6.2."

C. M. Perfetti and B. T. Rearden, "Continuous-Energy Monte Carlo Methods for Calculating Generalized Response Sensitivities Using TSUNAMI-3D."

S. W. D. Hart, "Problem-Dependent Doppler Broadening of Continuous-Energy Cross Sections in the KENO Monte Carlo Computer Code."

B. T. Rearden, L. M. Petrie, D. E. Peplow, K. B. Bekar, D. Wiarda, C. Celik, C. M. Perfetti, and M. E. Dunn, "Enhancements in Continuous-Energy Monte Carlo Capabilities for SCALE 6.2."

C. M. Perfetti and B. T. Rearden, "Quantifying the Effect of Undersampling in Monte Carlo Simulations Using SCALE."

M. A. Jessee, W. A. Wieselquist, T. M. Evans, S. P. Hamilton, J. J. Jarrell, K. S. Kim, J. P. Lefebvre, R. A. Lefebvre, U. Mertyurek, A. B. Thompson, and M. L. Williams, "Polaris: A New Two-Dimensional Lattice Physics Analysis Capability for the SCALE Code System."

SCALE 6.2 Status

Development and testing of SCALE 6.2 continues, as the team prepares advanced and robust features for the community. Many of these advancements are documented in recent SCALE publications. Some features that are currently in beta testing include the following:

- The continuous-energy Monte Carlo capabilities are substantially improved in terms of accuracy and memory requirements (Figure 5).
- The *Sourcerer* sequence provides a hybrid technique for reliable fission source convergence for KENO.
- KENO is enhanced with problem-dependent Doppler broadening, parallel capabilities (Figure 6), fission source convergence diagnostics, and resonance upscattering techniques.
- New continuous-energy Monte Carlo capabilities are introduced for radiation shielding with MAVRIC/Monaco, sensitivity analysis with TSUNAMI, and depletion with KENO/TRITON.
- New 56 and 252 energy-group neutron libraries provide improved accuracy relative to the previous libraries for light-water-reactor systems.
- The *Sampler* stochastic sampling tool operates with any response from most SCALE sequences to propagate cross-section uncertainties and quantify uncertainties and correlations due to uncertainties in input parameters.
- The new *ORIGAMI* tool provides convenient characterization of used nuclear fuel with axially and radially varying burnup with ORIGEN.
- The new *Polaris* tool provides rapid lattice physics analysis of PWR fuel assemblies with simplified input.

SCALE 6.2 is currently in its third beta release, with a production release anticipated in late 2014 or early 2015.

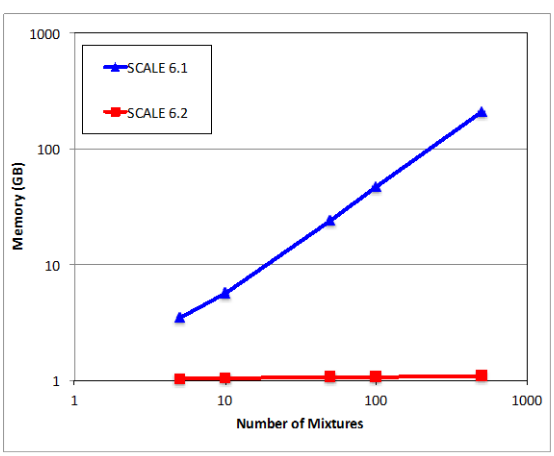

Figure 5. Memory requirements for continuous-energy (CE) KENO calculations using many mixtures with SCALE 6.1 and SCALE 6.2

SCALE 6.1.3 Update

The SCALE 6.1.3 update is available to provide compatibility with additional Linux operating systems. This comprehensive update includes enhancements previously released as SCALE 6.1.1 and SCALE 6.1.2 but provides no additional updates in functionality. This update is recommended for all users of SCALE 6.1 and 6.1.1 and for Linux users of 6.1.2. Details of the enhancements and instructions for requesting and installing this update are available at http://scale.ornl.gov/downloads_scale6-1.shtml.

SCALE Quality Assurance Program

The SCALE quality assurance (QA) program was updated in 2013 to provide improved high-quality software and data to the user community. The new QA program is compliant with ISO 9001-2008, DOE 414.1D, and the ORNL Standards Based Management System and is consistent with NRC requirements from NUREG/BR-0167 as well as ASME NQA-1. With the new SCALE QA program, a streamlined Kanban process is implemented with continual integration of new features and an automated test system that performs approximately 70,000 tests per day on Linux, Macintosh, and Windows operating systems. The QA program provides for rapid introduction of new features for deployment to end users. The updated QA plan was implemented after the deployment of SCALE 6.1 and is in use for the development of SCALE 6.2. However, the SCALE Team makes no guarantees regarding the performance of SCALE for any specific purpose, and users should independently submit the software to their own site- or program-specific testing and validation prior to use. See http://scale.ornl.gov/moreinfo.shtml to download a copy of the SCALE QA plan.

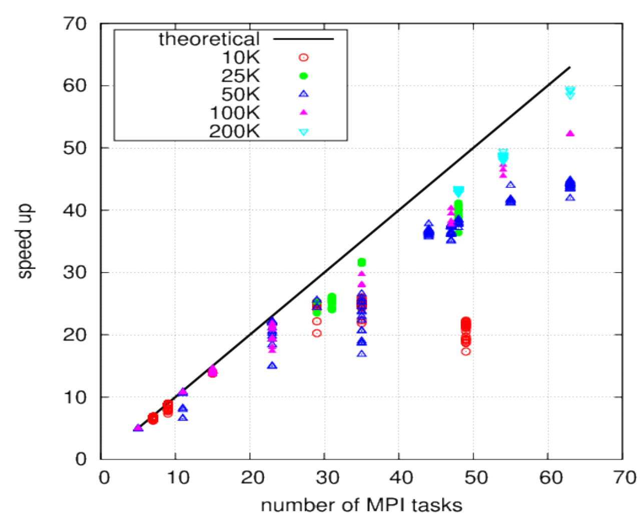

Figure 6. Speed up of parallel KENO calculations with number of particles per generation and processors (MPI Tasks)

SCALE Spotlight

SCALE is developed, tested, documented, and maintained by approximately 40 talented and diverse staff members within the Reactor and Nuclear Systems Division at Oak Ridge National Laboratory. The SCALE Spotlight provides a profile of a team member in each edition.

Dr. Mark L. Williams

Dr. Mark L. Williams (on right)

Position:

Distinguished Scientist in Reactor Physics Group

Focus areas:

Lattice Physics; Sensitivity/Uncertainty Analysis; Nuclear Data

Most memorable projects:

I began working at ORNL in 1974 and have had the opportunity to work on a wide variety of memorable projects in reactor physics and shielding. I took a 20-year "vacation" from ORNL during 1983–2003 when I was a physics professor at Louisiana State University but continued collaborating on SCALE development. During this period, several LSU graduate students and I developed the CENTRM and PMC modules, which are still used for self-shielding in SCALE. I returned to ORNL in 2003 and continue to work on SCALE development. This is an exciting time to be involved with SCALE because the entire structure of the system is being redesigned and modernized.

Life outside of work:

My wife and I are originally from Louisiana, so we enjoy having crawfish and shrimp boils for family and friends. We have two grown kids with the youngest graduating from college next year. I'm an avid reader, and I like going to baseball and football games, attending concerts, and taking photographs of the beautiful East Tennessee scenery.

Technical Support and Training

The SCALE Team is dedicated to supporting all SCALE users, but the team can only provide limited complimentary technical support for inquiries submitted to scalehelp@ornl.gov. For basic help in getting started with SCALE, new users are encouraged to attend the public training courses where the capabilities of SCALE are presented in detail.

A new venue is now available to facilitate interaction between SCALE users and developers. The SCALE Users Group is a new forum hosted by Google and available at https://groups.google.com/forum/#!forum/scale-users-group.

The primers distributed with SCALE for KENO V.a, KENO-VI, TSUNAMI, and TRITON provide detailed step-by-step instructions to assist new users in learning how to use these modules for criticality safety, sensitivity/uncertainty, lattice physics, and source term calculations. Direct links to the SCALE primers are available at http://scale.ornl.gov/training_primers.shtml.

If your team could benefit from customized technical support or training, additional options are available. The SCALE Team can provide direct support or travel to your site to present customized hands-on courses to provide the expertise needed to solve challenging application scenarios. Please contact scalehelp@ornl.gov for more information.

SCALE Leadership Team

The SCALE Leadership Team consists of the SCALE manager, line managers, program managers, and developers. The Leadership Team meets regularly to discuss the current status and make programmatic and managerial decisions regarding SCALE.

Members of the SCALE Leadership Team are as follows:

Brad Rearden – Manager, SCALE Code System

Steve Bowman – Group Leader, Reactor Physics

Mike Dunn – Group Leader, Nuclear Data and Criticality Safety

Bob Grove – Group Leader, Radiation Transport

Matt Jessee – Senior Developer, Reactor Physics

Douglas Peplow – Senior Developer, Radiation Transport

Mark Williams – Distinguished Developer, Nuclear Data and Reactor Physics

Upcoming SCALE Training Courses

Training courses are provided by developers and expert users from the SCALE Team. Courses provide a review of theory, description of capabilities and limitations of the software, and hands-on experience running problems of varying levels of complexity.

Please see http://scale.ornl.gov/training_2014_summer.shtml for more information.

Dates	Course	Registration Fee
August 4–8, 2014	**SCALE Criticality Safety Calculations** Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA Introductory through advanced criticality calculations using KENO V.a and KENO-VI; resonance self-shielding techniques	$2000
August 11–15, 2014	**SCALE Sensitivity and Uncertainty Calculations** Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA TSUNAMI: 1D, 2D, and 3D k_{eff} sensitivity/uncertainty analysis; 2D generalized sensitivity analysis for lattice physics; reactivity sensitivity analysis; advanced S/U methods for code and data validation using trending analysis and data assimilation (data adjustment) techniques; k_{eff} burnup credit validation	$2000
August 18–22, 2014	**SCALE Lattice Physics and Depletion** Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA 2D lattice physics calculations; 1D, 2D, and 3D depletion calculations; resonance self-shielding techniques including Monte Carlo Dancoff factors for non-uniform lattices; generation of libraries for ORIGEN-ARP	$2000
August 25–28, 2014	**SCALE/ORIGEN Stand-alone Fuel Depletion, Activation, and Source Term Analysis Course** Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA Isotopic depletion, activation analysis, and source term characterization using ORIGEN/OrigenArp	$1800

**Full-time university students can register at a reduced rate. Both professional and student registration fees are discounted $200 for each course over one.*

All attendees must be licensed users of SCALE 6.1, which is available from ORNL/RSICC in the USA, the OECD/NEA Data Bank in France, and the RIST/NUCIS in Japan.

Class size is limited, and course may be canceled if minimum enrollment is not obtained one month prior to the course. Course fees are refundable up to one month before each class.

FOREIGN NATIONAL VISITORS TO ORNL - Payment MUST be received at least one week prior to attending the training course. All foreign national visitors must register 40 days before the start date of the training course they plan to attend.

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