scale Newsletter

Nuclear Systems Modeling & Simulation

Number 44 Spring 2012

In This Issue

Over 4000 distributions of SCALE!

SCALE 6.1 was released through the Radiation Safety Informational Computational Center (RSICC) in July 2011 and subsequently distributed through the Nuclear Energy Agency (NEA) Data Bank. As of the end of April 2012 there have been over 1000 distributions of SCALE 6.1, including over 500 distributions to individuals who had not previously used any version of SCALE. There are now over 4000 unique users of SCALE versions 5.0–6.1, representing 40 different nations. The SCALE Team is thankful to our valued users for helping us achieve this milestone. The rate of distribution of recent versions of SCALE is shown below in Fig. 1.

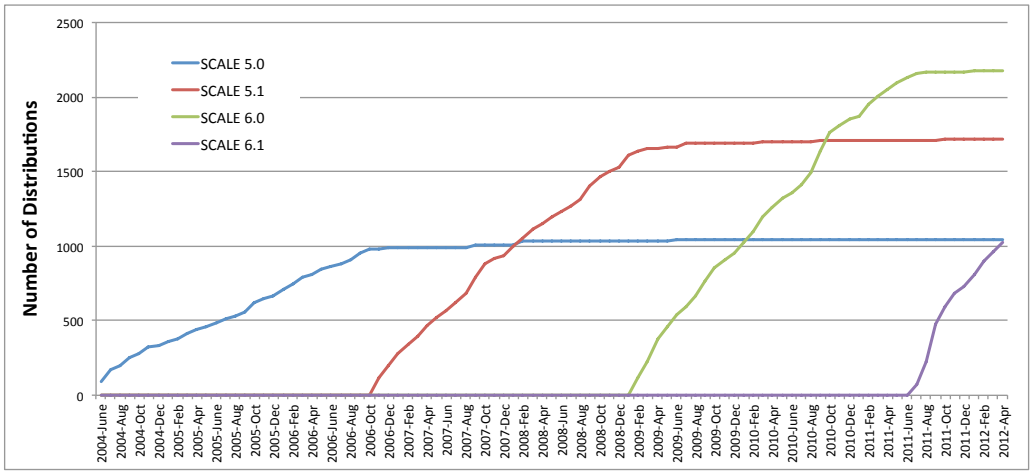
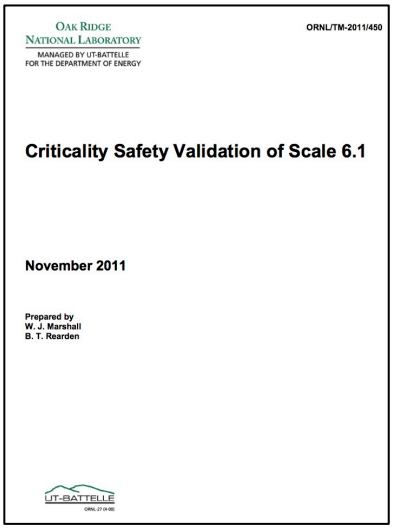


Fig. 1. Number of distributions of SCALE 5.0–6.1 as a function of time.

Criticality Safety Validation of SCALE 6.1

The performance of SCALE 6.1 for a wide range of critical benchmark experiments is documented in a recent report. More than 350 cases from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* have been prepared and reviewed within the Verified, Archived Library of Inputs and Data (VALID) maintained by the Reactor and Nuclear Systems Division at Oak Ridge National Laboratory (ORNL). The performance of the KENO V.a and KENO-VI Monte Carlo codes from SCALE 6.1 with ENDF/B-VII.0 cross-section data in 238-groups and continuous energy (CE) is assessed using the VALID models of benchmark experiments. The SCALE tools for sensitivity and uncertainty (S/U) analysis are applied to determine the uncertainty in each computed k_{eff} value due to uncertainties in the nuclear data. The S/U tools are further utilized to examine selected systems to identify potential causes of unexpected results. This report is available online at
http://info.ornl.gov/sites/publications/Files/Pub33149.pdf


OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

ORNL/TM-2011/450

Criticality Safety Validation of Scale 6.1

November 2011

Prepared by
W. J. Marshall
B. T. Rearden

UT-BATTELLE

Recent Publications

The SCALE Team recently published a number of articles detailing practical uses of SCALE and the development of new methods that will be available in future releases.

Applications of SCALE to Burnup Credit Analysis

J. M. Scaglione, D. E. Mueller, J. C. Wagner, and W. J. Marshall, *An Approach for Validating Actinide and Fission Product Burnup Credit Criticality Safety Analyses-Criticality (k_{eff}) Predictions*, NUREG/CR-7109 (ORNL/TM-2011/514)

G. Radulescu, I. C. Gauld, G. Ilas, and J. C. Wagner, *An Approach for Validating Actinide and Fission Product Burnup Credit Criticality Safety Analyses-Isotopic Composition Predictions*, NUREG/CR-7108 (ORNL/TM-2011/509)

Publications at PHYSOR 2012

April 2012, Knoxville, TN, USA

Bradley Rearden, Lester Petrie, Douglas Peplow, Matthew Jessee, Dorothea Wiarda, Mark Williams, Robert Lefebvre, Jordan Lefebvre, Ian Gauld, and Sedat Goluoglu
Enhancements in SCALE 6.1

Anselmo Cisneros and Dan Ilas
Neutronics and Depletion Methods for Parametric Studies of Fluoride-Salt-Cooled High Temperature Reactors with Slab Fuel Geometry and Multi-Batch Fuel Management Schemes

Cole Gentry, Ivan Maldonado, Andrew Godfrey, and Jess Gehin
Application of Fully Ceramic Micro-Encapsulated Fuels for Transuranic Waste Recycling in PWRs

Nathan George, Ivan Maldonado, Kurt Terrani, Andrew Godfrey, and Jess Gehin
Neutronics Studies of Uranium-Based Fully Ceramic Micro-Encapsulated Fuel for PWRs

Dan Ilas
SCALE Validation for Prismatic High-Temperature Gas-Cooled Reactors

Dan Ilas, David Holcomb, and Venugopal Varma
Advanced High-Temperature Reactor Neutronic Core Design

Ryan Kelly and Dan Ilas
Verification of a Depletion Method in SCALE for the Advanced High Temperature Reactor

Carolyn McGraw and Germina Ilas
PWR ENDF/B-VII Cross-Section Libraries for ORIGEN-ARP

Harold Smith
Modeling Depletion Simulations for a High-Burnup, Highly Heterogeneous BWR Fuel Assembly with SCALE

Artem Yankov, Ben Collins, Matthew Jessee, and Tom Downar
A Generalized Adjoint Approach for Quantifying Reflector Assembly Discontinuity Factor Uncertainties

Artem Yankov, Markus Klein, Matthew Jessee, Winfried Zwermann, Kiril Velkov, Andreas Pautz, Ben Collins, and Tom Downar
Comparison of XSUSA and "Two-Step" Approaches for Full-Core Uncertainty Quantification

Mark Williams and Kang-Seog Kim
The Embedded Self-Shielding Method

Mark Williams, Doro Wiarda, Harold Smith, Matthew Jessee, Brad Rearden, Winfried Zwermann, Markus Klein, and Andreas Pautz
Development of a Statistical Sampling Method for Uncertainty Analysis with SCALE

Christopher Perfetti, William Martin, Bradley Rearden, and Mark Williams
Development of Continuous-Energy Eigenvalue Sensitivity Coefficient Calculation Methods in the Shift Monte Carlo Code

Christopher Perfetti, William Martin, Bradley Rearden, and Mark Williams
Determining Importance Weighting Functions for Contributon Theory Eigenvalue Sensitivity Coefficient Methodologies

Kang Seog Kim and Mark L. Williams
The Method of Characteristics for 2-D Multigroup and Pointwise Transport Calculations in SCALE/CENTRM

Recent Publications on the Use of SCALE for Reactor Physics Applications

Brian Ade and Ian Gauld
Decay Heat Calculations for PWR and BWR Assemblies Fueled with Uranium and Plutonium Mixed Oxide Fuel Using SCALE, ORNL/TM-2011/290, Oak Ridge National Laboratory (2011)

Dan Ilas
Development of a SCALE Model for High Flux Isotope Reactor Cycle 400, ORNL/TM-2011/367 (2012)

Ron Ellis
Comparison of Calculated and Measured Neutron Fluence in Fuel/Cladding Irradiation Experiments in HFIR, ANS Transactions **105**, 808 (2011)

Extended Uses of MeshView

MeshView is a utility program distributed with SCALE that is used to visualize data generated on a spatial grid, especially dose and flux data from the shielding sequences of SCALE. The documentation and user guidance for MeshView is included in the *meshview.pdf* file located in the MeshView directory available under the root SCALE installation directory (e.g. c:\scale6.1\Meshview). Some extended applications of MeshView are shown below.

Visualization of Fission Source Distribution

Since SCALE 6.0, an option has been available in KENO V.a and KENO-VI to write mesh-based fission source density information to a file. The feature was implemented for use in criticality accident alarm system calculations, but it provides a convenient means of visualizing the fission source distribution. The fission source tally simply accumulates the fission sites, and energy-dependence is represented by multiplying the energy-independent tally by the fission spectrum. This optional feature is activated by specifying *cds=yes* in the KENO *Parameters* block and specifying a user-defined spatial mesh using the *gridGeometry* block. The fission source data is tabulated on the user-specified mesh during the KENO calculation. At the end of the calculation, the resulting mesh-based fission source data is placed in the return directory with the extension *.3dmap*. MeshView can be used to visualize the fission source from the *.3dmap* file. The absolute or relative uncertainty in the fission source tallies can also be displayed, as well as a wide variety of 2D plots displaying the fission neutron generation along X, Y, Z, or energy axes.

Because the mesh data defined in *gridGeometry* is independent of the model geometry specification, it is completely flexible in cutting across unit, array, or hole boundaries. Repeated elements in an array are tabulated separately because of this decoupling. The mesh will also tabulate fission density within each mesh cell, regardless of the contents of that cell. It is therefore important for users to verify that mesh grid is defined as intended during the KENO calculations.

Currently, MeshView cannot display flux or reaction rate data from KENO, as the file formats are not compatible.

Radial and axial views of a fuel rod array in a water tank are shown below in Fig. 2 and Fig. 3, respectively. The array contains water holes, HEU rods, and LEU rods. The water rod locations appear as white spaces in the figures because there are no fission tallies in those mesh cells.

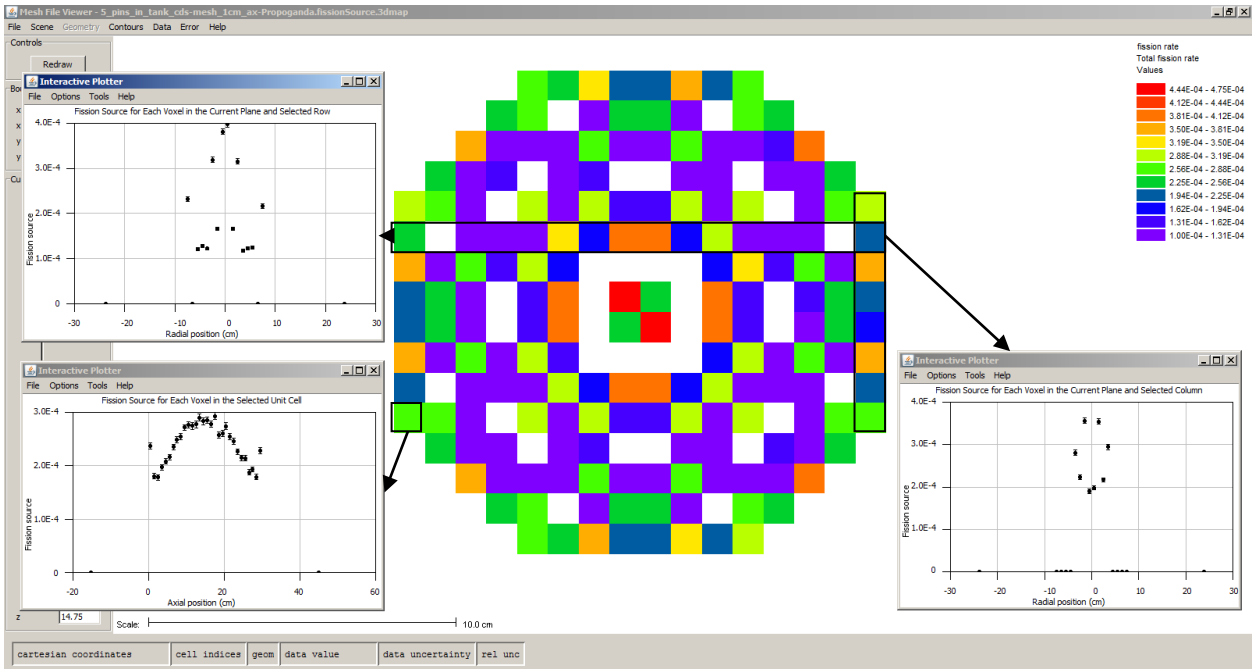


Fig. 2. Radial view of fission source distribution for a fuel rod array in a water tank.

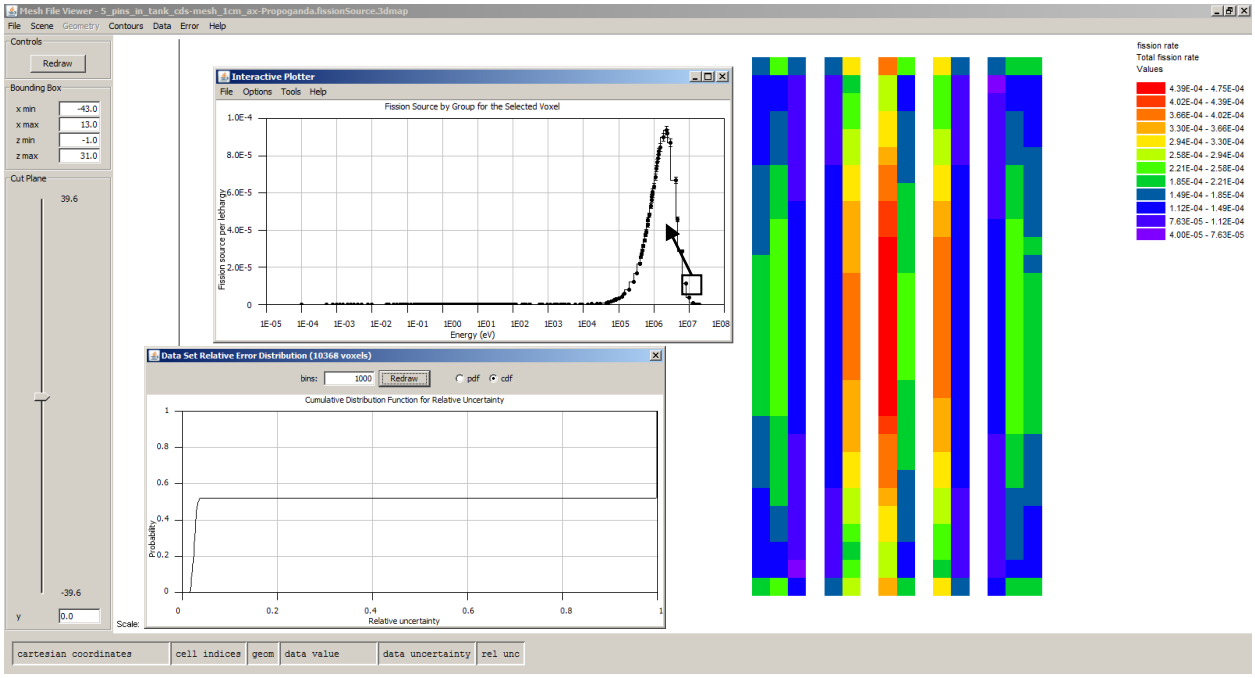


Fig. 3. Axial view of fission source distribution for a fuel rod array in a water tank.

Visualization of KENO Grid Geometry Superimposed on Problem Geometry

Using the *.3dmap* file, MeshView can display the mesh boundaries (SCENE menu – Show Mesh option) with or without data (DATA Menu – None option). This image can be captured, exported, and overlaid on an image of the KENO geometry. This is especially useful for reviewing mesh boundaries for sensitivity calculations. The scaling and alignment are left to the user, so this technique should not necessarily be viewed as confirming that the grid geometry has been correctly implemented. It is most useful for generating figures for reports, presentations, and other similar documents. An example is given in Fig. 4 for the same sample problem used in the previous section.

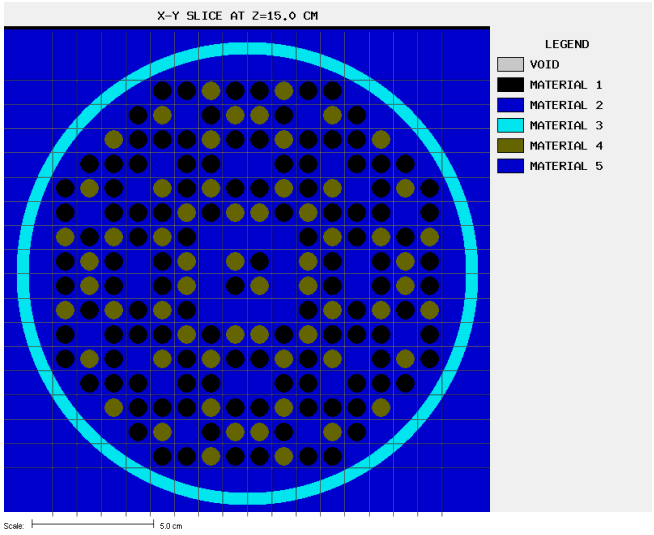


Fig. 4. MeshView overlay of gridGeometry with KENO material plot.

SCALE 6.1 Known Issues

Since SCALE 6.1 was released on July 22, 2011, end users and the SCALE development team have identified a few issues that impact the performance of individual parts of the code package. To keep users informed of the latest information, items are cataloged on the SCALE website (http://scale.ornl.gov/known_issues.shtml).

Further information and discussion opportunities are available in the SCALE 6 User Notebook (http://scale.ornl.gov/notebooks.shtml).

Many of these known issues are corrected in the SCALE 6.1.1 patch described below, while other issues will be resolved in SCALE 6.2.

Error in ENDF/B-VII.0 Decay Data

An error in the nuclear decay data for ^{234}Th has been identified in ENDF/B-VII.0, which is used for the SCALE decay library. A review of the problem indicates that the error was introduced in the evaluated ENDF/B-VII.0 decay sub-library released by the National Nuclear Data Center (NNDC) in December 2006. The NNDC has confirmed the problem and recently released an updated decay library with ENDF/B-VII.1. Currently, ORNL is working closely with NNDC to identify the nature and extent of the nuclear data evaluation problem and is preparing a patch for the ENDF/B-VII.0-based decay library distributed with SCALE 6.1. It is important to note that ORNL has performed extensive validation using the ENDF/B-VII.0-based decay library in SCALE 6.1 and has NOT identified any discrepancies for benchmark problems involving irradiated fuel isotopic compositions, decay heat, and source terms. The error has been observed for problems involving the decay of ^{238}U. As an example, the gamma ray spectra calculated using SCALE 6.0 (ENDF/B-VI decay data) and SCALE 6.1 (ENDF/B-VII.0 decay data) are shown in Fig. 5. The spectrum obtained using ENDF/B-VII.0 data is significantly over estimated, caused primarily by incorrect production of ^{234}Pa from ^{234}Th decay. Additional information on the error in ENDF/B-VII.0 and decay evaluation improvements for ENDF/B-VII.1 are posted on the NNDC website (http://www.nndc.bnl.gov/exfor/endfb7.1_decay.jsp).

MacOS System Requirements

The SCALE 6.1 Readme states that the system will operate on Mac OSX version 10.5 or newer, where Mac OSX 10.6 or newer is actually required to properly execute SCALE 6.1.

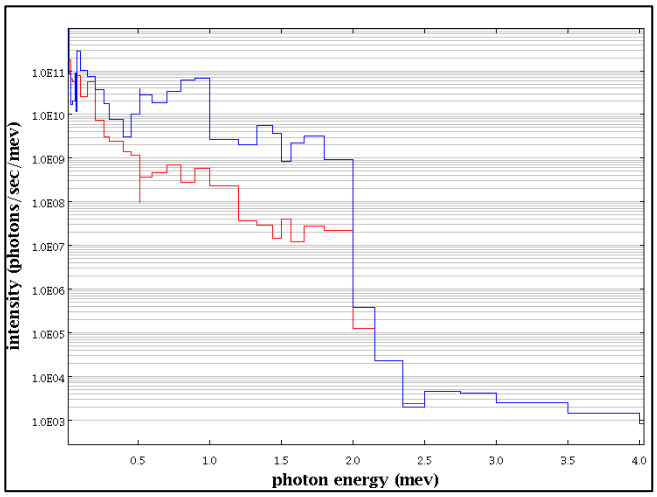


Fig. 5. Comparison of gamma ray spectrum for the decay of low enriched uranium fuel after 10 years cooling (SCALE 6.0 in red and SCALE 6.1 in blue).

Problem with Bound BeO in Continuous Energy KENO Calculations

Internal testing of continuous-energy calculations with KENO has revealed a considerable non-conservative change in k_{eff}, on the order of 20%, for cases involving BeO. Users who properly validate continuous-energy KENO calculations for these systems would notice a strong systematic bias for bound BeO cases prior to use in safety calculations. Nevertheless, **users should not use *be-beo* in continuous-energy KENO calculations**. Multigroup calculations with *be-beo* are not affected. Additional details are provided in the Known Issues posting on the SCALE website, and this issue will be corrected in SCALE 6.2.

Optional Output Edit in STARBUCS

In STARBUCS burnup credit loading curve search calculations, an optional input *prt=short* may be used within the *READ SEARCH* input block to restrict the final output to contain only relevant information for a burnup loading curve calculation. In SCALE 6.1, this optional input causes the calculation to fail.

Users should only use the default parameter *prt=long*, which retains all SCALE output information for the last step of the iterative fuel enrichment search process. As *prt=long* is the default option in STARBUCS, there is no need for this input option to be specified in a STARBUCS input file.

SCALE 6.1.1 Update

A new update is available for SCALE 6.1 to provide enhanced performance in the areas detailed below. This update can be requested from the SCALE website at http://scale.ornl.gov/downloads_scale6-1.shtml and is recommended for all users.

CENTRM

CENTRM was updated to correct an issue that can lead to non-conservative k_{eff} values when using the 44-group ENDF/B-V data with CENTRM for high-leakage models with trace-element number densities below ~10^{-9} atoms/barn-cm when running SCALE 5.1–SCALE 6.1. The effect on the 238-group ENDF/B-V, VI, and VII libraries is minimal. There is no effect on continuous-energy Monte Carlo calculations.

In the dozens of test cases examined thus far, the discrepancy appears only in cases that meet ALL of the following conditions.

(1) Calculations are performed with SCALE 5.1, 6.0 or 6.1.
(2) The number density of at least one nuclide has a small fractional concentration of 10^{-8} or less relative to the total mixture number density. Typically this corresponds to an absolute concentration less than ~10^{-9} to 10^{-10} atoms/barn-cm, but greater than zero.
(3) The SCALE 44-group ENDF/B-V library or a user-generated broad group library with few groups in the U-238 resolved resonance range (1 eV-4 KeV) is used.
(4) CENTRM is used for resonance self-shielding. This is the default behavior in SCALE 6.1, but NITAWL processing is the default behavior for SCALE 5.1 and 6.0 for the ENDF/B-V cross-section data, so the user must explicitly request CENTRM processing to observe the discrepancy with SCALE 5.1 or 6.0.
(5) The system is sensitive to the high-energy portion of the resolved range, which most commonly occurs for high-leakage systems. Low-leakage criticality and depletion models examined realized only a minimal impact.

Impact of CENTRM error on computed results:

(1) Continuous-energy KENO calculations do not use CENTRM and are not affected.
(2) The impact for all 238-group calculations examined thus far is small, on the order of a few pcm.
(3) Eigenvalues and isotopic concentrations computed for the 44-group ENDF/B-V depletion cases examined are not significantly affected, because these are low-leakage systems [reflected lattice geometries]. For most cases that meet all of the above criteria, including burned fuel criticality safety calculations that include small concentrations of fission products, the discrepancy introduces an error on the order of 100 pcm.

In a contrived case that artificially introduces a trace material into a plutonium nitrate system, a discrepancy of ~3% delta-k between the SCALE 6.1 and corrected SCALE 6.1.1 result has been observed. However, the SCALE development team has not observed an experimental benchmark or operational safety-related problem that exhibits an error on the order of this contrived numerical case.

After applying the patch, users should repeat any calculations where this discrepancy could affect results.

Lattice Physics Enhancements

Several minor updates for lattice physics calculations have been included for TRITON and NEWT. Users will realize improved performance where these specific features are utilized. The following issues have been resolved.

(1) Homogenization of kinetic parameters in NEWT: The delayed neutron fraction, beta, is currently homogenized by forward fission weighting. In this formulation, beta should be weighted by the nu-fission reaction rate. The current coding uses the fission reaction rate (i.e., without the nu). Users should expect differences in the homogenized values of kinetic parameters, which will impact subsequent transient analysis.
(2) *TRITON TRACE* Block: An issue was identified using the *TRACE* block in TRITON. The *TRACE* block now supports any nuclide in the ORIGEN light-element library. Previously in SCALE 6.1, only trace amounts of nuclides from the AMPX cross-section library could be added to depletion materials. The ORIGEN light-element library contains more nuclides than are available in the AMPX cross-section library.
(3) Depletion File ft71f001 Index Listing: TRITON provides an output edit for a table of contents of the data in the ORIGEN nuclide inventory file (i.e., ft71f001). This file can be used in follow-on ORIGEN-ARP and OPUS analyses. It was identified that the record numbers were not properly displayed for the two cumulative datasets (system-sum of materials and selected-sum of materials). This edit was corrected.
(4) KENO Depletion Message: TRITON increases the user-defined KENO parameters NSK and GEN for depletion analysis. A message was added to the TRITON output to notify users of the modified values.
(5) NEWT *ARRAY* block: Two issues were addressed for the NEWT *ARRAY* block. An error message was added in the case where an array is used in the model geometry without being defined in the *ARRAY* block. Second, a code bug was removed so that the model geometry may include multiple placements of the same array definition.

(6) CENTRM Cross-section processing defaults: TRITON supports several sets of CENTRM cross-section processing defaults: *parm=2region*, *parm=centrm*, and *parm=(xslevel=1/2/3/or 4)*. An error was identified in depletion calculations if the user supplied *parm=centrm*. In this case, TRITON continued to use the depletion default set, which has been slightly modified to decrease run-time without significantly impacting depletion analysis. This error was resolved in this patch. For depletion calculations (i.e. *=t-depl*, *=t-depl-1d*, *=t5-depl*, *=t6-depl*) that use *parm=centrm*, users can expect a small deviation (~50 pcm change in multiplication factor as a function of burnup) and slightly longer run-times for depletion models that utilize the *parm=centrm* option when using the SCALE 6.1.1 update.

MAVRIC/Monaco Enhancements

A few minor issues were identified with the SCALE fixed-source Monte Carlo code Monaco and an associated utility, especially related to seldom-used optional features. Users should review any results produced with these features using SCALE 6.1.

(1) When specifying the special distribution *pwrNeutronAxialProfileReverse* or *pwrGammaAxialProfileReverse* for a spatial source distribution, the un-reversed profile was erroneously returned.

(2) The sum of the point detector group-wise results may be higher than the point detector energy-integrated (total) results. The reported total is correct. The group-wise values are high due to rejecting negative contributions (which happen a small fraction of the time due to the multigroup energy/angle physics).

(3) If a source specification utilizes different Watt spectra distributions in multiple sources, the energies sampled for one source may include energies from the wrong distribution.

(4) The utility program *mim2wwinp* does not format MCNP *.wwinp files correctly for photon-only problems. MCNP interprets a *.wwinp with only one particle listed as neutrons, even in a "mode p" problem. The *.wwinp file produced by SCALE needs to specifically identify that there are 0 neutron groups for photon-only problems.

ORIGEN Data Enhancements

Three issues are corrected within the ORIGEN depletion and decay libraries.

(1) origen.rev03.jeff200g – The energy group boundaries of the 200-group JEFF-based ORIGEN library were inadvertently generated using constant lethargy boundaries instead of the boundaries of the SCALE 200-neutron and 47-gamma group cross section libraries. The library was regenerated to include the corrected boundaries. No other changes were made. All calculations performed with the previous version of the *jeff200g* library should be discarded and repeated with the current library.

(2) The fission product yield library used by COUPLE was modified to include ternary yields of H-3, He-3, and He-4 based on data from the JEF-2.2 fission yield library. In the previous library these fission products are only generated as by-products of neutron reactions other than fission, and not directly from fission. Cumulative yields are applied for H-3 and He-4, and direct yields are used for He-3 since it is a decay product of H-3. Direct yields for He-3 are zero for all fission nuclides.

(3) The ORIGEN decay libraries were updated to provide correct natural abundances of several elements. Previously, the use of natural isotopic abundances (NEX1=4) for input element concentrations entered in gram units may have resulted in incorrect isotopic concentrations for Mg, Ge, Kr, Sr, and Te. If atom units (gram atoms) were used, incorrect isotopic concentrations may have occurred for F, Na, Mg, Al, P, Sc, Mn, Co, Ge, As, Kr, Sr, Y, Nb, Rh, Te, I, Cs, Pr, Tb, Ho, Tm, and Au. The libraries origen.rev02.decay.data and origen.rev02.end7dec were updated.

KENO-VI Hexagonally-Pitched Arrays

KENO-VI was updated to correct an issue that occasionally caused a calculation to fail when tracking in a hexagonally-pitched array. Previous calculations that encountered this error failed, and the results of other calculations are not affected.

Other Enhancements

The SCALE 6.1 distribution included some sample problem output data that were generated with a prerelease version of SCALE and were not consistent with those produced by the final release of SCALE 6.1. Additionally, some of the sample problems were verified using output that included timing information, such as Figure of Merit data from Monte Carlo calculations. This update provides revised *.out* and *.table* files for all sample problems, updates in the XML files that drive the sample problems, corrections in platform-specific information in three Windows sample problem inputs, and provides an updated differencing tool that is used for comparing sample problem outputs.

Additionally, KENO3D and OrigenArp example files that are referenced in some publications but were not included in SCALE 6.1 are also installed with this update, and an updated version of GeeWiz is provided to correct minor issues.

SCALE 6.2 Preview

The SCALE Team is actively developing a number of enhancements for distribution in SCALE 6.2, including the following.

Enhancements in the KENO Monte Carlo Codes

The KENO Monte Carlo codes of SCALE are commonly used in criticality safety calculations as well as S/U analysis and depletion. Recently significant technical advancements were made to facilitate the use of the KENO codes.

Parallel Calculations with KENO

Parallel computation capabilities were added to KENO to provide faster results on multicore PCs and Linux clusters. When using 20 processors, the calculation can now run up to 16 times faster than a serial calculation. Thus, in the same runtime SCALE users can obtain (1) more precision for a single calculation or (2) more variants of a base calculation to explore additional upset conditions. The accelerated capabilities are especially useful for performing S/U analysis or Monte Carlo depletion on Linux clusters. KENO V.a has been enhanced to utilize OpenMP threaded parallel calculations on multi-core computers as well as Message Passing Interface (MPI) domain replication calculations on multi-node clusters. KENO-VI has been enhanced for MPI calculations. The speed-up realized for a graphite-moderated reactor model is shown in Fig. 6. The code parallel performance is very good up to eight processors, greater than 93%. The parallel performance then diminishes as a function of increasing the number of processors but is still above 80%.

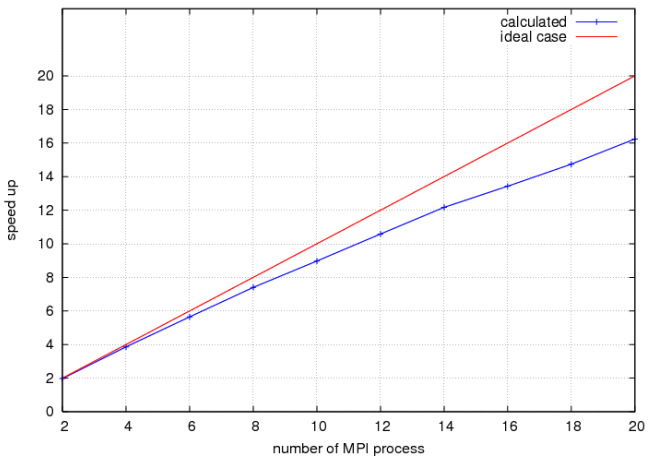


Fig. 6. Speed-up for MPI calculations for a graphite-moderated reactor model.

Reduced Memory Requirements for CE

Continuous-energy calculations in KENO through SCALE 6.1 have been performed using a "unionized energy grid," where material-dependent cross-section data are generated for each user-defined mixture. This feature reduces the run-time for KENO CE calculations by a factor of 2 or more but results in substantially increased memory usage for a problem with many materials, making it impossible to perform CE calculations for problems with multiple spent fuel mixtures. An option will be available in SCALE 6.2 to disable the unionized energy grid to enable models with many mixtures to execute with substantially reduced memory requirements.

Source Convergence Diagnostics

Fission source convergence diagnostic techniques were implemented to provide improved confidence in the computed results. Confirming convergence of the fission source in addition to k_{eff} is especially useful for flux tallies as needed for reaction rate calculations and sensitivity analysis studies using the TSUNAMI tools of SCALE. An example Shannon Entropy plot for an Organisation for Economic Co-operation and Development (OECD) benchmark model is shown in Fig. 7.

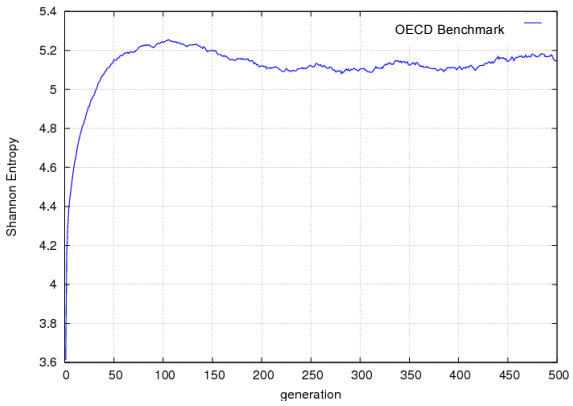


Fig. 7. Shannon entropy variation during the simulation; NPG = 10,000, GEN = 500.

Continuous-Energy Monte Carlo Depletion

SCALE 6.1 provides two Monte Carlo depletion sequences, T5-DEPL and T6-DEPL, that use standard SCALE multigroup cross-section processing capabilities with KENO V.a and KENO-VI, respectively. A new CE-based Monte Carlo depletion capability will be supported through the T6-DEPL sequence and can be utilized by simply changing the input library specification. CE depletion is especially useful for models with complex geometry that present difficulties in obtaining accurate resonance self-shielded multigroup data, and for models with many depletion regions where run-time to generate and store the resonance self-shielded cross-section data for each material is prohibitive.

Improved Continuous-Energy Cross Section Data

The *Criticality Safety Validation of SCALE 6.1* report, described on page 1 in this newsletter, demonstrates systematic biases for CE Monte Carlo calculations, especially for water-moderated mixed-oxide lattices. Further investigations into the CE data generated by the AMPX code system revealed a need for improvement in the S(α,β) treatment, especially for forward-peaked kinematics. These and other improvements are currently under development for SCALE 6.2. The calculated to experiment ratios (C/E) for the MIX-COMP-THERM (MCT) benchmarks examined in the validation report are shown in Fig. 8, where the SCALE 6.1 multigroup (MG) and CE results are supplemented with preliminary SCALE 6.2 CE results. The updated CE data mitigate the systematic bias trend, especially for the MCT-004 series of benchmarks.

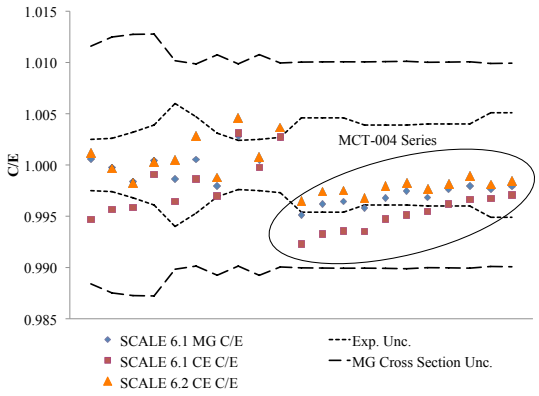


Fig. 8. C/E results for MIX-COMP-THERM benchmarks.

Additionally, the use of BeO data in CE calculations will be corrected in SCALE 6.2.

Continuous-Energy Fixed-Source Monte Carlo Calculations with Automated Variance Reduction

The SCALE fixed-source Monte Carlo capability with automated variance reduction is being enhanced to enable continuous-energy (CE) calculations. The new CE capabilities will provide enhanced solution fidelity while still implementing the unique acceleration techniques of the FW-CADIS (Forward-Weighted Consistent Adjoint Driven Importance Sampling) methodology.

The implementation of CE fixed-source physics demonstrated here currently exists as a prototype capability. In this example, different methods are applied to compute the dose rates external to a radioactive material transport packaging system that contains a cobalt-60 source.

A simple model of the package consisting of steel and tungsten is shown in Fig. 9. The inner-most cylinder contains 1.0 Ci of cobalt-60.

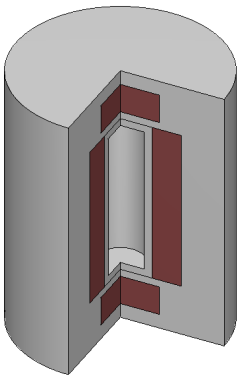


Fig. 9. Simple cask geometry showing tungsten (brown) and steel (gray).

One major drawback of the current SCALE multigroup (MG) approach to shielding calculations is in the representation of discrete gammas, such as the decay radiation from common isotopic sources such as cobalt-60. The cobalt-60 produces two high-energy gamma rays when it decays (1173230 eV with intensity 99.85% and 1332490 eV with intensity 99.9826%). In the SCALE MG calculations, a cobalt-60 source spectrum is represented by broad probability distribution functions, which must fit into a predefined group structure. This is shown in Fig. 10 for the fine 47-group structure and the broad 19-group structure used for gammas.

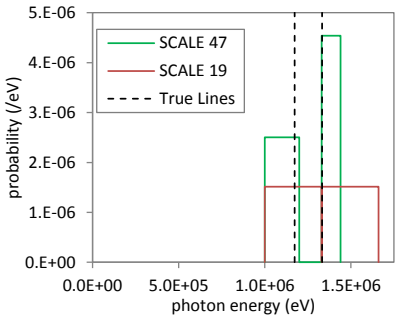


Fig. 10. The representation of a cobalt-60 source using the SCALE 47-group and 19-group structures. The actual cobalt lines are also shown as black dotted lines.

With the FW-CADIS automated variance reduction available in the MAVRIC sequence of SCALE, an importance map can be used to spend more time on the particles that are traveling towards the outer surface of the package and less time on particles that scatter back towards the innermost cylinder. The two required coarse-mesh discrete-ordinates calculations were performed automatically by MAVRIC in less than 20 minutes. The importance map was then employed by two different Monaco calculations: a SCALE 6.1 MG calculation using 47 photon groups and a prototypic SCALE 6.2 CE calculation. Results should be different between the MG and CE due to two reasons: (1) representation of the discrete gamma line source and (2) transport effects from

the averaging of cross sections over finite energy ranges. Results for the CE calculation (600 minutes) using the importance map (19-group) for optimizing the calculation of dose rate outside the cask are shown in Fig. 11. Note that since dose rates inside the package are not of concern, that region was excluded from the mesh tally. Due to the optimization that focused the Monte Carlo calculation on dose rates outside the cask, values of the dose rate inside the cask may be underestimated. Also note that voxels along the outer cylindrical edge of the package could show low dose rates, since the voxel value is an average and only part of the voxel is actually outside the package.

The same importance map was used to optimize a 47-group calculation (480 minutes), with dose rates shown in Fig. 12. The ratio of the 47-group calculation to the CE calculation is shown in Fig. 13. For this MG calculation, the dose rate varies from the CE calculations by up to a factor of 1.5 in either direction, indicating improvement in the results realized through CE treatment, especially of the line sources.

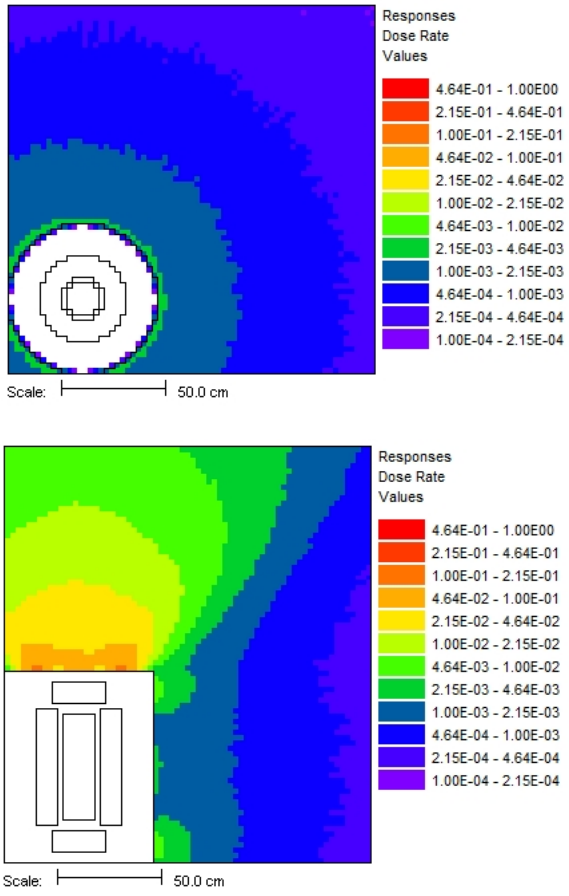


Fig. 11. Dose rates (mrem/hr/Ci) from the CE calculation, showing the midplane views of the cask (z=0 above and y=0 below).

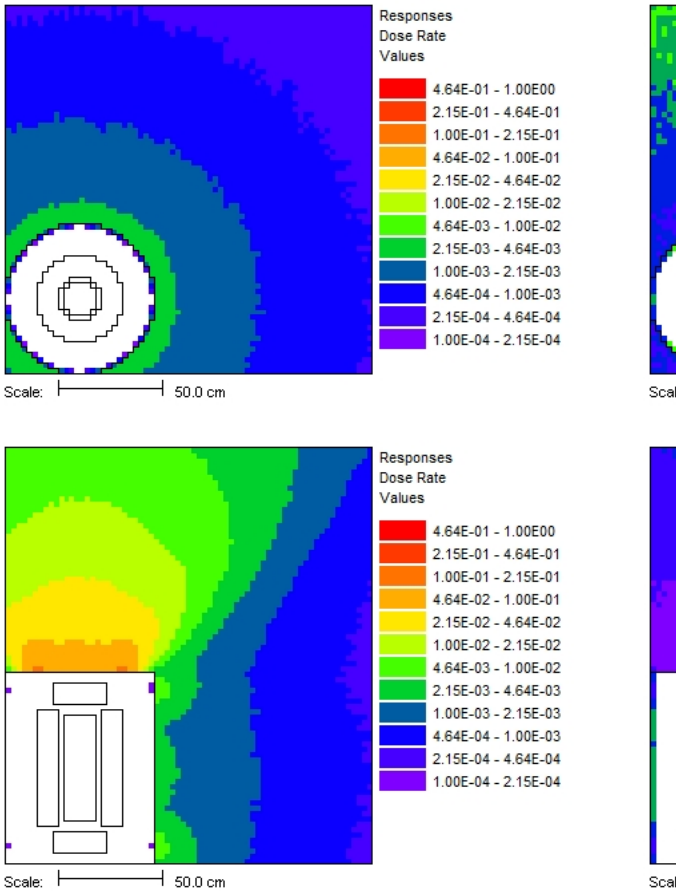


Fig. 12. Dose rates (mrem/hr/Ci) from the 47-group calculation, showing the midplane views of the cask (z=0 above and y=0 below).

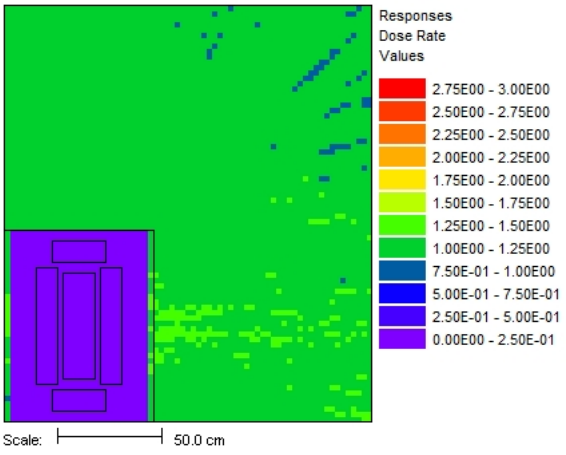


Fig. 13. Ratio of the 47-group MG computed dose rates to the CE dose rates (y=0 left and z=0 right).

Mixture Limit Enhancement

Since the first release of SCALE in 1980, there has been a limitation on the number of materials that could be utilized in a single model. A limit of 2,147 mixtures was imposed by an internal data structure in the AMPX nuclear data file format. This limit was due to storing the mixture number and the nuclide identifier both within a single integer, an attribute of the AMPX MG file format that predates the initial version of SCALE by nearly two decades. For 32-bit integers, the largest number that can be represented is 2^{31}, or 2,147,483,648. In sharing a single integer to represent both the mixture number and the nuclide identifier, the leading 4 digits were used to represent the mixture number (M) and the trailing 6 digits were used to represent the nuclide identifier as a ZA number, as shown below.

M	M	M	M	Z	Z	Z	A	A	A

For example, ^{235}U (ZA is 92235) in mixture 135 would be represented as 0135092235. This system works fine as long as the mixture number does not exceed 2,147, at which point a numeric overflow would occur in the calculation. For approximately 50 years this file format has been hard coded into over 100 modules throughout SCALE and AMPX, requiring a significant task to update and test every code that reads, writes, or utilizes this format.

With an expanding need for Monte Carlo reactor calculations with many more than 2,147 depletion regions, it became necessary to resolve this legacy issue. As this task was initiated, other limitations in the AMPX MG data format were noted such as an upper limit of 999 energy groups, due to another legacy instance of sharing an integer for more than one value. There were also restrictions that prevented inclusion of new types of data, such as photo-neutrons produced from high-energy gamma interactions.

In order to provide a lasting resolution to these format limitations that impact simulations, a centralized data Resource for MG data was developed and connected to all SCALE modules. The centralized Resource provides a single modular and extensible component that provides the connection between the data file and the computational codes. The data file can be updated as needed, and only the single Resource module needs to reflect this change. The update is transparent to the numerous computational codes that access the data.

As a basic feature, the data Resource and associated code changes enable the use of separate integers for the mixture number and the nuclide ZA identifier. Thus, the mixture limit for SCALE 6.2 will be over 2 billion, which will hopefully be sufficient for the next 50 years.

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. Lester M. Petrie, Jr.

Position: Research Staff, SCALE Technical Lead

Working on SCALE since the late 1970s
(since the beginning)

Focus Areas: Criticality Safety, Shielding, Cross Sections

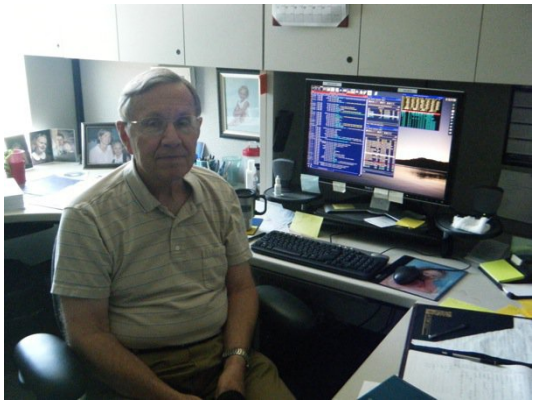


Fig. 14. Dr. Lester M. Petrie, Jr.

Most memorable projects:

Obviously, SCALE is one of the most memorable projects. I have been responsible for KENO development for most of the past 40 years, and responsible for keeping SCALE integrated together for much of that period.

I served on an international criticality safety committee investigating methods and data. Early in my career, I was fortunate enough to help design some criticality safety experiments, and then observe the actual execution of some of the experiments. In the 1980s, I served on the DOE Language Working Group, which was tasked with extending Fortran 77 to allow more optimum use of the supercomputers of that era. While DOE never did anything with the committee design, it provided some influence on the Fortran 90 standard.

Life outside of work:

I enjoy spending time with my family. For our 50th wedding anniversary, my wife and I went to California with our whole family and had a great time. We enjoy traveling and have visited various places in Europe several times, Alaska, Hawaii, and many parts of the US. I enjoy photography, and unfortunately, I enjoy eating.

Fall 2012 SCALE Training Courses

Date	Title	Location	Registration Fee
Oct 8-12	SCALE Criticality Safety Calculations Course *Introductory through advanced criticality calculations using KENO V.a and KENO-VI; Resonance self-shielding techniques*	ORNL Oak Ridge, TN, USA	$2000
Oct 15-19	SCALE Criticality and Shielding Course *Basic criticality calculations with KENO-VI; shielding analysis with automated variance reduction using MAVRIC; criticality accident alarm system analysis*	ORNL Oak Ridge, TN, USA	$2000
Oct 22-26	SCALE Lattice Physics and Depletion Course *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*	ORNL Oak Ridge, TN, USA	$2000
Oct 29-31	SCALE/ORIGEN Activation and Decay Calculations Course *Isotopic depletion/decay and source term characterization using ORIGEN/ORIGEN-ARP*	ORNL Oak Ridge, TN, USA	$1500

Foreign National Visitors: You **must** register **at least 40 days** in advance to obtain security clearance.

Payment must be received at least one week prior to training course.

For more information and online registration, please visit
http://scale.ornl.gov/training.shtml

SCALE Newsletter
Oak Ridge National Laboratory
Post Office Box 2008
Bldg. 5700
Oak Ridge, TN 37831-6170

Fax: 865-574-3527
E-mail: scalehelp@ornl.gov

SCALE Web Site:
http://scale.ornl.gov

SCALE Electronic Notebook:
http://scale.ornl.gov/notebooks.shtml

Find us on Facebook
http://facebook.com/Scale.codes

SCALE Newsletter is published twice a year by the Reactor and Nuclear Systems Division of the Oak Ridge National Laboratory*

*Managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725

SCALE Newsletter is sponsored by U.S. Nuclear Regulatory Commission, Division of Spent Fuel Storage and Transportation, and the U.S. Department of Energy.