OAK RIDGE National Laboratory

# SCALE Newsletter

Number 48 Spring 2016

## In This Issue



scale
Nuclear Systems Modeling & Simulation

## SCALE 6.2 Special Edition

SCALE 6.2 represents one of the most comprehensive revisions in the history of SCALE, providing several new capabilities and significant improvements in many existing features.

New capabilities include

- evaluated nuclear data file (ENDF)/B-VII.1 nuclear data libraries—continuous energy (CE) and multigroup (MG) with enhanced group structures,
- neutron covariance data based on ENDF/B-VII.1 and supplemented with ORNL data,
- covariance data for fission product yields and decay constants,
- stochastic uncertainty and correlation quantification for any SCALE sequence with Sampler,
- parallel calculations with KENO,
- problem-dependent temperature corrections for CE calculations,
- CE shielding and criticality accident alarm system analysis with MAVRIC,
- CE Monte Carlo depletion with TRITON,
- CE sensitivity/uncertainty analysis with TSUNAMI-3D,
- simplified and efficient light water reactor (LWR) lattice physics with Polaris,
- large-scale detailed spent fuel characterization with ORIGAMI and ORIGAMI Automator,
- advanced fission source convergence acceleration capabilities with Sourcerer,
- nuclear data library generation with AMPX, and
- integrated user interface with Fulcrum.

Enhanced capabilities include

- accurate and efficient CE Monte Carlo methods for eigenvalue and fixed source calculations;
- improved MG resonance self-shielding methodologies and data;
- resonance self-shielding with modernized and efficient XSProc integrated into most sequences;
- accelerated calculations with TRITON (generally 4x faster than SCALE 6.1);
- spent fuel characterization with 1470 pre-generated burnup libraries representing 61 reactor fuel types for use in ORIGEN and ORIGAMI;
- modernization of ORIGEN (Chebyshev Rational Approximation Method [CRAM] solver, API for high-performance depletion, new keyword input format);
- extension of the maximum mixture number to values well beyond the previous limit of 2147 to ~2 billion;
- nuclear data formats enabling the use of more than 999 energy groups;
- updated standard composition library to provide more accurate use of natural abundances; and
- numerous other enhancements for improved usability and stability.

The user documentation for SCALE has also been substantially updated and reorganized.

# Updates in SCALE 6.2

## Nuclear Data

### ENDF/B-VII.1 Cross-section Libraries

ENDF/B-VII.1 nuclear data libraries are introduced in SCALE 6.2. CE data are available for general-purpose neutron, gamma, and coupled neutron/gamma calculations. MG neutron libraries in the 252- and 56-group structure are available, where the 252-group library is for general-purpose applications and the 56-group library is intended for light water reactor (LWR) analysis. Coupled neutron/gamma MG libraries are available in a fine 200-neutron/47-gamma group structure and a broad 28-neutron/19-gamma structure.

### Neutron Cross-section Covariance Data

Updated cross-section covariance libraries are provided with SCALE 6.2 for use with the sensitivity and uncertainty modules. The data has been assembled from a variety of sources, including high-fidelity covariance evaluations from ENDF/B-VII.1, other domestic and international evaluations, as well as approximate uncertainties obtained from a collaborative project performed by Brookhaven National Laboratory, Los Alamos National Laboratory, and ORNL. In addition, the covariance library now uses a 56-group structure for broad group analysis, which is suitable for most applications, as well as the 252-group structure for fine group analysis, such as for energy-dependent reaction rates. These libraries are generated for compatibility with the ENDF/B-VII.1 56-group lattice physics library, 252-group criticality library, and CE analysis. The current SCALE covariance library spans the full energy range of the MG cross-section libraries. The new 56-group and 252-group covariance libraries (56groupcov7.1 and 252groupcov7.1) are recommended for all applications. However, the previous library (44groupcov) distributed with SCALE 6.0 and SCALE 6.1 is retained for backwards compatibility. Covariance data are available for 456 materials, including some duplication for materials with multiple thermal scattering kernels. The SCALE 6.2 56-group covariance library (56groupcov7.1) is the default library for uncertainty calculations, but other libraries can be accessed by setting the appropriate parameter in the sensitivity/uncertainty analysis codes.

### Continuous-energy Data Processing

Investigations into the CE data generated by the AMPX code system for deployment in SCALE 6.0 and 6.1 revealed a need for improvement in the S($\alpha$,$\beta$) treatment, especially for forward-peaked kinematics. The SCALE 6.2 ENDF/B-VII.0 and ENDF/B-VII.1 data libraries have been generated using new AMPX processing procedures, and the benchmark testing results with SCALE 6.2 show substantially improved results relative to SCALE 6.0 and 6.1. Select critical benchmark results for thermal mixed oxide (MOX) systems are provided in Figure 1, which shows that the bias in the SCALE 6.2 ENDF/B-VII.0 CE results is reduced relative to SCALE 6.1. Additional testing has revealed that biases for burned LWR fuel as large as 1000 pcm are resolved with the improved treatment.

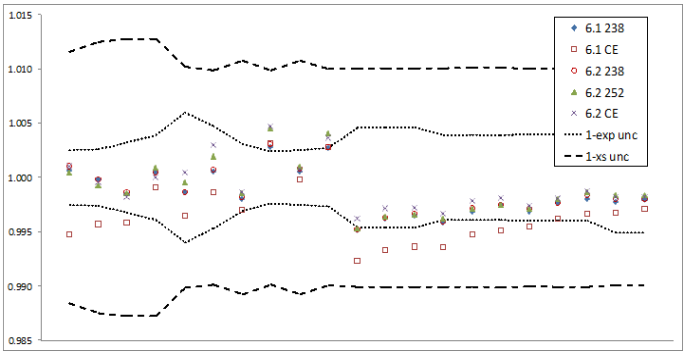



**Figure 1. SCALE calculated to experimental results for International Criticality Safety Benchmark Evaluation Project (ICSBEP) thermal mixed oxide critical systems.**

Additionally, the probability tables that provide CE treatment in the unresolved resonance range have been improved, primarily through the inclusion of additional resolution and error correction. Testing with the new probability tables has shown reduced biases for systems that are sensitive to the intermediate energy range.

Historically, only neutron CE data libraries with a specific reaction subset of the ENDF libraries have been supported in KENO Monte Carlo criticality safety codes. To support CE depletion, sensitivity analysis, and coupled neutron-gamma shielding analysis, AMPX capabilities for the generation of CE neutron data have been improved and extended. Capabilities were added to generate gamma interaction data and to produce gamma yield data from neutron interactions. In addition, wide ranges of neutron interactions were also added in order to support creating reaction responses in Monaco.

The improved CE data have been comprehensively reviewed, verified, and validated with approximately 5000 infinite medium eigenvalue tests, 6300 fixed-source transmission tests, and 400 criticality and shielding benchmark experiments to ensure robust and accurate calculations.

### Multigroup Data Processing

For MG analyses, ORNL has performed detailed comparisons between SCALE CE and MG results, and historically a bias of 200-500 pcm has been observed where the 238-group library is applied to LWR systems. The new 252-group structure for SCALE 6.2 provides a more detailed representation of the $^{238}$U resonance structure. AMPX has been used to develop new 56- and 252-energy-group ENDF/B-VII.1 neutron cross-section libraries. In addition to the new group structures, these libraries have been generated using a new weighting spectrum with improved resonance self-shielding parameters. Specifically, for actinides and hydrogen in $H_2O$, a temperature-dependent CE flux spectrum has been generated with the CE CENTRM module for a PWR pin cell, and the CE flux spectrum has been used as a weighting function for library

generation. Intermediate resonance parameters (lambdas) for all isotopes have been included in the library, which provides a capability for improved self-shielding with the Bondarenko method and Polaris. Bondarenko shielding factors, as a function of background cross section and temperature, were computed for most nuclides using CE spectra calculated by CENTRM for homogeneous mixtures of the resonance material and hydrogen, corresponding to the respective background cross section. For the nuclides $^{235}U$, $^{238}U$, $^{239}Pu$, $^{240}Pu$, and $^{241}Pu$, the Bondarenko factors are based on CENTRM CE calculations for heterogeneous pin cell models that span the range of anticipated self-shielding conditions. The thermal cutoff for moderators and the free-gas approximation has been raised from 3 eV to 5 eV. The new library has been tested by analyzing a wide variety of critical benchmark experiments and by comparing results with CE Monte Carlo results. The 252-group results presented in Figure 1 demonstrate consistent performance with the SCALE 6.2 CE results for the thermal MOX critical benchmark experiments. Based on additional studies with the 252-group library, computational benchmark comparisons with CE results at room temperature and elevated temperatures show agreement within 100 pcm in most cases.

### Nuclear Data File Formats

A new binary data format is introduced in SCALE 6.2 and applied to modernize the format of the AMPX MG cross section data libraries, replacing the AMPX Working and Master formats that were designed in the 1960s. The previous formats were restricting the extension of capabilities desired to provide improved physics.

BOFF (Binary Object Formatted File) is a binary data format designed for flexibility and compactness and is intended to compete with native binary file formats that incorporate optimizations implicit to the developer and the data being stored. BOFF revolves around the steadfast data structures of primitive, array, and object data and can provide backward and forward data format compatibility. BOFF provides the capability to store data in a hierarchical manner utilizing objects, arrays, and keyed-values. The BOFF format is implemented in the AMPX MG format to provide the ability to incorporate additional data in future updates.

### Modernized Resonance Self-Shielding

Several SCALE sequences have been updated to perform resonance self-shielding of MG cross sections and one-dimensional neutron transport calculations using the modern XSProc module. XSProc provides the capabilities of BONAMI, CENTRM, PMC, WORKER, and XSDRN and has been demonstrated to produce equivalent results to the prior independent codes. With XSProc, runtime and memory requirements are substantially improved, especially when performing calculations with many unit cells. Generally, speedups in self-shielding of about 3x are realized, but in an extreme test case using an as-loaded spent nuclear fuel storage package with hundreds of unique materials, the cross section processing and cell homogenization time was reduced from 5 days to 3.7 minutes, while still obtaining equivalent results. XSProc is implemented across most SCALE sequences, as shown in Table 1, where modernized sequences with XSProc and legacy sequences that run that stand-alone codes are identified.

**Table 1. SCALE Sequence Modernization**

| Sequence | Modern | Legacy |
|---|---|---|
| CSAS-MG | ✓ | |
| CSAS1 | ✓ | |
| CSAS1X | ✓ | |
| CSAS5 | ✓ | |
| CSAS6 | ✓ | |
| CSASI | ✓ | |
| CSASIX | ✓ | |
| MAVRIC | ✓ | |
| STARBUCS | | ✓ |
| T-NEWT | ✓ | |
| T-XSDRN | ✓ | |
| T-XSEC | ✓ | |
| T5-DEPL | ✓ | |
| T6-DEPL | ✓ | |
| T-DEPL | ✓ | |
| T-DEPL-1D | ✓ | |
| TSUNAMI-1D | ✓ | |
| TSUNAMI-2D | | ✓ |
| TSUNAMI-3D_K5 | ✓ | |
| TSUNAMI-3D_K6 | ✓ | |

XSProc provides for infinite homogeneous medium, lattice cell, multiregion, and double heterogeneous cell types. For all but the double heterogeneous cells, a new capability is implemented for accelerated self-shielding using intermediate resonance (IR) approximation Bondarenko treatment for the full energy range (PARM=BONAMI) as well as the more rigorous option of CE treatment in the resolved resonance range (PARM=CENTRM), with default treatment set as CE. Only the CENTRM path is available for double heterogeneous cell types.

XSProc provides capabilities for

- resonance self-shielding of microscopic data,
- generation of macroscopic cross sections for mixtures,
- one-dimension MG transport calculations to calculate eigenvalues and flux weighting functions,
- group collapsing of cross sections using flux spectra from the one-dimensional eigenvalue calculation or user input fixed source spectra, and
- spatial homogenization of cross sections across material zones.

Sequence-specific control for the generation of on-disk or in-memory data libraries for microscopic or macroscopic data containing selected reaction cross sections and scattering data is available with this modernized tool.

### CENTRM

A new two-dimensional CENTRM option is available to explicitly treat the boundary of square-pitched LWR fuel pins with a Method-of-Characteristics (MoC) CE transport option, resulting in approximately a 100 pcm reduction in bias between MG and CE calculations. This is now the

default option for fuel lattice calculations using CENTRM through XSProc within SCALE sequences.

New options are available in CENTRM/PMC to address the effects of resonance self-shielding on scattering matrices, using the *N2D=* option in *centrm data* in *celldata*. *N2D=2* performs self-shielding corrections on the 0th order scattering data (like the default *N2D=-1* method) but also corrects the higher order Legendre moments with corresponding higher order fluxes. *N2D=-2* similarly treats the higher order Legendre moments and explicitly treats within-group elastic scattering removal. The impact of these options is demonstrated on the IEU-MET-FAST-005-001 fast system with a steel reflector with $k_{eff}$ results shown in Figure 2. Here it is observed that the use of the *N2D=2* and *-2* options produces MG results that are more consistent with the reference CE Monte Carlo results. However, these results are not universal for all calculations, so the *N2D=2* and *-2* options should be applied after careful investigation of each system type. In particular, the use of this option for systems with large reflectors is not recommended.

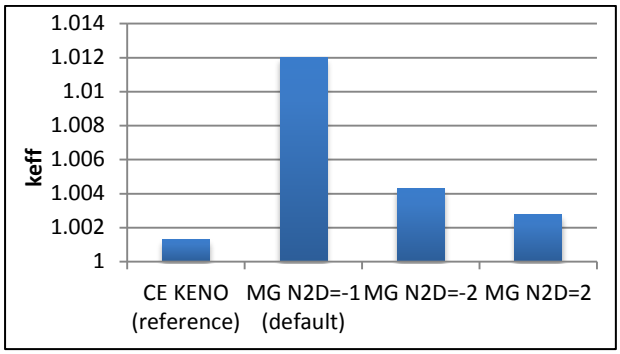



**Figure 2. $k_{eff}$ values for IEU-MET-FAST-005-001 with different MG options.**

## Bondarenko Self-Shielding

BONAMI has been rewritten as part of the overall SCALE modernization effort. BONAMI now implements IR approximation theory as well as the previous narrow resonance (NR) approximation. The IR approximation allows for improved accuracy for systems with overlapping resonances and provides a rapid self-shielding option using only full-range Bondarenko factors. This technique produces accurate results and provides up to a 10x speedup relative to CE treatment with CENTRM. IR theory is described in the updated BONAMI section, Section 8.2. To enable this option, set *PARM=BONAMI* on the sequence specification record (e.g., *=t-depl PARM=BONAMI*) and *IROPT=1* in the *more data* section of *celldata*.

## Double Heterogeneity Treatments

The DoubleHet cell types for the treatment of tristructural isotropic (TRISO) fuels has been updated within XSProc to provide more accurate results and accommodate all lattice cell types with cylindrical, spherical, and slab geometry, including annular and asymmetrical arrangements, for high temperature gas reactor (HTGR), fluoride-salt cooled high-temperature reactor (FHR), and fully ceramic microencapsulated (FCM) fuels.

## Graphical User Interface – Fulcrum

Fulcrum is a cross-platform graphical user interface designed to create, edit, validate, and visualize SCALE input, output, and data files. Historically, SCALE has provided several special-purpose graphical user interfaces, which operate only on specific platforms and are loosely integrated with SCALE's computational and data components. Fulcrum, in contrast, is designed to provide a single user interface that directly integrates with SCALE's internal resources to provide a consistent experience between Fulcrum and SCALE's command line interface.

The concept of Fulcrum is based on decades of feedback from our user community through the release of numerous interfaces. In contrast to the SCALE 6.1 GeeWiz interface with many layers of dialog boxes, Fulcrum directly connects the user with the text form of the input file, while providing inline features to assist with building correct inputs. Fulcrum provides input editing and navigation, interactive geometry visualization for KENO V.a, KENO-VI, and NEWT, job execution, overlay of mesh results within a geometry view, and plotting of data from most SCALE file formats. An error checker interactively identifies poorly formed input with spelling errors or data entry omissions for all SCALE sequences. The input validation engine identifies allowed data ranges and interdependencies in the input and reports inconsistencies to the user. Fulcrum can interactively process standard composition data to produce a mixing table, list expanded input aliases for review, provide an internal listing of input (as is required for Sampler material and geometry perturbation analysis), and launch SCALE calculations.

The layout of panels in Fulcrum is highly configurable to accommodate the preferences of users, as shown in Figure 3.

As Fulcrum is a new user interface, users are directed to the *Help* menu within the application itself for *Help documentation*.

Fulcrum replaces the following SCALE 6.1 user interfaces:

- GeeWiz
- Javapeño
- MeshView
- ChartPlot
- OrigenArp
- PlotOpus
- KENO3D

KENO3D, Javapeño, and MeshView are deployed with SCALE 6.2 for backwards compatibility with some functions, but the use of Fulcrum is strongly recommended.

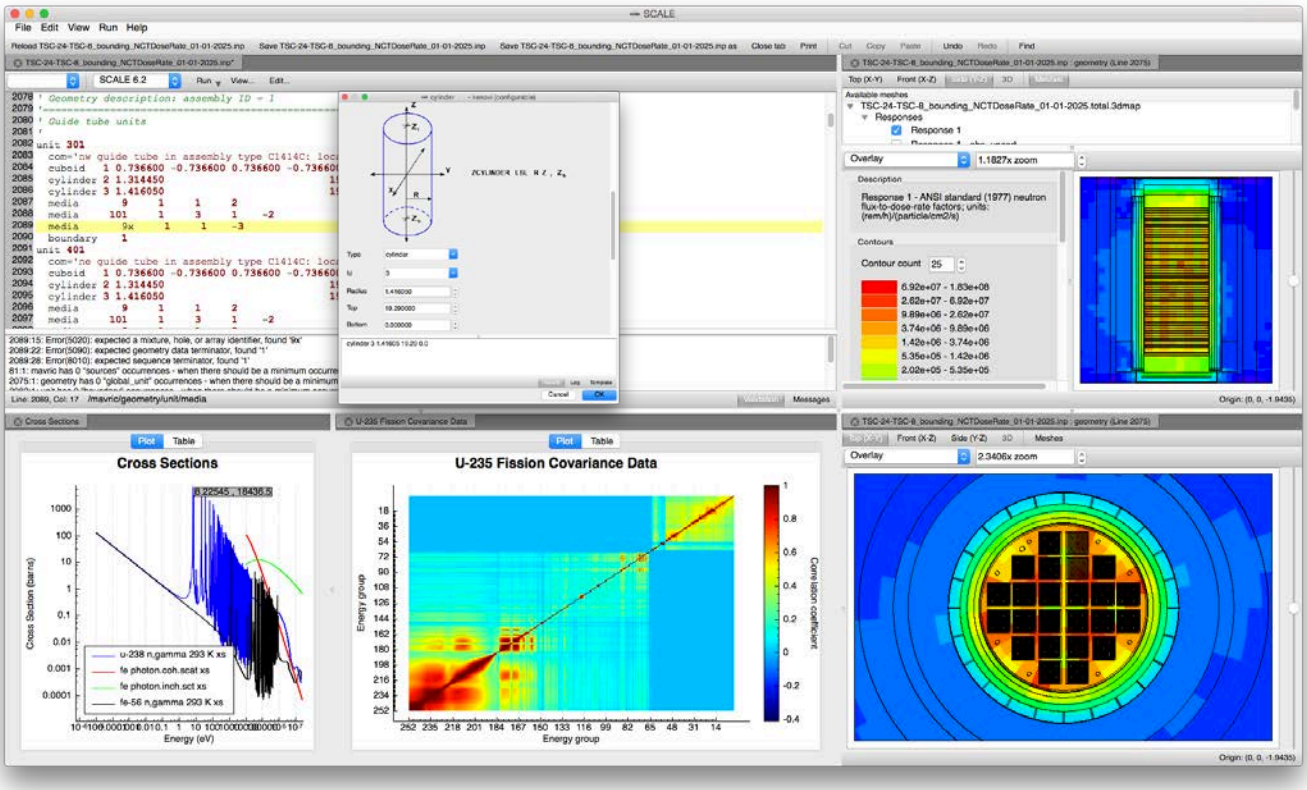



**Figure 3. SCALE Graphical User Interface – Fulcrum.**

The Fulcrum user interface provides numerous features, such as

- operates on all supported platforms, Linux, Mac and Windows;
- can edit, view, and run multiple inputs simultaneously;
- context aware auto-completion input generation menus are presented when *ctrl+space* is pressed within an input file,
- graphical forms-based input is available to assist users with the creation of sequence blocks and specific input components (press *ctrl+space* and select a *configurable* item);
- input is validated as it is entered, and erroneous or missing input is identified in the *Validation* panel;
- geometry models can be visualized for sequences that use KENO V.a, KENO-VI, Monaco, and NEWT (*View…* menu shown in toolbar associated with relevant input file);
- Fulcrum is pre-configured to run SCALE 6.2, but can be custom configured for other codes;
- associated files (such as *.out*, *.msg*, plot, or data files) are shown in contextual pop-up menu for each input file in the navigation panel and can be opened (right-click on input file name in navigation panel);
- associated files not supported in Fulcrum open a local tool for appropriate viewing (e.g. .html files launch the system web browser); and
- mesh tallies stored in *.3dmap* files can be overlaid with geometry view (*Meshes* on toolbar in geometry view, right click in *Available Meshes* panel to load a *.3dmap* file);
- data plotting is available for the following SCALE files:
  - MG and CE cross section data;
  - cross-section covariance data;
  - ORIGEN gamma data;
  - ORIGEN concentration file (*f71*) with integrated unit conversion (OPUS capability);
  - sensitivity data file (*.sdf*);
  - KENO reaction rate and flux file (*.kmt*);
  - Ptolemy plot file (*.ptp*) (previously Javapeño 2D plot, *.plt*); and
  - MAVRIC Chart Plot file (*.chart*).
- data files with file extensions (e.g. *.sdf*, *.kmt*, etc.) are accessed through *File/Open file…*;
- other file types, especially SCALE nuclear data files, have a specific menu item in the *File* menu (e.g., *Open continuous-energy library…*);
- plots can now be saved in an editable format as a SCALE Plot File (.spf);
- data tables are available for data shown in a plot;
- geometry volumes can be computed for KENO and Monaco models; and
- inline help is available.

## Criticality Safety

KENO has been substantially improved for SCALE 6.2, especially for the accuracy and efficiency of CE calculations, CE temperature corrections, source convergence diagnostics and acceleration, and parallel capabilities.

### Reduction in Memory Requirement of CE Internal Storage

Numerous improvements were made to enhance the CE capabilities of KENO, especially to reduce the memory requirements of the calculations. CE calculations now require 40–99% less memory than previous versions with no loss of accuracy in the results. Improved memory efficiency will be observed for all calculations, but especially for models with many materials and/or temperatures. Models that previously would have required hundreds of GB of memory with SCALE 6.0 and 6.1 can now be performed with only a few GB of memory.

User controllable options:

- *UUM:* Optional *unionization* of mixture-dependent cross-section data results in a 50-90% reduction in memory requirements for a single material, with no additional memory required for the use of the same nuclide in more than one mixture. Previous burned fuel calculations that would have required hundreds of GB of memory can now be run with just a few GB through the use of the default setting of *UUM=no* in the KENO parameter data.
- *M2U:* Optional nuclide level energy grid unionization (map2union) controls the unionization of all reaction types within a single nuclide. The default behavior, *M2U=yes,* reduces runtime. Optionally disabling map2union (*M2U=no*) results in an ~20% reduction in memory with an ~10% increase in runtime.

Other internal optimizations include

- removed redundant copies of temperature-independent data to improve memory efficiency for models with multiple temperatures, resulting in >50% memory savings for the addition of each temperature relative to the techniques implemented in SCALE 6.0 and 6.1.
- Kinematics (scattering) data structures were updated to optimize data storage, especially with an updated structure in the CE data itself. These updates result in an ~40% reduction in memory requirements using the same runtime.
- Changed internal data storage precision from double precision to single precision where possible, resulting in a 15–45% reduction in memory requirements, depending on the nuclides used in the model.
- Introduced optional data loading by filtering data during reading instead of loading all available data whether it is needed or not. Filtering methods such as energy range, reaction types, data types, etc., result in an ~20% reduction in memory requirements.

### Problem-Dependent Doppler Broadening

The CE data libraries distributed with SCALE are provided with about five temperatures per isotope. The Doppler broadening temperature corrections using only a few temperatures may not match the desired temperature of the calculation. In previous versions of SCALE, KENO would select the nearest available temperature, which could be several hundred degrees from the desired temperature, producing results that vary significantly from those that would be produced at the correct temperature.

New methods have been developed and implemented in SCALE 6.2 to provide *problem-dependent* temperature corrections by Doppler broadening data for the full energy range to the requested temperature when the cross sections are loaded for the calculation including the thermal scattering data, the pointwise data in the resolved resonance region, and the probability table data in the unresolved resonance region. The runtime penalty for this methodology is negligible, as all temperature corrections are performed as the calculation begins and typically require only a few seconds to a few minutes, depending on the number of nuclides and temperatures used.

The eigenvalues computed for a typical fresh pressurized water reactor (PWR) pin cell using the nearest selected CE temperature, and problem-dependent CE temperature treatments, are shown in Figure 4. Problem-dependent Doppler broadening is controlled with *DBX=0* to select the nearest temperature, *DBX=1* to perform problem-dependent corrections for the resolved and unresolved resonance ranges, and *DBX=2* (default) to also perform corrections for the S(α,β) thermal scattering data.

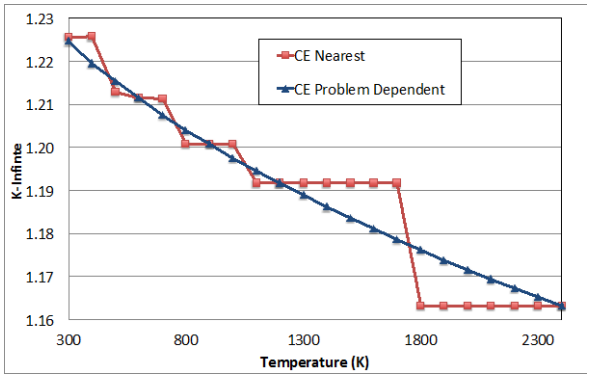



**Figure 4. Eigenvalues computed for a PWR pin cell with different temperature treatments.**

### Doppler Broadened Rejection Correction

The implementation of Doppler Broadened Rejection Correction (DBRC) techniques provides further enhancements for calculations with elevated temperatures. DBRC in KENO presents a reactivity correction of approximately 300 pcm relative to the default methodology for a 1200K LWR fuel pin, consistent with that predicted with MCNPX by the originators of the methodology. DBRC is enabled with *DBR=* in the KENO parameter data. Available options are *DBR=0* to disable the correction (default), *DBR=1* to perform DBRC for $^{238}$U only, and *DBR=2* to perform DBRC for all major actinides. The use of DBRC only impacts calculations at elevated

temperatures, and there is a runtime penalty for the use of this methodology. As such, it is not recommended for calculations near room temperature.

## Distributed Memory Parallelism via MPI

In addition to the numerous improvements described that directly affect solution accuracy and efficiency, parallel computation capabilities, especially for Linux clusters, have been added to KENO to provide reductions in wall clock time, especially for S/U analysis or Monte Carlo depletion on computer clusters. By introducing a simple master-slave approach via Message Passing Interface (MPI), KENO runs different random walks concurrently on the replicated geometry within the same generation. The fission source and other tallied quantities are gathered at the end of each generation by the master process; then, they are processed either for final edits or next-generation.

The parallel performance of KENO as used in a CE calculation for a graphite-moderated reactor model is shown in Figure 5. These tests were conducted on a heterogeneous Linux cluster where the size of the nodes varies from 4 to 16 cores with differing processor speeds, much like SCALE users may encounter in practice. Tests were conducted with systematically increasing numbers of particles per generation, and various combinations of options were enabled to develop the distributions of speedups for each number of MPI processes shown in the figure. With larger numbers of particles per generation, KENO provides nearly linear speedup on 64 processors.

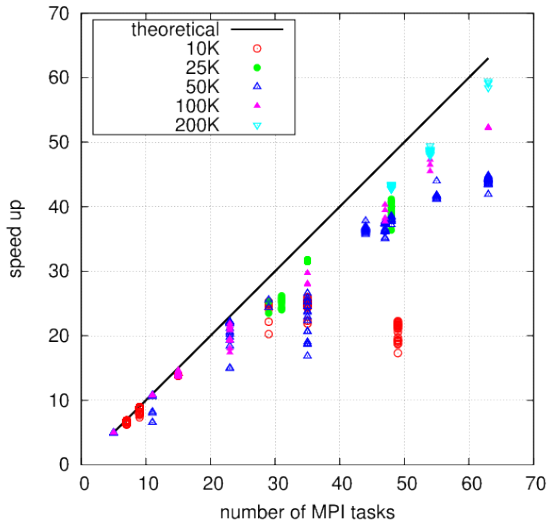



**Figure 5. Speedup for parallel KENO-VI calculations for a graphite-moderated reactor model.**

## Reaction Tallies

User-configurable reaction rate tallies are now available within KENO CE calculations. The tallies are specified in the *REACTION* block of KENO. The KMART modules continues to provide reaction rate calculations for MG calculations.

## Fission Source Convergence Diagnostics

Prior to SCALE 6.2, KENO provided only plots of $k_{eff}$ by generation and average $k_{eff}$ for visual inspection of source convergence, followed by a $\chi^2$ statistical assessment of convergence. With SCALE 6.2, Shannon Entropy fission source convergence diagnostic techniques have been implemented in KENO to provide improved confidence in the computed results, as well as reduced simulation times in some cases. Confirming the convergence of the fission source distribution is especially useful to avoid the false convergence of $k_{eff}$ and neutron flux tallies that can be caused by insufficient sampling of important portions of the system. Source convergence diagnostics are enabled with *SCD=yes* (default) in the KENO parameter data.

## Sourcerer - Hybrid Method for Starting Source Distribution

The *Sourcerer* sequence introduced in SCALE 6.2 uses the Denovo discrete-ordinates code to generate a starting fission source distribution in a KENO Monte Carlo calculation. Initial studies have shown that using a starting fission distribution that is similar to the true fission distribution can both reduce the number of skipped generations required for fission source convergence and significantly improve the reliability of the final $k_{eff}$ result.

For many criticality safety applications, the additional step of performing a deterministic calculation to initialize the starting fission source distribution is not necessary. However, for the most challenging criticality safety analyses, such as spent-nuclear-fuel-loaded transportation packages with a mixed loading of low- and high-burnup fuel, even a low-fidelity deterministic solution for the fission source produces more reliable results than the typical starting distributions of uniform or cosine functions over the fissionable regions, as demonstrated in a recent study. In that study, a cask holding 24 spent fuel assemblies was examined using a uniformly distributed starting source and a deterministically calculated starting source. Multiple clones of KENO were run (with different random number seeds) for different values of skipped cycles. The number of clones that gave an incorrect result for $k_{eff}$ was then tabulated. The results from that study, presented in Figure 6, show that using a deterministic starting source significantly increases the $k_{eff}$ reliability.

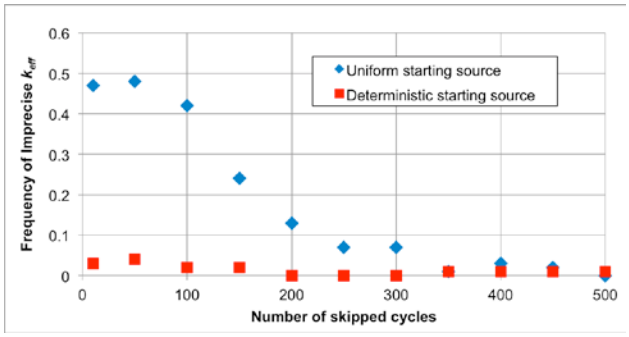



**Figure 6. Fraction of failure to agree with the reference $k_{eff}$ value for KENO calculations with different starting sources.**

## Reactor Physics

### Polaris – New Advanced Lattice Physics Module

Polaris is a new 2D lattice physics code for SCALE that utilizes a new MG self-shielding method called the Embedded Self-Shielding Method (ESSM) and a new MoC transport solver. Polaris provides simplified input, where only a few lines are required to describe the entire model, compared to TRITON.

The ESSM approach computes MG self-shielded cross sections using Bondarenko interpolation. The background cross section utilized in the interpolation is determined by a series of 2D MoC fixed-source calculations, similar to the subgroup method that does not require explicit *celldata* input. Additionally, heterogeneous lattices are explicitly treated without the need to externally compute Dancoff factors.

Polaris currently employs ESSM with either the 252-group or 56-group ENDF/B-VII.1 libraries. Each library contains cross sections, IR parameters, and full-range Bondarenko factors for all nuclides.

Polaris utilizes the self-shielded cross sections within a MG 2D eigenvalue calculation using the new MoC transport solver. The MoC solver has been developed within Denovo, which was originally developed for parallel 3D Cartesian mesh MG discrete-ordinates ($S_N$) calculations. Polaris also provides a critical spectrum calculation for correcting the flux distribution for computing both few-group homogenized cross-section edits and depletion reaction rates.

Polaris is integrated with ORIGEN for depletion calculations. The depletion of each pin, or radial subregion of the pin, is based on the local normalized flux distribution. Cross-section values in the ORIGEN transition matrix are updated from the MG self-shielded cross sections and the MG flux distribution for each depletion region. The critical-spectrum correction to the flux distribution for depletion is controlled by an input user option. The cross-section updates are performed in-memory as compared to the file-based approach previously utilized in the TRITON lattice physics sequence. Polaris supports branch calculations for the generation of few-group constants for reactor core simulators.

### Continuous-Energy Monte Carlo Depletion

SCALE 6.1 provided MG Monte Carlo depletion that coupled SCALE MG cross-section processing capabilities with KENO and ORIGEN. A new CE-based KENO/ORIGEN Monte Carlo depletion capability has been developed 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 MG data, and for models with many depletion regions where runtime to generate and store the resonance self-shielded cross-section data for each material is prohibitive.

### Lattice Physics with TRITON

Two-dimensional lattice physics calculations with TRITON will realize substantial speedups due to the use of XSProc for resonance self-shielding as well as numerous optimizations within the NEWT code. Speedups of 2-6x faster calculations are common, and some models have realized speedups of 30x relative to previous versions of NEWT. Calculation times for 1470 TRITON calculations used to generate the ORIGEN reactor libraries for SCALE 6.1.3 and SCALE 6.2 are shown in Figure 7. The average calculation time was reduced by a factor of 4.

A material SWAP capability is now available within the TIMETABLE block of TRITON. This feature allows a user to switch the material present during a depletion calculation and is especially useful for removable absorber materials.

The ASSIGN capability of TRITON is available for many calculations, where the same resonance self-shielding calculation can be applied to many similar materials. Unfortunately, ASSIGN is not yet implemented for BRANCH, TIMETABLE, or SWAP calculations.

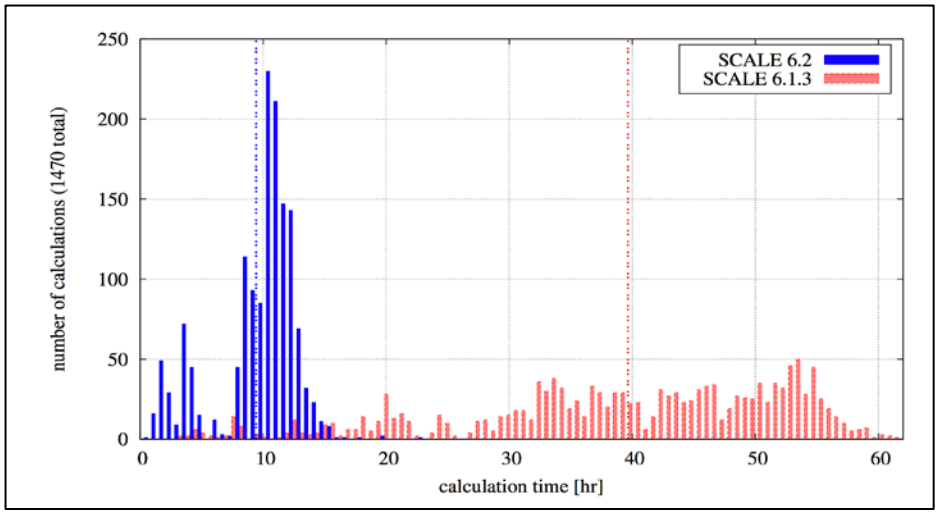



**Figure 7. Comparison of calculation times for 1470 TRITON calculations.**

### Bias Reduction for Depletion

Historical SCALE biases for LWR fuel have been mitigated as a result of the numerous enhancements included in SCALE 6.2.

Figure 8 shows the results for a reference PWR pin cell burnup calculation using SCALE 6.1 and SCALE 6.2. Here, the SCALE 6.2 CE results are the reference, and the SCALE 6.1 CE results are simply eigenvalue statepoints using the isotopics provided by the SCALE 6.2 results, as CE depletion is not available in SCALE 6.1. The 1000 pcm bias in the SCALE 6.1 CE results are due to erroneous treatment of thermal scattering data in the AMPX CE data distributed with SCALE 6.1. The SCALE 6.1 TRITON 238-group results using the default settings from SCALE 6.1 demonstrate the typical 400–500 pcm bias observed for SCALE 6.1 LWR calculations. The SCALE 6.2 TRITON 252-group results apply the improved nuclear data library, the CENTRM MoC solver, and the enhanced within group treatment for CENTRM/PMC, *N2D*=-2. The SCALE 6.2 Polaris results apply the default settings in Polaris with the ESSM methodology and IR factors on the library. These calculations demonstrate the impact of improvements in both the MG libraries and resonance self-shielding techniques, as well as improvements in the CE treatments from SCALE 6.1 to SCALE 6.2.

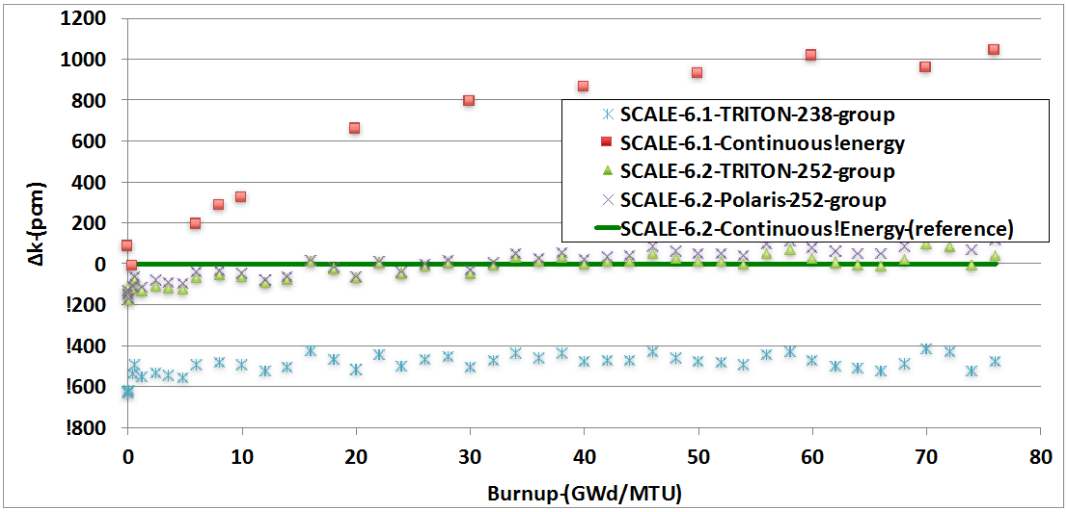



**Figure 8. Comparison of computational biases as a function of burnup.**

## Radioactive Source Term Characterization

### ORIGEN

SCALE includes the ORIGEN code and its comprehensive depletion, activation, decay, gamma-ray, and x-ray library with over 2,200 nuclides. ORIGEN and its nuclear data libraries have been updated to provide convenient modular interfaces within SCALE, and these interfaces also provide easy access to ORIGEN's robust capabilities by other software packages.

The input for ORIGEN has been updated to provide a modern interface using SCALE's new Standard Object Notation (SON). The legacy FIDO input interface will continue to be supported for backwards compatibility, but users are encouraged to begin using the modern input through input files as well as the forms-based input in Fulcrum. An excerpt from an example problem is included to show this new structured and keyword-based input.

The ENDF/B-VII.1-based fission product yields used by ORIGEN are updated to provide improved agreement with burst fission experiments for $^{235}$U, $^{238}$U, $^{239}$Pu, and $^{241}$Pu. The changes correct inconsistencies that were introduced in ENDF/B when updating the nuclear decay data in ENDF/B-VII.1 and not updating the fission product yields that are based on evaluations from the 1990s. These yield adjustments improve the consistency between the direct fission yields and decay data and the cumulative yields.

```
=origen
'three cycles of irradiation plus decay
bounds {neutron="xn27g19v7.0" gamma="xn27g19v7.0"}
case(c1){
    lib{ file="ft33f001" pos=1 }
    time=[8i 50 500]
    power=[10r40]
    mat{ iso=[u235=4e3 u238=960e3] }
}
case(c2){
    lib{ pos=2 }
    time=[8i 550 1000]
    power=[10r40]
}
case(c3){
    lib{ pos=3 }
    time=[8i 1050 1500]
    power=[10r40]
}
case(cool){
    time{ start=0 t=[20L 0.001 100] units=YEARS }
    save{ file="snf.f71" time_offset=1500 }
    gamma{ sublib=ALL brem_medium=UO2 }
    print{ neutron{ spectra=yes } }
    neutron{ alphan_medium=UO2 }
}
end
```

ORIGEN has been enhanced to provide an alternative solver based on the Chebyshev Rational Approximation Method (CRAM). When compared to a robust reference solution for a depletion problem, the traditional matrix power series and Bateman solver predicts isotopic concentrations with an average relative error of about 10E-5, where the CRAM solver produces an average relative error of about 10E-15 for the same case. The CRAM solver can also handle essentially arbitrary step lengths through internal substepping with minimal computational cost, so the runtimes are generally faster for large depletion problems. The previously mentioned depletion case required 550 ms to execute 8 substeps with the traditional solver, where CRAM completed the more accurate calculation in 44 ms. However, CRAM is slower than the traditional solver for decay problems or problems with small libraries. CRAM is currently available as an optional solver in stand-alone ORIGEN calculations.

## ORIGAMI – New Advanced Used Fuel Assembly Characterization

SCALE 6.2 includes the new ORIGAMI (ORIGEN Assembly Isotopics) tool to compute detailed isotopic compositions for LWR assemblies containing $UO_2$ fuel by using the ORIGEN transmutation code with pre-generated ORIGEN libraries, for a specified assembly power distribution. The assembly may be represented by a single lumped model with only an axial power distribution, or by a square array of fuel pins with variable pin-powers as well as an axial distribution. In either case, ORIGAMI performs ORIGEN burnup calculations for each of the specified power regions to obtain the spatial distribution of isotopes in the burned fuel. Multiple cycles with varying burn-times and down-times may be used. ORIGAMI produces files containing SCALE- and MCNP-formatted composition data for axial burnup distribution at the last time-step, as well as a file containing the axial decay-heat at the final time-step, and a file specifying the energy-dependent radioactive source for use in shielding calculations.

## ORIGAMI Automation Tool

ORIGAMI Automator, a graphical user interface integrated with Fulcrum, facilitates the quantification of isotopics as a function of time for a large set of fuel assemblies (Figure 9). This tool was developed to support the US Nuclear Regulatory Commission (NRC) in MELCOR analyses but can be adapted to many other uses. The ORIGAMI Automator is an integrated graphical user interface that leverages many modern components developed for SCALE 6.2 to enable the analyst to (1) easily create, view, and edit the reactor site and assembly information, (2) automatically create and run ORIGAMI inputs, and (3) analyze the results from ORIGAMI. The Automator uses the standard ORIGEN binary concentrations files produced by ORIGAMI, with concentrations available at all time points in each assembly's life. ORIGAMI Automator enables plotting of results such as mass, concentration, activity, and decay heat using an OPUS component. The ORIGAMI Automator Primer includes a description and user guide, a step-by-step tutorial for a simplified scenario, and appendices that document the file structures used.

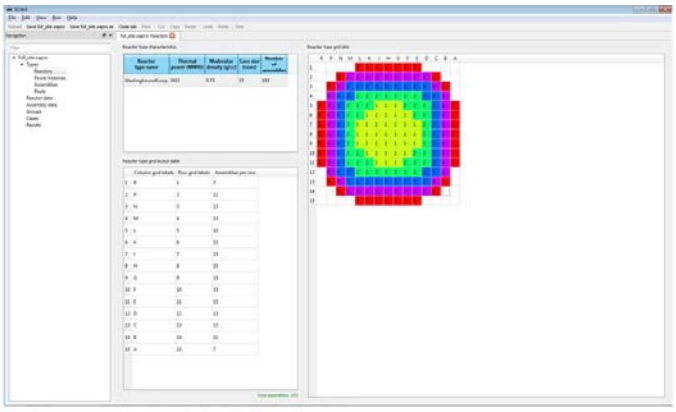


**Figure 9. ORIGAMI Automator**

## ORIGEN Reactor Libraries

A new series of 1470 pre-generated burnup libraries representing 61 reactor fuel types for use in ORIGEN and ORIGAMI are introduced to SCALE 6.2. These libraries are generated under quality assurance with TRITON using the ENDF/B-VII.1 252-group nuclear data library through the use of a new template and script system. These libraries replace the ORIGEN-ARP libraries that were generated with previous versions of SCALE with varying levels of quality assurance. Libraries are available for a variety of fuel assemblies for commercial and research reactors, as detailed in Table 2 and Table 3.

**Table 2. Assembly and Lattices Types with Available ORIGEN Reactor Libraries**

| Assembly type | | Lattice types |
|---|---|---|
| PWR | Babcock & Wilcox | 15×15 |
| | Westinghouse | 14×14, 15×15, 17×17, 17×17-OFA |
| | Combustion Engineering | 14×14, 16×16 |
| | Siemens | 14×14, 18×18 |
| BWR | ABB | 8×8-1 |
| | Atrium | 9×9-9, 10×10-9 |
| | General Electric | 8×8-4, 9×9-7, 7×7-0, 8×8-1, 8×8-2, 9×9-2, 10×10-8 |
| | SVEA | 64(8×8-1), 96(10×10-4), 100(10×10-0) |
| MOX | BWR Lattices | ABB 8×8-1, Atrium 9×9-9, 10×10-9; GE 7×7-0, 8×8-1, 8×8-2, 9×9-2, 10×10-8; SVEA-64, 96, 100 |
| | PWR Lattices | Siemens 14×14, 18×18; CE 14×14, 16×16; B&W 15×15; Westinghouse 14×14, 15×15, 17×17, 17×17-OFA |
| Other | AGR | |
| | CANDU | 19-pin, 28-pin, 37-pin |
| | IRT | 2M, 3M, 4M |
| | Magnox | |
| | RBMK | |
| | VVER-440 | flat, radial enrichments (3.82, 4.25, 4.38) |
| | VVER-1000 | flat enrichment |

**Table 3. Additional Information for ORIGEN Reactor Libraries**

| Assembly type | Enrichments [%] | Coolant/ moderator densities [g/cm$^3$] | Maximum burnup [GWd/MTU] |
|---|---|---|---|
| PWR LEU | 0.5, 1.5, 2, 3, 4, 5, 6 | ~0.73 | 70.5 |
| BWR LEU | 0.5, 1.5, 2, 3, 4, 5, 6 | 0.1, 0.3, 0.5, 0.7, 0.9 | 70.5 |
| PWR MOX | * | ~0.73 | 70.5 |
| BWR MOX | * | 0.1, 0.3, 0.5, 0.7, 0.9 | 70.5 |
| AGR | 0.5, 1.5, 2, 3, 4, 5 | 1.65 | 48.7 |
| CANDU | 0.711 | 0.8445 | 13.7 |
| IRT | 19.75, 36, 80, 90 | 0.989 | 159 |
| Magnox | 0.7, 0.8, 0.9, 1 | 1.628 | 13.7 |
| RBMK | 1.8, 2.2, 2.6, 3 | 0.15, 0.28, 0.41, 0.54, 0.67, 0.8 | 24.3 |
| VVER-440 | 1.6, 2.4, 3.6, profiled | 0.73 | 70.5 |
| VVER-1000 | 0.5, 1.5, 2, 3, 4, 5, 6 | 0.7145 | 70.5 |

* Pu contents [%]: 4, 7, 10; $^{239}$Pu contents [%]: 50, 55, 60, 65, 70

## Radiation Shielding

The SCALE fixed-source Monte Carlo capability with automated variance reduction has been enhanced to enable CE calculations. The new CE capabilities provide enhanced solution fidelity while still implementing the unique acceleration techniques of the FW-CADIS (Forward-Weighted Consistent Adjoint Driven Importance Sampling) methodology for deep penetration shielding and criticality accident alarm system modeling.

### Continuous-energy Shielding Calculations

Prior to SCALE 6.2, the MAVRIC/Monaco capabilities relied on the MG approach for radiation transport. The MG approach is suitable for many applications but can be problematic for others, such as deep penetration shielding through iron, where the MG-averaged cross section for capture resonances may not accurately represent the true transmission of neutrons due to fine "windows" through (i.e., minima in) the cross section. Additionally, MG cannot adequately resolve discrete gamma emission lines, such as those of $^{60}$Co. With the CE treatment introduced in SCALE 6.2, improved solution fidelity is available. The generation of CE nuclear data and the implementation of CE physics in Monaco are based on a first-principles approach, where the simulation is represented as realistically as possible. This approach will lead to higher-fidelity results, but runtimes may be substantially increased over more approximate methods.

Monaco also includes capabilities to import sources generated with ORIGAMI and to access gamma sources directly from ORIGEN data.

## Sensitivity and Uncertainty Analysis

### CE Eigenvalue Sensitivity Analysis

With SCALE 6.2, the MG eigenvalue sensitivity and uncertainty analysis methods that use KENO for transport analysis are extended to provide CE capabilities through the implementation of the CLUTCH (Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization) and IFP (Iterated Fission Probability) methods. CLUTCH is an efficient methodology that has been demonstrated to provide high-fidelity results with manageable runtimes and memory requirements. State-of-the-art sensitivity methods make CE calculations easier to use than MG in several ways; for example, CE calculations do not require resonance self-shielding calculations to determine implicit sensitivity effects, the simulation of a separate adjoint transport calculation, or the use of a flux mesh for tallying fluxes and flux moments.

The new capabilities enable improvements in sensitivity coefficient accuracy compared to MG. Table 4 compares the accuracy of the total nuclide sensitivity coefficients estimated by each sensitivity method for the MIX-COMP-THERM-004-001 system. The MG analysis produced a $^{238}$U total nuclide sensitivity that disagreed with the reference direct perturbation sensitivity by 2.80 effective standard deviations ($\sigma_{eff}$), while the CE methods (IFP and CLUTCH) sensitivities were within almost 1 standard deviation of the reference sensitivity coefficients for all of the nuclides examined.

**Table 4. MIX-COMP-THERM-004-001 Total Nuclide Sensitivity Coefficient Comparison.**

| Sens-itivity | Reference | MG TSUNAMI | CE TSUNAMI IFP | CE TSUNAMI CLUTCH |
|---|---|---|---|---|
| $H_2O$ | 0.2935 ± 0.0179 | 0.2805 ± 0.0088 (-0.65 $\sigma_{eff}$) | 0.2733 ± 0.0052 (-1.08 $\sigma_{eff}$) | 0.2793 ± 0.0065 (-0.75 $\sigma_{eff}$) |
| $^{238}$U | -0.0061 ± 0.0003 | -0.0050 ± 0.0002 (2.80 $\sigma_{eff}$) | -0.0055 ± 0.0003 (1.16 $\sigma_{eff}$) | -0.0057 ± 0.0001 (1.14 $\sigma_{eff}$) |
| $^{239}$Pu | 0.1262 ± 0.0087 | 0.1264 ± 0.0014 (0.02 $\sigma_{eff}$) | 0.1188 ± 0.0020 (-0.83 $\sigma_{eff}$) | 0.1190 ± 0.0001 (-0.83 $\sigma_{eff}$) |
| $^{240}$Pu | -0.03777 ± 0.00350 | -0.03750 ± 0.00011 (0.08 $\sigma_{eff}$) | -0.03738 ± 0.00060 (0.11 $\sigma_{eff}$) | -0.03743 ± 0.00002 (0.10 $\sigma_{eff}$) |
| $^{241}$Pu | 0.00589 ± 0.00042 | 0.00599 ± 0.00004 (0.24 $\sigma_{eff}$) | 0.00567 ± 0.00014 (-0.50 $\sigma_{eff}$) | 0.00579 ± 0.00003 (-0.24 $\sigma_{eff}$) |

Figure 10 compares the figures of merit for the nuclide sensitivity coefficients presented in Table 4. Figure 10 indicates that the CE sensitivity calculations are of a comparable efficiency to the MG calculations, and in some cases the CE CLUTCH method is more efficient than MG method.

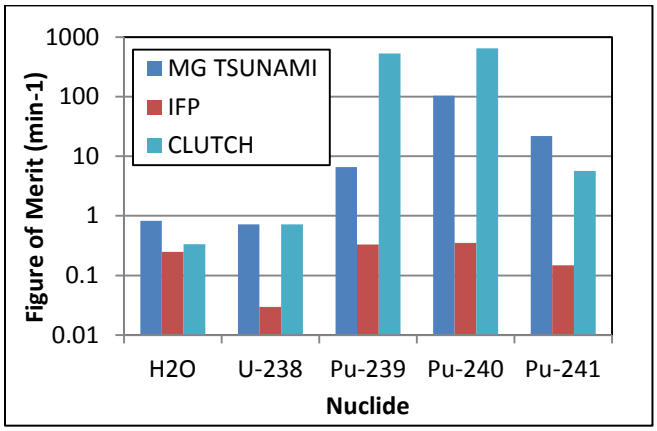



**Figure 10. MIX-COMP-THERM-004-001 total nuclide sensitivity Figure of Merit comparison.**

Table 5 gives the amount of computational memory required by each method for the sensitivity coefficient calculations. These memory requirements were obtained by subtracting the memory requirements of each eigenvalue-only calculation from the memory requirements of each sensitivity coefficient calculation. As seen below, the CLUTCH method excels in terms of memory usage and can readily compute sensitivities for complex systems on a typical personal computer.

**Table 5. Sensitivity Method Memory Usage for MIX-COMP-THERM-004-001.**

| MG TSUNAMI | CE TSUNAMI | |
|---|---|---|
| | IFP | CLUTCH |
| 13,785 MB | 10,643 MB | 63 MB |

TSUNAMI-3D also includes a Generalized Perturbation Theory (GPT) capability to compute the sensitivity of ratios of reaction rates to cross section data by introducing the GEneralized Adjoint Responses in Monte Carlo (GEAR-MC) method. The two GEAR-MC implementations are available for use in CE Monte Carlo simulations.

GPT sensitivity coefficients now share the same input as the previous MG GPT methods implemented in TSUNAMI-1D and TSUNAMI-2D. The Definitions block is used to define reaction rates in terms of material, reactions and energy ranges, and the *SystemResponses* block is used to define ratios for which sensitivity coefficients will be computed. A separate SDF file is generated for each ratio defined in *SystemResponses* detailing the sensitivity of the reaction rate ratio to the cross-section data on an energy dependent basis. The uncertainty in each ratio due to cross-section covariance data is also provided in the output file.

## Sampler

A new stochastic uncertainty quantification capability is introduced with the SCALE 6.2 *Sampler* module that implements stochastic techniques to quantify the uncertainty in any computed result from any SCALE sequence due to uncertainties in

- neutron cross sections,
- fission yield and decay data, and
- any user input parameter, such as geometry, material density, isotopic composition, temperature, etc.

Sampler propagates these uncertainties through complex analysis sequences, such as depletion calculations, and provides the variation in the output quantities due to variations in any combination of input data, as shown in Figure 11. Correlations between systems with shared uncertainties are also computed, which is especially useful for quantifying correlated uncertainties in benchmark experiments, required for generalized linear least-squares techniques implemented by the SCALE module TSURFER.

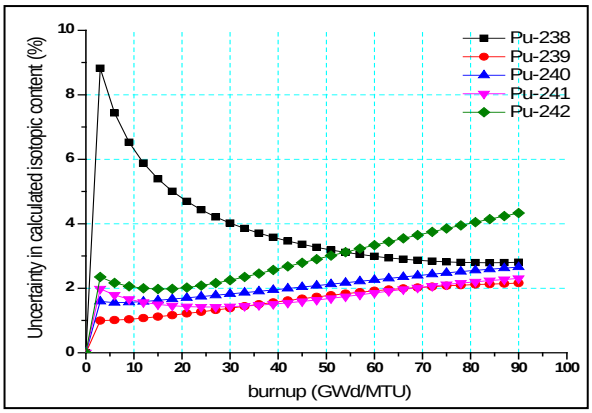



**Figure 11. Uncertainty in plutonium isotopics as function of burnup.**

Uncertainty libraries for fission product yields are implemented from ENDF/B-VII.1 data for the major actinides $^{235}$U, $^{238}$U, $^{239}$Pu, and $^{241}$Pu. These libraries are used directly by Sampler to assess uncertainty in fission product concentrations due to yield uncertainties. Covariance data are developed from fission models and a Bayesian method applied to ensure that uncertainties in the cumulative fission yields are consistent with the independent yields in each chain. The decay uncertainty data has four major components: decay constant uncertainty, q-value uncertainty, fraction of q value in photons, and branch ratio uncertainty. Perturbation factors for these four components are generated using uncertainties from the ENDF/B-VII.1 library. Correlations are accounted for decays with multiple decay modes to ensure the sum of branching is unity. No uncertainties are applied for data that does not have associated uncertainty information. Perturbations are applied using the covariance information to provide 1000 ORIGEN fission product yield and 1000 decay libraries. Currently, decay data sampling is available for ORIGEN and ORIGAMI calculations but is not operational with TRITON calculations without additional user-supplied preliminary calculations.

### Other Updates

SCALE 6.2 includes a number of other improvements, such as the extension of the maximum allowed number of materials from around 2,147 to around 2 billion. Some older features are removed such as ENDF/B-V and -VI nuclear data, the point kernel shielding capability, and a material optimization search sequence. Additionally, the default temperature for materials with no temperature explicitly specified has been modified from 300K to 293K for improved consistency between MG and CE calculations.

### Missing Cross-Section Messages

There are several nuclides that occur in natural abundance distributions for elements that are not present in the current generation of nuclear data libraries. For example, the natural abundance for oxygen contains 0.205% $^{18}$O, but ENDF evaluations do not provide cross sections for this isotope.

In previous versions of SCALE, the Standard Composition Library made several non-physical adjustments to facilitate the use of nuclear data libraries with missing nuclides. In the case of $^{18}$O, the standard compositions *UO2*, *O*, and others assumed oxygen to consist of 100% $^{16}$O instead of its true natural abundance. If the user input the standard composition name *OXYGEN*, the true natural abundances would be used and the calculation would immediately stop on an error that $^{18}$O was not present on the nuclear data library.

In SCALE 6.2, this behavior has changed in that true natural abundances are consistently applied for all standard composition materials (i.e., *UO2, O,* and *OXYGEN* now all include natural abundances for $^{16}$O, $^{17}$O, and $^{18}$O), warning messages are presented for missing nuclides, and the calculations continue without error. For example, for a very simple input of natural abundance *UO2* at 0.95% theoretical density, the following warning is produced:

```
Nuclide 8018 is not contained in the specified
library.
Attempting to use element 8000 failed.
It is also not contained in the library
'Because nuclide 8018 is missing from the cross
section library, its mixture 1 composition
definition follows:
o-16 1 0 0.0463287 end
o-17 1 0 1.76478e-05 end
o-18 1 0 9.52052e-05 end
u-234 1 0 1.25392e-06 end
u-235 1 0 0.000167282 end
u-238 1 0 0.0230522 end
*** The above edits can be used to fix the
composition input by removing or redistributing
the atomic density of the missing nuclide(s).
*** Warning - 1 issue(s) with the composition
input resulting in removal of 1 nuclide(s) with a
total of 9.52052e-05 atoms/barn-cm.
*** Mixture 1 density updated to 10.4092 grams/cc
```

The calculation then proceeds with the number density for the missing nuclide set to 0.00. The explicit number densities of every nuclide in the mixture are provided so that the user has a choice of accepting adjusted material composition or updating the input for the model to compensate for the missing material in some other way such as increasing the density of some other nuclide. In most cases, the missing nuclides do not make up a large fraction of the natural abundance and making some other adjustments will have a negligible impact on computed results. The isotopes that occur in the Standard Composition Library but have no corresponding nuclear data in ENDF/B-VII.0 or -VII.1 are shown in Table 6.

.

**Table 6. Isotopes with No ENDF/B-VII.0 or –VII.1 Nuclear Data**

| Element | SCALE standard composition ID | Missing Isotopes | ZA numbers | % Abundance |
|---|---|---|---|---|
| oxygen | 8000 | 18 | 8018 | 0.20 |
| neon | 10000 | 21, 22 | 10021, 10022 | 0.27, 9.25 |
| ytterbium | 70000 | All(1) | (1) | |
| osmium | 76000 | All(2) | (2) | |
| platinum | 78000 | All(3) | (3) | |
| tantalum | 73000 | 180m | 1073180 | 0.01 |

(1) no data for any of the seven naturally occurring ytterbium isotopes
(2) no data for any of the seven naturally occurring osmium isotopes
(3) no data for any of the six naturally occurring platinum isotopes

## 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 international standards in ISO 9001-2008, US Department of Energy Order 414.1D, and the ORNL Standards-Based Management System, and it is consistent with US NRC guidelines in NUREG/BR-0167 as well as ASME NQA-1. SCALE QA program implements a streamlined Kanban process with continuous integration of new features and an automated test system that performs approximately 100,000 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. 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.

## Nuclear Data Processing with AMPX

SCALE 6.2 also includes the AMPX cross-section processing software package that has been developed and maintained at ORNL for more than 40 years and is completely independent of any other cross-section–processing software package. AMPX is used to process ENDF nuclear data evaluations, as well as other data sources that use the ENDF format, to provide nuclear data libraries for use in modern transport code packages. AMPX is primarily used to provide nuclear data libraries for the SCALE code package, but AMPX can be used to produce data libraries that can be used by other transport codes. AMPX provides CE and MG neutron and gamma cross-section data. Also, AMPX provides cross-section uncertainty or covariance data for use with sensitivity/uncertainty analysis tools. Furthermore, AMPX can be used to process ENDF/B evaluations to produce depletion and decay libraries needed by depletion codes such as ORIGEN.

The last major public release of the AMPX code package was in 1992 when AMPX-77 was released through RSICC. In the past few years, the development, maintenance, quality assurance, and deployment of AMPX has been synchronized with SCALE such that the distribution of SCALE 6.2 includes both code systems. As a result, this AMPX release represents the culmination of significant modernization to the cross-section processing code package. Although AMPX and SCALE modernization is still in progress, one of the major objectives of the code modernization effort was to bring AMPX under a formal software quality assurance plan. To achieve this objective, ORNL merged the AMPX software repository (including software configuration control) and build system with SCALE. Merging the AMPX and SCALE development infrastructure offers many advantages with the primary motivation being software quality assurance. The merger also allows AMPX to use the same continuous integration testing that SCALE now uses. Although AMPX and SCALE are now developed under the same infrastructure, both code packages can be distributed together or separately. The combined code package release provides significant modeling and simulation capabilities by allowing users to generate and test nuclear data libraries for their specific radiation transport application needs.

## SCALE Workshop PHYSOR 2016

### Introduction to Depletion and Lattice Physics Tools in SCALE 6.2: TRITON and Polaris Workshop

Sunday, May 1, 2016, 8:00 AM – 5:00 PM
Sun Valley, Idaho, USA

The first 4 hours of the workshop will focus on TRITON by introducing users to the basic and recently added features. The last 4 hours will focus on the new lattice physics tool, Polaris. If possible, the participants are encouraged to request the SCALE code system and install it on a laptop prior to the conference in order to follow along with the exercises.

## 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


T. M. Pandya, S. R. Johnson, T. M. Evans, G. G. Davidson, S. P. Hamilton, and A. T. Godfrey, "Implementation, Capabilities, and Benchmarking of Shift, a Massively Parallel Monte Carlo Radiation Transport Code," *J. Comp. Phys.,* **308**, 239–272 (2016).

S. W. D. Hart, C. Celik, G. I. Maldonado, and L. Leal, "Creation of Problem-dependent Doppler-broadened Cross Sections in the KENO Monte Carlo Code," *Ann. of Nucl. Energy*, **88**, 49–56 (2016).

M. T. Pigni, S. Croft and I. C. Gauld, "Uncertainty Quantification in (α,n) Neutron Source Calculations for an Oxide Matrix," accepted for publication in *Prog. Nucl. Energ.* (2016).

I. C. Gauld, J. M. Giaquinto, J. S. Delashmitt, J. Hu, G. Ilas, T. J. Keever, and C. Romano, "Re-evaluation of Spent Nuclear Fuel Assay Data for the Three Mile Island Unit 1 Reactor and Application to Code Validation," *Ann. of Nucl. Energy,* **87**, 267–281 (2016).

U. Mertyurek and I. C. Gauld, "Development of ORIGEN Libraries for Mixed-Oxide (MOX) Fuel Assembly Designs," *Nucl. Eng. Des.*, **297**, 220–230 (2016).

M. Pigni, M. W. Francis, and I. C. Gauld, "Investigation of Inconsistent ENDF/B-VII.1 Independent and Cumulative Fission Product Yields with Proposed Revisions," *Nucl. Data Sheets*, **123**, 231–236 (2015).

I. C. Gauld, M. Pigni, and G. Ilas, "Validation and Testing of ENDF/B-VII Decay Data," *Nucl. Data Sheets*, **120,** 33–36 (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. Tech.* **188**(2) 154–157 (2014).

C. M. Perfetti, B. T. Rearden, and W. R. Martin, "SCALE Continuous-Energy Eigenvalue Sensitivity Coefficient Calculations," *Nucl. Sci. Eng.* **182**(3), 332–353 (2016).

C. M. Perfetti and B. T. Rearden, "Development of a Generalized Perturbation Theory Method for Uncertainty and Sensitivity Analysis Using Continuous-Energy Monte Carlo Methods," *Nucl. Sci. Eng.* **182**(3), 354–368 (2016).

M. L. Williams, D. Wiarda, W. J. Marshall, and B. T. Rearden, "Covariance Applications in Criticality Safety, Light Water Reactor Analysis, and Spent Fuel Characterization," *Nucl. Data Sheets*, **123**, 92–96 (2015).

B. T. Rearden, L. M. Petrie, D. E. Peplow, K. B. Bekar, D. Wiarda, C. Celik, C. M. Perfetti, A. M. Ibrahim, S. W. D. Hart, M. E. Dunn, and W. J. Marshall, "Monte Carlo Capabilities of the SCALE Code System," *Ann. of Nucl. Energy*, **82**, 130–141 (2015).

### Technical Reports

M. W. Francis, C. F. Weber, M. T. Pigni, I. C. Gauld, *Reactor Fuel Isotopics and Code Validation for Nuclear Applications*, ORNL/TM-2014/464, UT-Battelle, LLC, Oak Ridge National Laboratory, 2015.

### Conference Proceedings

**ANS MC2015 - Joint International Conference on Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) and the Monte Carlo (MC) Method, April 2015, Nashville, TN, USA**

J. Hu, I. Gauld, and A. Worrall, "Spent Fuel Modeling And Simulation Using ORIGAMI for Advanced NDA Instrument Performance Assessment."

B. T. Rearden, K. B. Bekar, C. Celik, C. M. Perfetti, and S. W. D. Hart, "Advancements in Monte Carlo Capabilities for SCALE 6.2."

B. T. Rearden, R. A. Lefebvre, J. P. Lefebvre, K. T. Clarno, M. L. Williams, L. M. Petrie, Jr., U. Mertyurek, B. R. Langley, and A. B. Thompson, "Modernization Strategies for SCALE 6.2."

F. Bostelmann, F. P. Weiß, A. Aures, K. Velkov, W. Zwermann, B. T. Rearden, M. A. Jessee, M. L. Williams, D. Wiarda, W. A. Wieselquist, "Uncertainty and Sensitivity Analysis in Criticality Calculations with Perturbation Theory and Sampling."

**American Nuclear Society 2015 International High-Level Radioactive Waste Management Conference, April 2015, Charleston, SC, USA**

J. Peterson, I. Gauld, S. Bowman, "Extended Burnup Summary of $UO^2$ and MOX Fuel."

**European Safeguards Research and Development Association Symposium, May 2015, Manchester, UK**

I. Gauld, J. Hu, P. DeBaere, S. Vaccaro, P. Schwalbach, H. Liljenfeldt, S. Tobin, "In-field Performance Testing of the Fork Detector for Quantitative Spent Fuel Verification."

ICNC 2015 – International Conference on Nuclear Criticality Safety, September 2015, Charlotte, NC, USA

B. J. Ade, W. J. Marshall, S. M. Bowman, I. C. Gauld, G. Ilas, J. S. Martinez, "Coolant Density and Control Blade History Effects in Extended BWR Burnup Credit."

C. M. Perfetti and B. T. Rearden, "SCALE 6.2 Continuous-Energy TSUNAMI-3D Capabilities."

C. M. Perfetti and B. T. Rearden, "Diagnosing Undersampling in Monte Carlo Eigenvalue and Flux Tally Estimates."

E. L. Jones, G. I. Maldonado, W. J. Marshall, C. M. Perfetti, and B. T. Rearden, "Investigation of the Continuous-Energy Sensitivity Methods in SCALE 6.2 Using TSUNAMI-3D."

B. T. Rearden et al., "Criticality Safety Enhancements for SCALE 6.2 and Beyond."

W. J. Marshall, M. L. Williams, D. Wiarda, B. T. Rearden, M. E. Dunn, D. E. Mueller, J. B. Clarity, and E. L. Jones, "Development and Testing of Neutron Cross Section Covariance Data for SCALE 6.2."

W. J. Marshall, B. T. Rearden, and E. L. Jones, "Validation of SCALE 6.2 Criticality Calculations Using KENO V.a and KENO-VI."

W. J. Marshall and B. T. Rearden, "Determination of Critical Experiment Correlations Using the Sampler Sequence within SCALE 6.2."

V. Sobes, B. T. Rearden, D. E. Mueller, W. J. Marshall, J. M. Scaglione, and M. E. Dunn, "Upper Subcritical Calculations Based on Correlated Data."

**American Nuclear Society Winter Meeting, November 2015, Washington, DC, USA**

G. Radulescu, R. A. Lefebvre, K. Banerjee, P. Miller, and J. M. Scaglione, "Shielding Analysis Capability of UNF-ST&DARDS."

V. Sobes, B. T. Rearden, D. E. Mueller, W. J. Marshall, J. M. Scaglione, and M. E. Dunn, "Upper Subcritical Limit Calculations with Correlated Integral Experiments."

**Waste Management 2016, March 2016, Phoenix, AZ, USA**

G. Radulescu and K. J. Connolly, "A Parametric Analysis of Factors Affecting Calculations of Estimated Dose Rates from Spent Nuclear Fuel Shipments."

**Spent Fuel Workshop 2016, May 2016, Stockholm, Sweden**

I. Fast, I. Gauld, F. Michel-Sendis and S. Caruso, "Importance of Available Experimental and International Reference Inventory Data for the Estimation of Realistic SNF Inventory Bandwidths."

**American Nuclear Society Annual Meeting, June 2016, New Orleans, LA, USA**

C. M. Perfetti and B. T. Rearden, "CE TSUNAMI-3D Algorithm Improvements in SCALE 6.2."

C. M. Perfetti and B. T. Rearden, "A New TSUNAMI-3D Capability for Calculating Undersampling Metrics and Biases."

Do you have a publication documenting the application of SCALE to a challenging analysis scenario? Submit your publication to scalehelp@ornl.gov and it may appear in a future edition of the SCALE Newsletter!

## SCALE Team

The SCALE team consists of 47 talented and diverse staff members from ORNL's Reactor and Nuclear Systems Division. Most of our team members hold advanced degrees in nuclear engineering, physics, and/or computer science. SCALE development, testing, deployment, and training are organized into task-oriented teams as shown below in Figure 12. Many other internal and external collaborators and students also contribute to SCALE on an ongoing basis.

A photo of the team members present for the release of SCALE 6.2 is shown in Figure 13.

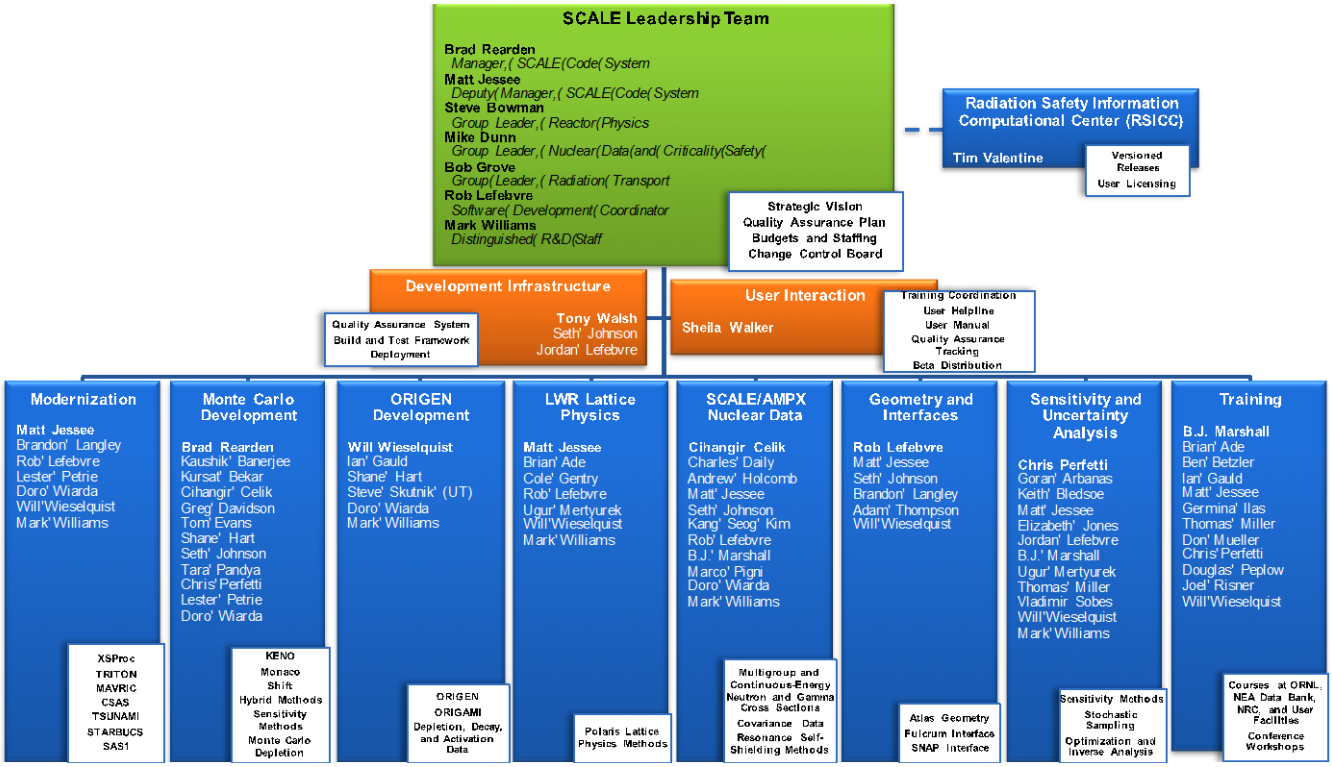
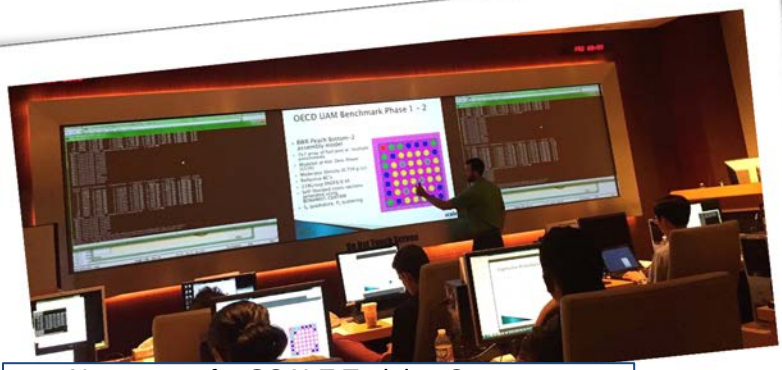



**Figure 12. SCALE Team Structure**

**Figure 13. SCALE 6.2 Team Photo - April 2016**

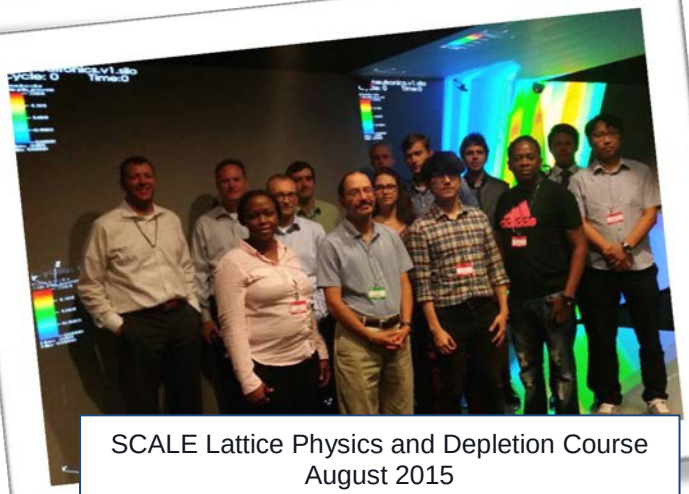
(Left to right. First Row: Jianwei Hu, Germina Ilas, Tara Pandya, Shane Hart, Lester Petrie, Brad Rearden, Bob Grove, Mike Dunn, Mark Williams, Georgeta Radulescu, Elizabeth Jones, Ian Gauld; Second Row: Matt Jessee, Steve Skutnik, Kevin Clarno, Tony Walsh, Cihangir Celik, Ron Ellis, Kursat Bekar, Doro Wiarda, Mark Baird; Back Row: Jordan Lefebvre, Rob Lefebvre, Adam Thompson, Andrew Holcomb, Rose Raney, Ugur Mertyurek, B. J. Marshall, Steve Bowman, Don Mueller, Ahmad Ibrahim, Brandon Langley, Douglas Peplow, Greg Davidson, Dan Ilas, Justin Clarity, Josh Peterson, and Will Wieselquist)

## Recent SCALE Photos



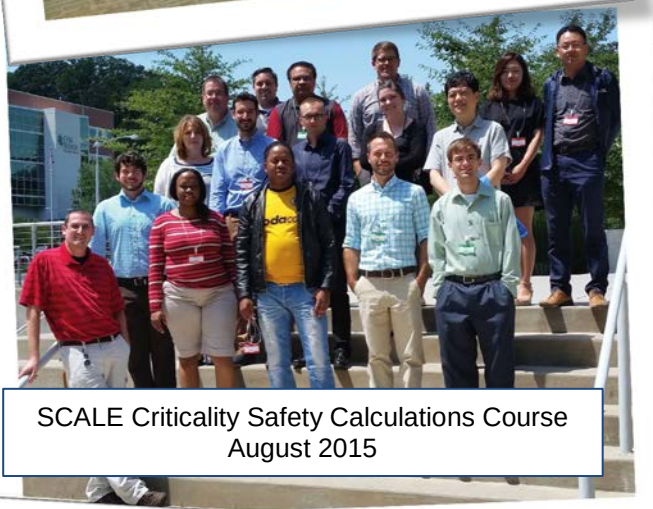
New venue for SCALE Training Courses – ORNL/CASL Virtual Office, Computing, and Community (VOCC)

SCALE Sensitivity and Uncertainty Calculations Paris – March 2015



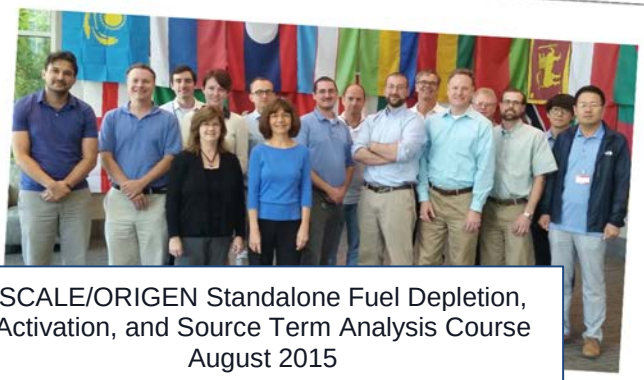
SCALE Lattice Physics and Depletion Course August 2015

SCALE Sensitivity and Uncertainty Calculations Course August 2015



SCALE Criticality Safety Calculations Course August 2015

SCALE/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis Course presented at Institute of Nuclear Physics in Tashkent, Uzbekistan September 2015

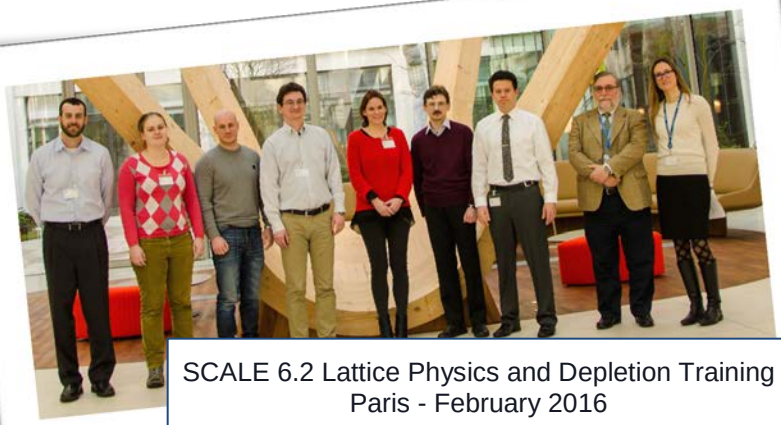


SCALE/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis Course August 2015

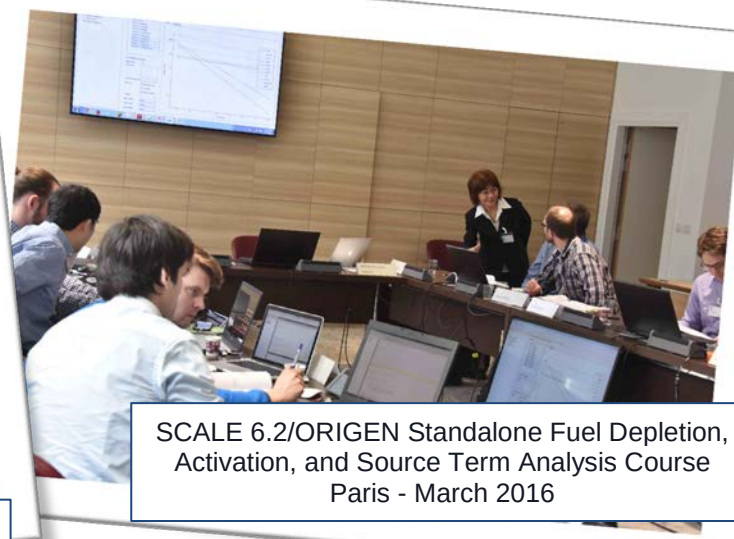
SCALE Training for TREAT Reactor Restart Team
Idaho National Laboratory
February 2016

SCALE 6.2/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis Course
February 2016

SCALE 6.2 Lattice Physics and Depletion Training
February 2016



SCALE 6.2 Lattice Physics and Depletion Training
Paris - February 2016



SCALE 6.2/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis Course
Paris - March 2016

## SCALE Spotlight

SCALE is developed, tested, documented, and maintained by over 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.

**Robert A. Lefebvre**

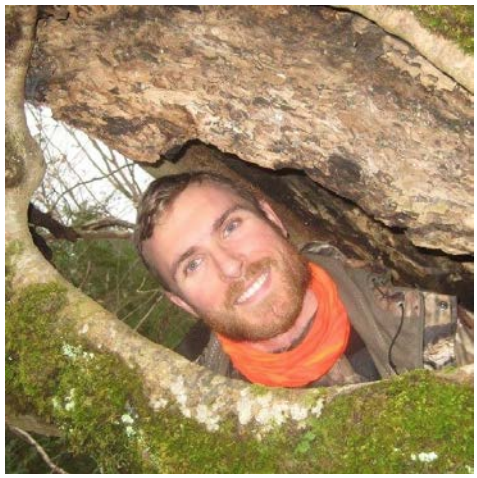


**Figure 14. Rob Lefebvre in the woods of East Tennessee**

**Positions:**
Research and Development Staff - Reactor Physics Group
SCALE Software Development Coordinator
SCALE Geometry and Interfaces Team Lead
UNF-ST&DARDS Development Lead

**Focus areas:**
Data Visualization, User Interfaces, and Software Engineering

**Most memorable projects:**
I joined ORNL in 2008 and prototyped a geometry visualization interface which used SCALE's KENO geometry module, after which I worked on the GeeWiz, Keno3D, and OrigenArp user interfaces. These experiences provided me insight into SCALE's user and developer community and led me down the path of SCALE modernization development with the intent of unifying the user-facing and developer-oriented software components of SCALE, which to date has culminated in the cross-platform Fulcrum user interface. While Fulcrum is not yet complete, it serves as a great foundation for the future, scalable from the new SCALE user to the most experienced. In attaining its current status, it definitely stands as my most memorable project.

**Life outside of work:**
I love spending time with my wife and kids. Any spare time I have I can usually be found canoeing the lakes and rivers or roaming the mountains and plateaus of East Tennessee.

## 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.

To facilitate interaction among SCALE users and with developers, the SCALE Users Group forum is hosted by Google is available at https://groups.google.com/forum/#!forum/scale-users-group.

SCALE primers 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

Matt Jessee – Deputy 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

Rob Lefebvre – SCALE Software Development Coordinator

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_2016_aug-sept.shtml for more information.

| Dates | Course | Registration Fee |
|---|---|---|
| **August 8–12, 2016** | **Introduction to New Features in SCALE 6.2**<br>Oak Ridge National Laboratory, Oak Ridge, TN, USA<br>This course highlights advancements in SCALE capabilities introduced in SCALE 6.2. The 5-day course is divided into two 2.5-day mini-courses that can be taken independently or as a set. Mini-course 1: SCALE 6.2 Lattice Physics and Stand-alone Fuel Depletion, Activation, and Source Term Analysis; Mini-course 2: SCALE 6.2 Monte Carlo Calculations and Uncertainty Analysis | $2000 (or $1000 for each 2.5 day mini-session) |
| **August 15–19, 2016** | **SCALE Criticality Safety Calculations**<br>Oak Ridge National Laboratory, Oak Ridge, TN, USA<br>Introductory through advanced criticality calculations using KENO V.a and KENO-VI; resonance self-shielding techniques | $2000 |
| **August 22–26, 2016** | **SCALE Sensitivity and Uncertainty Analysis for Criticality Safety Validation**<br>Oak Ridge National Laboratory, Oak Ridge, TN, USA<br>TSUNAMI: 1D and 3D $k_{eff}$ sensitivity/uncertainty analysis; 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 29–September 2, 2016** | **SCALE/ORIGEN Stand-alone Fuel Depletion, Activation, and Source Term Analysis Course**<br>Oak Ridge National Laboratory, Oak Ridge, TN, USA<br>Isotopic depletion, activation analysis, and source term characterization using ORIGEN and the new ORIGAMI tool for convenient characterization of used nuclear fuel with radially and axially varying burnup. | $2000 |

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

All attendees must be licensed users of SCALE 6.2, 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 a course may be canceled if minimum enrollment is not obtained 1 month prior to the course. Course fees are refundable up to 1 month before each class.**

**FOREIGN NATIONAL VISITORS TO ORNL** - Payment MUST be received at least 1 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.

*SCALE Newsletter*
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U.S. Department of Energy, Nuclear Criticality Safety Program