Getting Started with SCALE 6.2.4

April 2020

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Introduction

The SCALE Code System is a widely used modeling and simulation suite for nuclear safety analysis and design that is developed, maintained, tested, and managed by the Reactor and Nuclear Systems Division (RNSD) of Oak Ridge National Laboratory (ORNL). SCALE provides a comprehensive, verified and validated, user-friendly tool set for criticality safety, reactor physics, radiation shielding, radioactive source term characterization, and sensitivity and uncertainty analysis. Since 1980, regulators, licensees, and research institutions around the world have used SCALE for safety analysis and design. SCALE provides an integrated framework with dozens of computational modules, including 3 deterministic and 3 Monte Carlo radiation transport solvers that can be selected based on the desired solution strategy. SCALE includes current nuclear data libraries and problem-dependent processing tools for continuous-energy (CE) and multigroup (MG) neutronics and coupled neutron-gamma calculations, as well as activation, depletion, and decay calculations. SCALE includes unique capabilities for automated variance reduction for shielding calculations, as well as sensitivity and uncertainty analysis. SCALE's graphical user interfaces assist with accurate system modeling, visualization of nuclear data, and convenient access to desired results. 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 CE and MG nuclear data libraries with enhanced group structures,
- Neutron covariance data based on ENDF/B-VII.1 and supplemented with ORNL data,
- Covariance data for fission product yields, decay constants, branching ratios, and decay heat,
- 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 depletion with T5-DEPL/T6-DEPL,
- CE sensitivity/uncertainty analysis with TSUNAMI-3D,
- Simplified and efficient light-water reactor (LWR) lattice physics with Polaris,
- Simplified spent fuel characterization with ORIGAMI and ORIGAMI Automator,
- Advanced fission source convergence acceleration capabilities with Sourcerer,
- Nuclear data library generation with AMPX,
- Integrated user interface with Fulcrum, and
- Many other new features.

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 4× faster than SCALE 6.1),
- Spent fuel characterization with 1,470 new reactor-specific libraries for ORIGEN,
- Keyword input for ORIGEN,
- Extension of the maximum mixture number to values well beyond the previous limit of 2,147 to ~2 billion,
- Expanded 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 around capabilities instead of the historical division of function modules, control modules, etc.

SCALE 6.2 was originally released in April 2016. Three minor updates have been released to provide numerous enhancements and increased stability. SCALE 6.2.1 was released in July 2016, SCALE 6.2.2 was released in February 2017, and SCALE 6.2.3 was released in March 2018. The current version, SCALE 6.2.4, was released in April 2020.

This start-up guide provides an overview of many of the updated features of SCALE 6.2, instructions on how to install SCALE, instructions on using all the features of the SCALE runtime environment command line interface, and instructions on how to build SCALE. Because SCALE 6.2.1, 6.2.2, 6.2.3, and 6.2.4 are minor updates, references to the updated version are used only when necessary.

The SCALE user manual provides comprehensive documentation of all computational capabilities, nuclear data, input requirements, and output edits. Additional resources are available in the SCALE primers, located in the *docs/primers* directory after installation. These primers provide step-by-step instructions for running SCALE. However, at the time of this release, not all primers have been updated to reflect the latest features and user interface of SCALE 6.2. Additional resources are available on the SCALE website at http://scale.ornl.gov or by e-mailing scalehelp@ornl.gov.

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 structures are available, where the 252-group library is for general-purpose reactor physics and criticality safety applications and the 56-group library is intended for light water reactor analysis. Coupled neutron/gamma MG libraries for shielding are available in a fine 200-neutron/47-gamma group structure and a broad 28-neutron/19-gamma structure. An additional 8-group neutron library is available for code testing purposes but is not intended for production use.

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 have been assembled from a variety 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 libraries now use 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, the 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 and comparisons with the new data. 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(α,β) 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 smaller than the bias in SCALE 6.1. Additional testing has revealed that biases

for burned light water reactor (LWR) fuel are resolved with the improved treatment. Additional details and further results are provided in Saylor et al. 2018.[1]

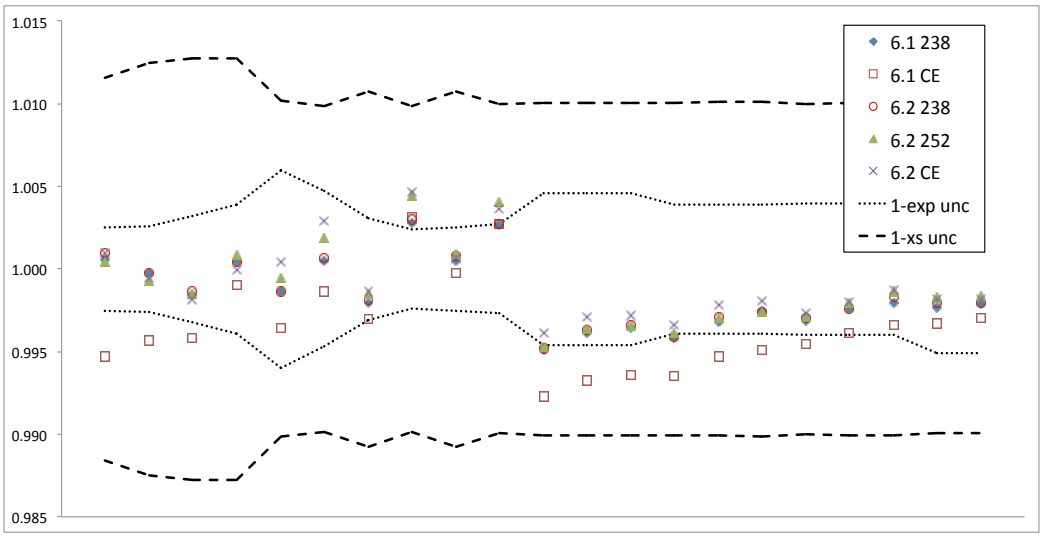

Figure 1. SCALE-calculated results for a selection of International Criticality Safety Benchmark Evaluation Project (ICSBEP) thermal mixed oxide critical systems.

Additionally, the probability tables for CE reactions in the unresolved resonance range have been improved, primarily through the inclusion of additional resolution and error correction.

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. Monaco now has the capability to model CE gamma interaction data and CE gamma yield data from neutron interactions. In addition, wide ranges of neutron reactions not needed for criticality calculations were also added to provide desired responses in Monaco.

The improved CE data have been comprehensively reviewed, verified, and validated, with approximately 5,000 infinite medium eigenvalue tests, 6,300 neutron and photon fixed-source transmission tests, and 600 criticality and shielding benchmark experiments to ensure robust and accurate calculations.

Multigroup Data Processing

ORNL has performed detailed comparisons between SCALE CE and MG results. Historically, a bias of 200–500 pcm has been observed for cases in which the earlier 238-group library is applied to LWR systems. AMPX has been used to develop new 252- and 56-energy-group ENDF/B-VII.1 neutron cross section libraries. The new 252-group structure for SCALE 6.2 provides a more detailed representation of the ^{238}U resonance structure and reduces the previous bias. In addition to the inclusion of the new group structures, these libraries have been generated using a new weighting spectrum with

improved resonance self-shielding procedures. For nuclides with atomic numbers of 40 and above, a CE flux spectrum computed with the CENTRM transport module for a pressurized water reactor (PWR) pin cell at 300K was used as a weighting function. Temperature-dependent thermal scatter matrices for all actinides and H_2O were processed with CE thermal flux at the corresponding temperatures. The standard AMPX weight function (i.e., fission spectrum + 1/E + Maxwellian) was used for nuclides with Z<40. 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 were computed with three different approaches, as a function of background cross section and temperature, depending on the nuclides. For nuclides with atomic numbers less than 40, the standard narrow resonance (NR) approximation was used. For all other actinides—except ^{91}Zr, ^{96}Zr, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu—the Bondarenko shielding factors were generated with CE spectra calculated by CENTRM for homogeneous mixtures of the resonance material and hydrogen, corresponding to the respective background cross section. Bondarenko factors for ^{91}Zr, ^{96}Zr, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu, are based on CENTRM CE calculations for *heterogeneous* pin cell models that span the range of anticipated self-shielding conditions. The thermal cutoff for bound and free-gas moderators 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. Most results lie within the experimental uncertainty, and the outliers are believed to be caused by deficiencies in the ENDF/B-VII.1 data. 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 has been introduced to SCALE 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.

The binary object formatted file (BOFF) is a binary data format designed for flexibility and compactness and is intended to compete with native binary file formats that incorporate optimization techniques 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 using 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 Material Input Processing and Resonance Self-Shielding

Most SCALE sequences now use the modern material and cross section processing module of SCALE, XSProc, which was developed for SCALE 6.2 to prepare data for CE and MG calculations. XSProc integrates and enhances the capabilities previously implemented

independently in BONAMI, CENTRM, PMC, WORKER, ICE, and XSDRNPM, along with some additional capabilities provided by MIPLIB and SCALELIB in earlier releases of SCALE. XSProc expands material input from Standard Composition Library definitions into nuclide number densities, and for MG calculations, it also performs resonance self-shielding, energy group collapse, and spatial homogenization calculations 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 the intermediate resonance (IR) approximation for the full energy range (PARM=BONAMI), as well as the more rigorous option of a deterministic CE treatment in the resolved resonance range (PARM=CENTRM). Only the CENTRM path is available for double heterogeneous cell types. Sequence-specific control for generation of on-disk or in-memory self-shielded MG libraries for microscopic or macroscopic data containing selected reaction cross sections and scattering data is available with this modernized tool.

XSProc runtime and memory requirements are substantially improved compared to legacy computations, especially when performing calculations with many unit cells. Generally, speedups in self shielding of about 3× 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 by 1,000× while still obtaining equivalent results. XSProc is implemented across most SCALE sequences, as shown in Table 1, for cases in which modernized sequences with XSProc and older legacy sequences that run that standalone 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	✓	

Missing Cross Section Messages

Several naturally occurring isotopes are not present in the SCALE nuclear data libraries. For example, the natural abundance for oxygen contains 0.20% ^{18}O, but ENDF evaluations do not provide cross sections for this isotope.

In previous versions of SCALE, the Standard Composition Library made several nonphysical adjustments to facilitate the use of nuclear data libraries with missing nuclides. In the case of ^{18}O, the standard compositions UO_2, O, H_2O, and others assumed oxygen to consist of 100% ^{16}O instead of its true natural abundance. If the user entered the standard composition name *OXYGEN*, then the true natural abundances would be used, and the calculation would immediately stop because ^{18}O was not present on the nuclear data library. For source terms calculations and nuclear heating analysis, the absence of ^{17}O can non-conservatively reduce results by several percent.

In SCALE 6.2, this behavior has been changed because natural abundances are consistently applied for all standard composition materials. When isotopes without nuclear data are present in the input, the calculation continues with the isotopes removed from the model, which produces identical radiation transport and activation/depletion results similar to those obtained when using a zero-valued cross section for each missing isotope. The isotopes that occur in the Standard Composition Library but with no corresponding nuclear data in ENDF/B-VII.0 or -VII.1 are shown in Table 2.

In SCALE 6.2.2, an update was introduced for processing ^{18}O. If a composition contains ^{18}O, either explicitly or implicitly (such as UO_2), then SCALE internally introduces a zero-value cross section for ^{18}O, and a warning is provided in the message file. The radiation transport solution is unaltered, but output edits such as the KENO mixing table contain ^{18}O. The inclusion of ^{18}O in composition output edits allows users to verify that the input composition density is consistent with the density computed from the isotope concentrations. For depletion calculations, the zero-valued cross section for ^{18}O is replaced by the cross sections included in the JEFF-3.0/A neutron activation files.

For compositions containing isotopes other than ^{18}O that are shown in Table 2, a warning message is provided with explicit number densities of every nuclide in the composition so that the user has a choice of accepting the SCALE composition with decreased density or updating the composition input 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.

Table 2. 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 ENDF/B-VII data for any of the seven naturally occurring ytterbium isotopes
2. no ENDF/B-VII data for any of the seven naturally occurring osmium isotopes
3. no ENDF/B-VII data for any of the six naturally occurring platinum isotopes

CENTRM/PMC Improvements

A new two-dimensional (2D) unit cell geometry is available in CENTRM to explicitly treat the boundary of square-pitched reactor lattices using with a method-of-characteristics (MoC) CE transport option, typically resulting in approximately 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 the *centrm data* block within the *celldata* block. *N2D=2* corrects the higher order Legendre moments with corresponding higher order fluxes, and based on the consistent P_N approximation, *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 option produces MG results more consistent with the reference CE Monte Carlo results. However, these results are not universal for all calculations, so the *N2D=-2* option 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.

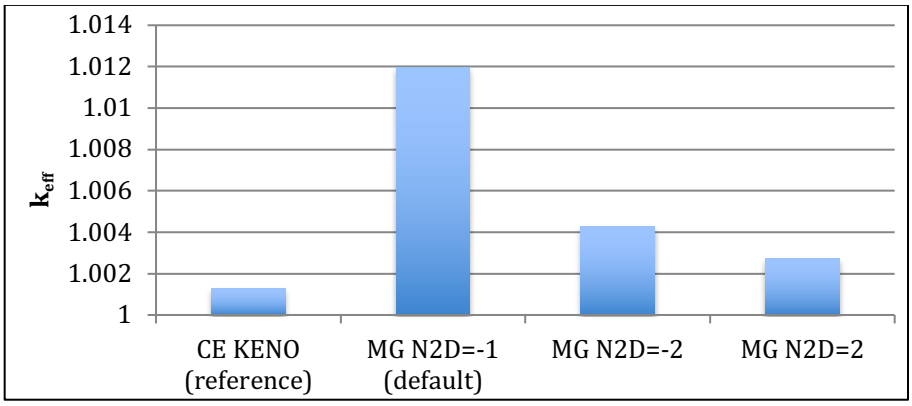

Figure 2. k_{eff} values for IEU-MET-FAST-005-001 with different MG options.

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 and provides a rapid self-shielding option using only full-range Bondarenko factors. This technique produces accurate results and provides up to a 10× speedup relative to CE treatment with CENTRM. IR theory is described in the updated BONAMI section, Section 7.3. 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 the *celldata* block.

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 intended 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 the 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 Hierarchical Input Validation Engine (HIVE) identifies allowed data ranges and interdependencies in the input and reports inconsistencies to the user. Fulcrum interactively processes standard composition data to produce a mixing table, lists expanded input aliases for review, provides an internal list of input as required for Sampler material and geometry perturbation analysis, and launches the SCALE sample problems.

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

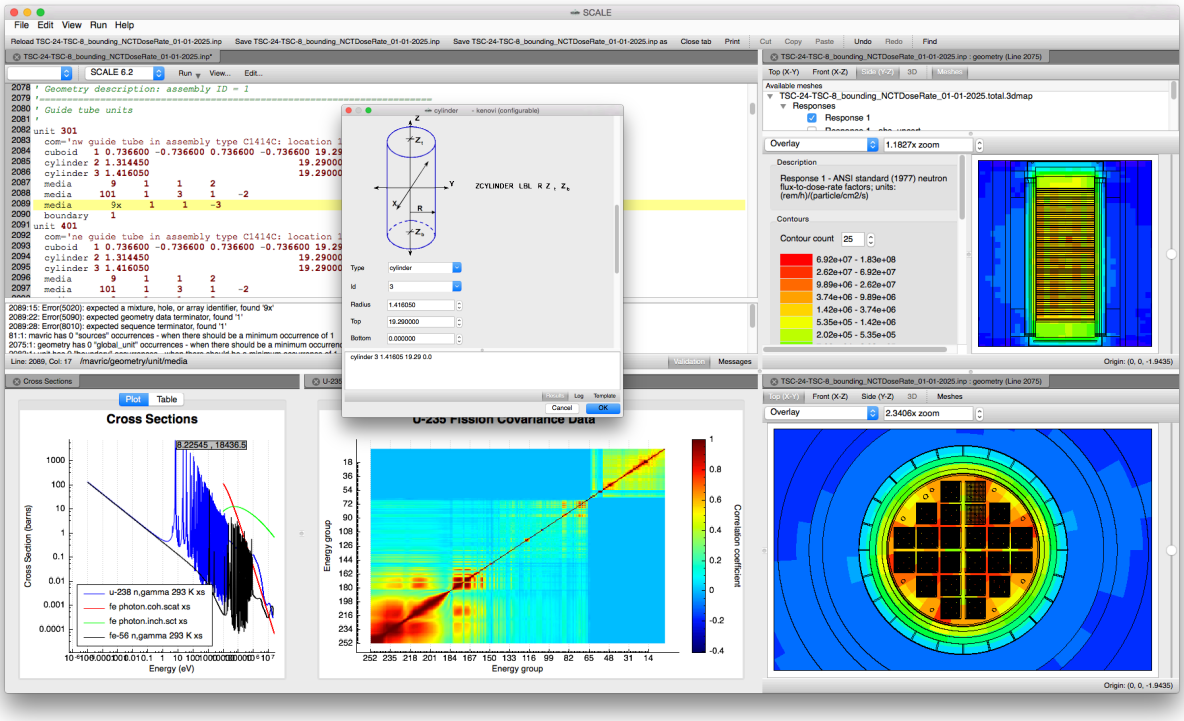

Figure 3. SCALE graphical user interface – Fulcrum.

The Fulcrum user interface provides numerous features, such as those described below.

- The interface operates on all supported platforms—Linux, Mac and Windows.
- The user 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 preconfigured 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 menus for each file in the navigation panel and can be opened by right clicking on the input file name in the navigation panel.
- Associated files not supported in Fulcrum open a local tool for appropriate viewing (e.g. .html files launch the system web browser).
- 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
  - UNF-STANDARDS time series
  - 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*)
  - MAVRIC Chart Plot file (*.chart*)
- Data files with file extensions (*.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.
- Online help is available.
- Many more features are included but are too numerous to list here.

As Fulcrum is a new user interface, users are directed to the *Help* menu within the application itself for *Help documentation*. A detailed introduction and tutorial to Fulcrum is available for download at http://scale.ornl.gov.

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. Previously 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,* in KENO parameter data helps to reduce runtime and was the default behavior in SCALE 6.0 and 6.1. Optionally disabling map2union (*M2U=no*) results in ~20% reduction in memory with ~10% increase in runtime.

Other internal optimizations include:

- Redundant copies of temperature-independent data were removed to improve memory efficiency for models with multiple temperatures. Previously, each set of temperature-dependent cross sections also included a redundant copy of the temperature-independent data, which caused an almost linear increase in memory for each new temperature. With this update, the temperature-independent data are shared by all 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 ~40% reduction in memory requirements using the same runtime.
- Internal data storage was changed from double to single precision where possible, resulting in a 15–45% reduction in memory requirements depending on the nuclides used in the model.
- Optional data loading was introduced 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., results in ~20% reduction in memory requirements.

Fission Source Convergence Diagnostics

Prior to the release of 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 χ^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 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.[2] Source convergence diagnostics are enabled with *SCD=yes* (default) in the KENO parameter data.

Problem-Dependent Doppler Broadening

The CE data libraries distributed with SCALE are provided with up to 9 temperatures per isotope. The Doppler broadening temperature corrections using only a few temperatures may not match the desired temperature of the calculation. When temperatures of the KENO model are different from those present on the library, KENO selects the nearest temperature, which can be several hundred degrees from the desired temperature, producing results that can vary significantly from those that would be produced at the correct temperature.

New methods have been developed and implemented to provide *problem-dependent* temperature corrections by Doppler broadening the point-wise data in the resolved resonance region and the probability tables in the unresolved resonance region when the cross sections are loaded for the calculation.[4] The thermal scattering data are also updated to the requested temperature. The runtime penalty for this methodology is negligible, as all temperature corrections are performed as the calculation begins, typically requiring only a few seconds to a few minutes depending on the number of nuclides and temperatures used.

The eigenvalues computed for a typical fresh 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 perform also corrections for the S(α,β) thermal scattering data.

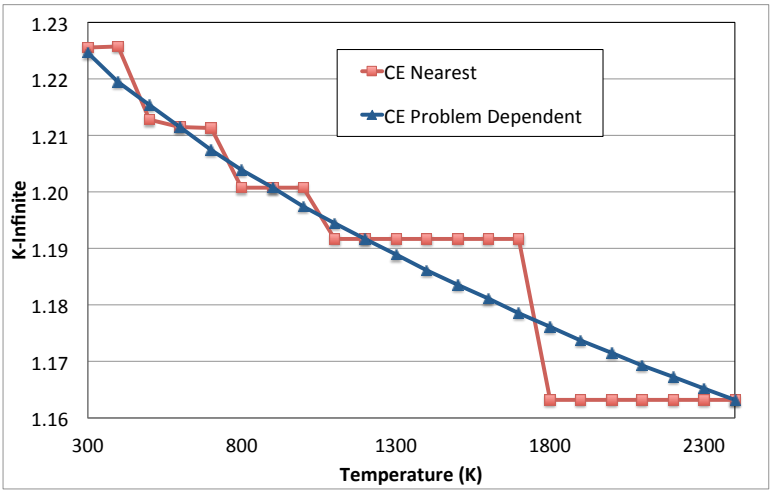

Figure 4. Eigenvalues computed for a PWR pin cell with different temperature treatments.

Doppler Broadened Rejection Correction

The implementation of Doppler Broadened Rejection Correction (DBRC) techniques provides further enhancements for calculations with elevated temperatures.[4] As shown in Table 3, DBRC in KENO presents a reactivity correction of approximately 300 pcm relative to the default methodology for a 1,200K LWR fuel pin, consistent with that predicted with MCNPX by the originators of the methodology.[5] 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.

Table 3. Effect of DBRC on k_{inf} for a LWR fuel pin at 1,200K

Case	Default	DBRC	Difference (pcm)
MCNPX	1.31137 +/- 9E-5	1.30791 +/- 9E-5	-346
KENO-VI	1.31029 +/- 15E-5	1.30730 +/- 15E-5	-299

Sourcerer - Hybrid Method for Starting Source Distribution

The *Sourcerer* sequence introduced in SCALE 6.2 uses the Denovo[6] discrete-ordinates code to generate a starting fission source distribution in a KENO Monte Carlo calculation. Initial studies[7,8] have shown that using a starting fission distribution 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.[9] 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, presented in Figure 5, show that using a deterministic starting source significantly increases the k_{eff} reliability. See the *Sourcerer* documentation in Section 2.4 for full details.

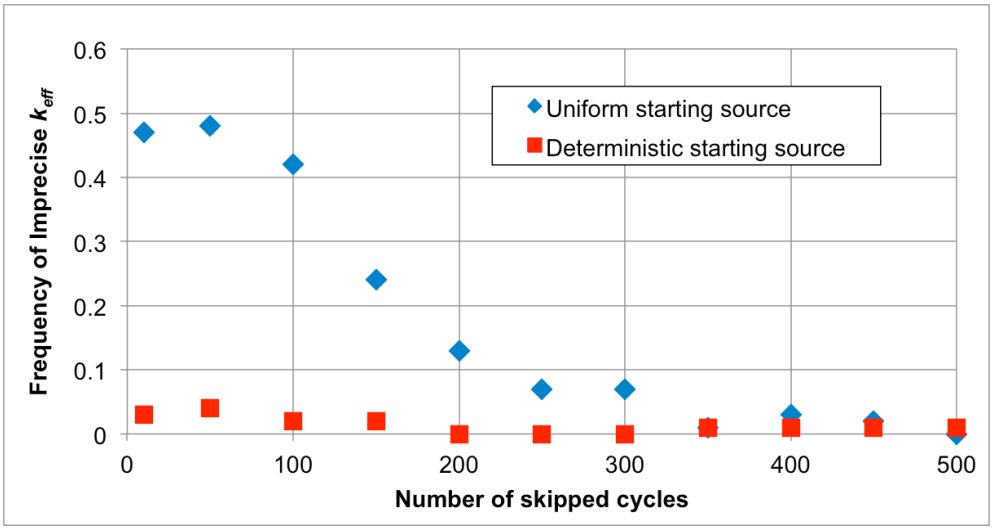

Figure 5. Fraction of failure to agree with the reference k_{eff} value for KENO calculations with different starting sources (Figure 4 from Ref. 9).

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 sensitivity and uncertainty (S/U) analysis or Monte Carlo depletion on computer clusters. By introducing a simple master-slave approach via message passing interface (MPI),[10] 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, and then they are processed either for final edits or next generations.

The parallel performance of KENO as used in a CE calculation for a graphite-moderated reactor model is shown in Figure 6. These tests were conducted on a heterogeneous Linux cluster in which 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 the 64 processors tested here and has been successfully demonstrated on hundreds of processors.

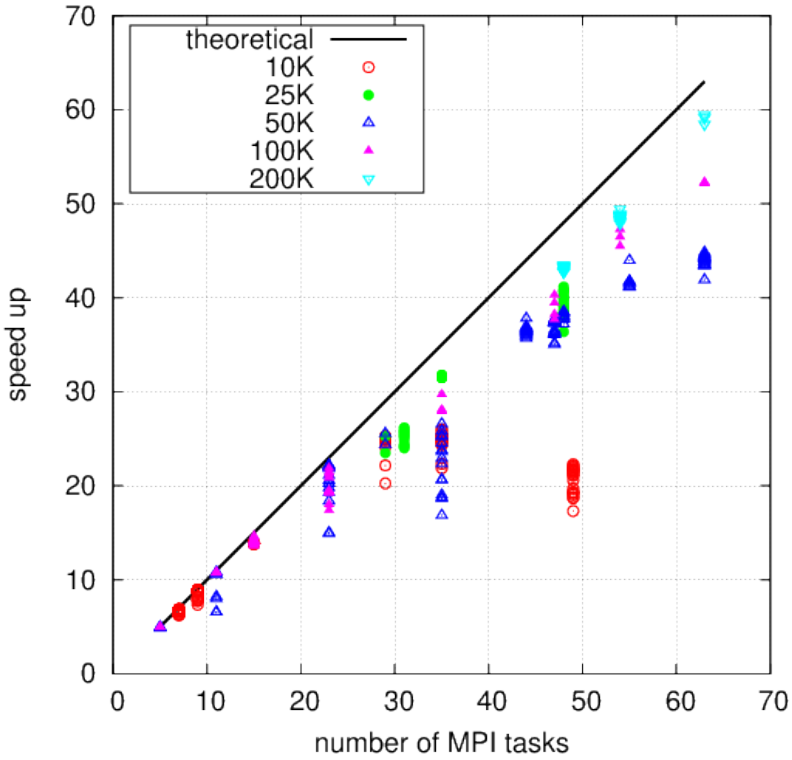

Figure 6. Speedup for parallel KENO-VI calculations for a graphite-moderated reactor model.

Reaction Tallies

User-configurable reaction rate tallies are now available within KENO CE calculations. The tallies are specified in the *REACTION* block of KENO.

Reactor Physics

Polaris – New Advanced Lattice Physics Module

Polaris is a new 2D lattice physics code for SCALE that uses a new MG self-shielding method called the Embedded Self-Shielding Method (ESSM)[11] and a new MoC transport solver. Polaris uses a simplified input, where only a few lines are required to describe the entire model. Polaris provides substantially reduced input requirements and improved runtime performance compared to TRITON (see Section 3.1).

The ESSM approach computes MG self-shielded cross sections using interpolation of the Bondarenko factors in the MG library. The background cross section used in the interpolation is determined by a series of 2D MoC fixed-source calculations similar to the subgroup method. Polaris does not require explicit *celldata* input, as needed in TRITON. Additionally, heterogeneous lattices are explicitly treated without the need to externally compute Dancoff factors. Additional details on ESSM are provided in a paper by Williams et al.[11]

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

Polaris uses the self-shielded cross sections to perform a MG 2D eigenvalue calculation with the new MoC transport solver developed for Denovo, a parallel 3D Cartesian mesh MG discrete ordinates (S_N) code.[6] 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 the 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. 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 capability that coupled the SCALE MG cross section processing methodology with KENO and ORIGEN. A new CE-based KENO/ORIGEN Monte Carlo depletion capability has been developed for SCALE-6.2 which can be activated 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 run-time to generate and store the resonance self-shielded cross section data for each material is prohibitive.

Lattice Physics with TRITON

2D 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 2–6× faster calculations are common, and some models have realized speedups of 30× relative to previous versions of NEWT. Calculation times for 1,470 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.

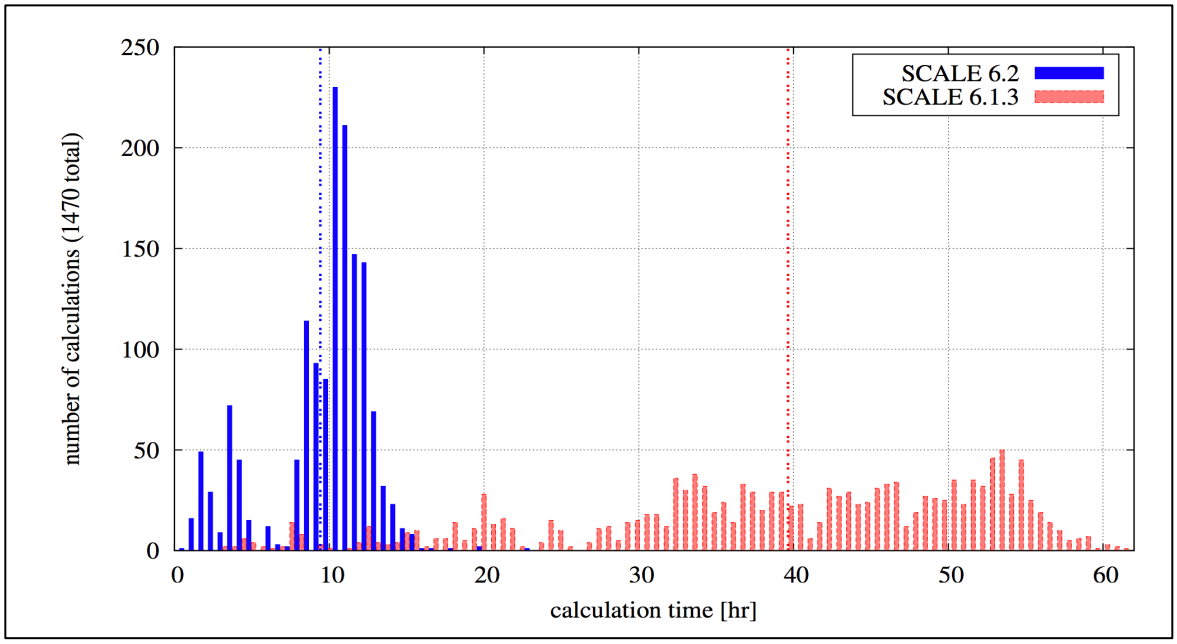

Figure 7. Comparison of calculation times for 1,470 TRITON calculations.

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, which is especially useful for modeling removable absorber materials.

Bias Reduction for Depletion

Historical SCALE biases 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 eigenvalue statepoints using the isotopics provided by the SCALE 6.2 results, as CE depletion is not available in SCALE 6.1. The 1,000 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 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.

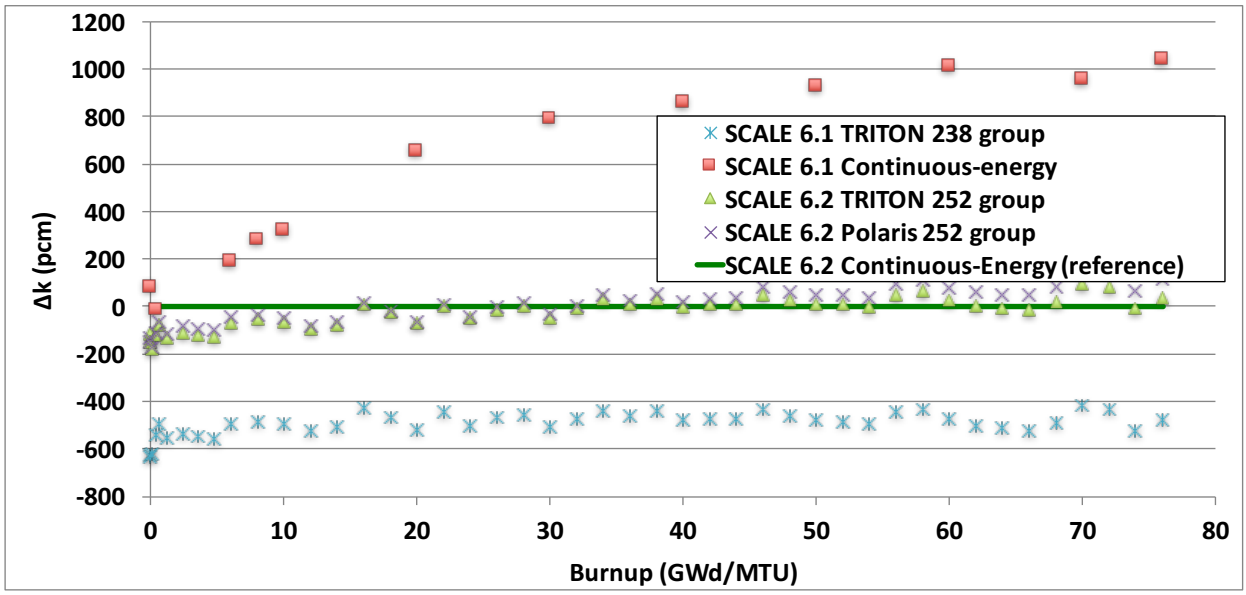

Figure 8. Comparison of computational biases as a function of burnup.

Radioactive Source Term Characterization

ORIGEN

SCALE includes the ORIGEN code with its comprehensive depletion, activation, decay, gamma-ray, and x-ray library for over 2,200 nuclides. ORIGEN and its nuclear data libraries have been updated in SCALE 6.2 to include convenient modular interfaces that provide easy access to ORIGEN's robust capabilities by other software packages.

The input for ORIGEN has been updated to provide a modern interface based on SCALE's 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 SON procedures through input files, as well as the forms-based input in Fulcrum. An excerpt from an example problem is included below to show this new structured, keyword-based input.

```
=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
```

The ENDF/B-VII.0-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 in ENDF/B-VII.0 introduced by updating the nuclear decay data in ENDF/B-VII.0, but not updating the independent and cumulative fission product yields. The yield adjustments improve the consistency between the direct fission yields, decay data, and the cumulative yields in ENDF/B-VII.0.

ORIGEN has been enhanced to provide an alternative solver based on the Chebyshev Rational Approximation Method (CRAM). When compared to an ultra high-precision reference for a depletion problem, ORIGEN's traditional matrix power series supplemented by Bateman solutions for short-lived isotopes, predicts isotopic concentrations with a max error of 0.1%, whereas the CRAM solver produces a max error an order of magnitude lower for the same case and achieves up to machine precision with time-step refinement. 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 also allows for time-dependent source terms and adjoint calculations, enabling the extension of ORIGEN to new classes of calculations. CRAM is currently available as an optional solver in stand-alone ORIGEN calculations, ORIGAMI, and in the Polaris lattice physics code.

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 with UO_2 fuel. ORIGAMI calls interfaces to the ORIGEN transmutation code, with pre-generated parameterized libraries (see next section) and 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 of the burned assembly.

ORIGEN Reactor Libraries

A new series of 1,470 pre-generated burnup libraries for use in ORIGEN and ORIGAMI are introduced in 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 are intended to replace the ORIGEN-ARP libraries that were generated with a previous version 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 4 and Table 5.

Table 4. Assembly and Lattice Types with Available ORIGEN Reactor Libraries

Assembly type (number of libraries)		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 (75)	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 (15)	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 (6)	
	CANDU (1)	19-pin, 28-pin, 37-pin
	IRT (12)	2M, 3M, 4M
	Magnox (4)	
	RBMK (24)	
	VVER-440 (3)	flat, radial enrichments (3.82, 4.25, 4.38)
	VVER-1000 (7)	flat enrichment

Table 5. Additional information for ORIGEN reactor libraries

Assembly type	Enrichments [%]	Coolant/moderator densities [g/cm^3]	Maximum burnup [GWd/MTU]	Number of libraries
PWR LEU	0.5, 1.5, 2, 3, 4, 5, 6	~0.73	70.5	7
BWR LEU	0.5, 1.5, 2, 3, 4, 5, 6	0.1, 0.3, 0.5, 0.7, 0.9	70.5	35
PWR MOX	*	~0.73	70.5	15
BWR MOX	*	0.1, 0.3, 0.5, 0.7, 0.9	70.5	75
AGR	0.5, 1.5, 2, 3, 4, 5	1.65	48.7	6
CANDU	0.711	0.8445	13.7	3
IRT	19.75, 36, 80, 90	0.989	159	12
Magnox	0.7, 0.8, 0.9, 1	1.628	13.7	4
RBMK	1.8, 2.2, 2.6, 3	0.15, 0.28, 0.41, 0.54, 0.67, 0.8	24.3	24
VVER-440	1.6, 2.4, 3.6, profiled	0.73	70.5	6
VVER-1000	0.5, 1.5, 2, 3, 4, 5, 6	0.7145	70.5	7

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

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. This tool was developed to support the US Nuclear Regulatory Commission (NRC) in MELCOR analyses, but it can be adapted to many other uses. The ORIGAMI Automator is an integrated graphical user interface that leverages many of the 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.

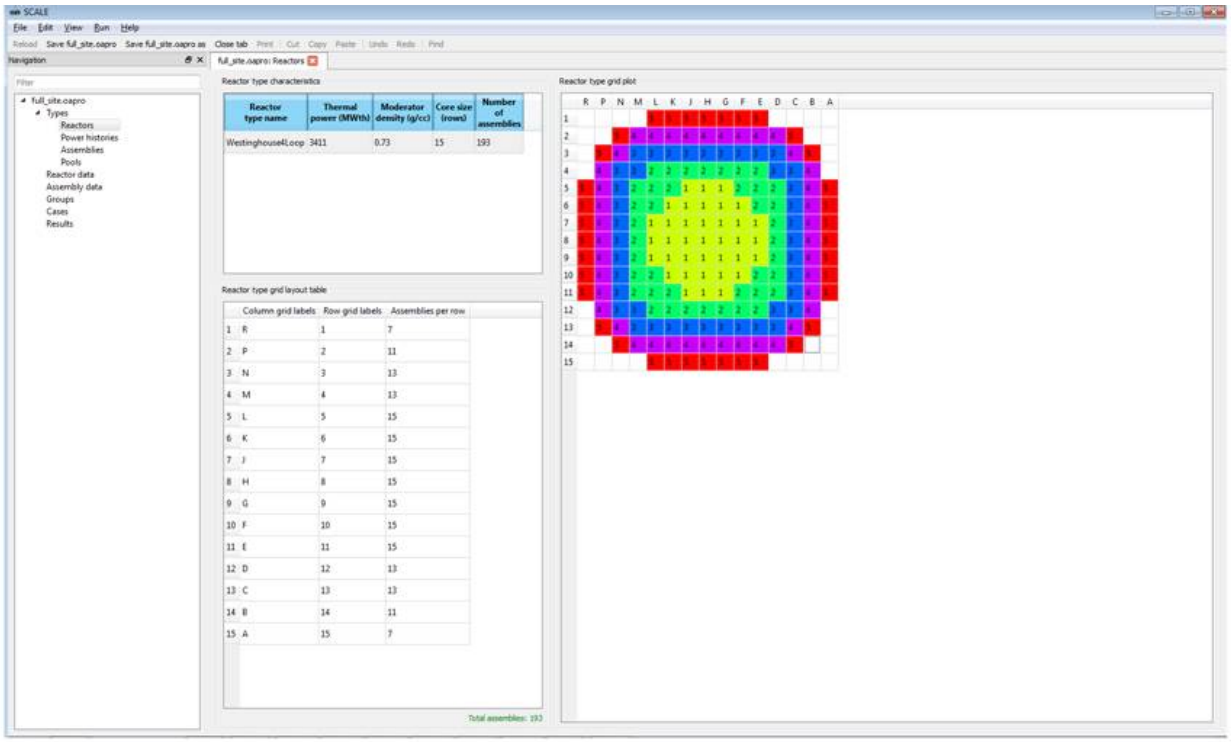

Figure 9. ORIGAMI Automator.

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 Forward-Weighted Consistent Adjoint Driven Importance Sampling (FW-CADIS) 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. For example, it is problematic for deep penetration shielding through iron, in which 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 in which 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 S/U analysis methods that use KENO for transport analysis are extended to provide CE capabilities through the implementation of the contributon-linked eigenvalue sensitivity/uncertainty estimation via tracklength importance characterization (CLUTCH) methodology and iterated fission probability (IFP) methods.[12] CLUTCH is an efficient methodology that has been demonstrated to provide high-fidelity results with manageable run-times 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 6 compares the accuracy of the total nuclide sensitivity coefficients estimated by the each sensitivity method for the MIX-COMP-THERM-004-001 system.[13] The MG analysis produced a ^{238}U total nuclide sensitivity that disagreed with the reference direct perturbation sensitivity by 2.80 standard deviations, while the CE methods (IFP and CLUTCH) sensitivities were within 1.25 standard deviation of the reference sensitivity coefficients for all of the nuclides examined.

Figure 10 compares the figures of merit for the nuclide sensitivity coefficients presented in Table 6. 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 the MG method. This is remarkable because of the use of CE physics, which can impose relatively long cross section lookup times, and it also indicates the efficiency of the CLUTCH method.

Table 6. MIX-COMP-THERM-004-001 nuclide sensitivity coefficient comparison

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

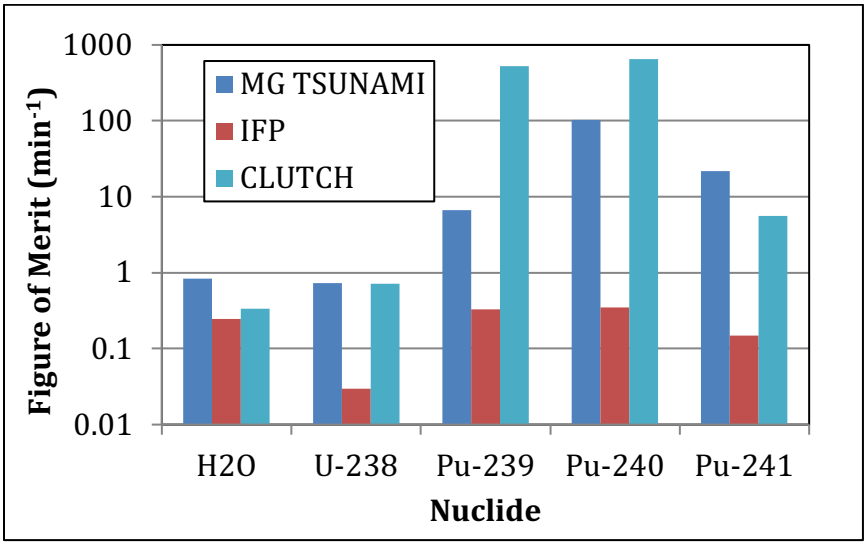

Figure 10. MIX-COMP-THERM-004-001 nuclide sensitivity figure of merit comparison.

Table 7 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 7. Sensitivity method memory usage.

Model	MG TSUNAMI	CE TSUNAMI	
		IFP	CLUTCH
MIX-COMP-THERM-004-001	13,785 MB	10,643 MB	63 MB

Sampler

A new stochastic uncertainty quantification capability has been added 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 user input parameters such as geometry, material density, isotopic composition, temperature, etc.

Sampler propagates these uncertainties through complex SCALE analysis sequences such as depletion calculations, and it provides the variation in the output quantities due to variations in any combination of input data, as shown in Figure 11.[14] 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.[15]

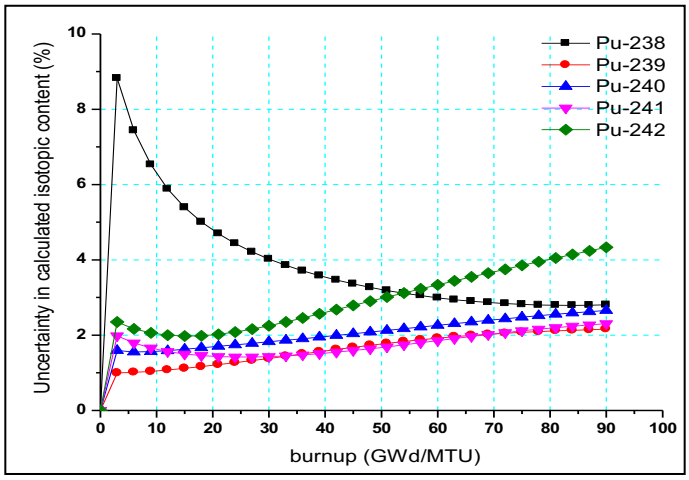

Figure 11. Uncertainty in plutonium isotopics as function of burnup.

The Medusa module of the XSUSA program[16] is used to generate perturbation factors for the 1D cross sections on the MG library, assuming that the probability density functions are multivariate normal distributions with covariances given in the SCALE nuclear data covariance library. 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, with independent correlations developed by ORNL using a Bayesian method applied to ensure that uncertainties in the cumulative fission yields are consistent with the independent yields in each chain.[17] Multiplicative perturbation factors for fission product yields have been generated with XSUSA. The decay uncertainty data has 4 major components: decay

constant uncertainty, q-value uncertainty, fraction of q value in photons, and branching ratio uncertainty. Perturbation factors for these 4 components are generated using uncertainties from the ENDF/B-VII.1 library. Correlations are defined for decays with multiple decay modes to ensure that the sum of branching is unity. No uncertainties are applied for data that do not have associated uncertainty information. Perturbations are applied using the covariance information with XSUSA to provide 1,000 ORIGEN decay libraries. At this writing, the uncertainty information has not been consolidated as a single file of perturbation factors.

Currently, decay data sampling is available for ORIGEN and ORIGAMI calculations but is not operational with TRITON and Polaris calculations without additional user-supplied preliminary calculations.

Sampler also provides the ability to perform multivariate parametric studies for variables with uniform distributions.

Note that Sampler can be built with MPI enabled for parallel computations (see “Build Instructions” below), but it can only sample the execution of serial codes. Threading is available with the default binary distribution (use the “-I” option of scalerte) when executing Sampler.

Other Updates

SCALE 6.2 includes a number of other improvements, such as the extension of the maximum allowed number of materials from around 2,000 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 300 K to 293 K for improved consistency between MG and CE calculations.

List of SCALE 6.2.4 Updates

SCALE uses a versioning scheme where new features are only introduced in a feature release, such as "6.2". The version number "6.2" describes the series, which began with 6.2.0 and follows with maintenance releases 6.2.1, 6.2.2, 6.2.3, and now 6.2.4. The maintenance releases are intended only to fix issues found by the user community while the next feature release is being developed. The following section presents the new fixes made in 6.2.4. The SCALE team will maintain a list of known (and unfixed) issues only for the latest maintenance release. See the website http://scale.ornl.gov for details.

The list below is organized by major sequence/module.

STDCOMP

Missing element isotopic distribution check

An issue has been fixed in SCALE 6.2.4 where the Standard Composition Library (STDCOMP) and related functions did not include an input check that certain elements must have user-defined isotopics. The elements listed in Table 7.2.2 have natural abundances which define a default isotopic distribution. Elements *not listed* in table include Tc, Pm, Po, At, Fr, Ac, Pa, and all actinides with atomic numbers greater than 92 (Np, Pu, Am, Cm, Bk, Cf, Es, etc.). For these elements, which are referred to as *non-naturally occurring elements*, the isotopic distribution is strongly dependent on the production source and decay time of the material, and ***the user is required to enter isotopic distributions*** for these elements or to simply enter the isotopic number densities directly. In SCALE versions 6.2.0-6.2.3, this check was not operating as intended.

The main area of concern, and why this was elevated to a high-priority fix, was that in SCALE 6.1 and previous versions, non-naturally occurring Pu was mapped to a fictitious "natural" abundance of 100% ^{239}Pu, mainly as a shortcut for defining limiting, maximum reactivity systems. This artificial behavior was removed in the SCALE 6.2 feature release. Because of the change in default behavior for Pu and the lack of a complete input check, an incomplete input that does not specify the isotopic distribution for materials with a non-naturally occurring element could have generated a non-conservative result in versions 6.2.0-6.2.3.

KENO

Doppler broadening rejection correction on Windows

An issue has been fixed in SCALE 6.2.4 where DBRC data was not being correctly loaded on Windows in 6.2.3, and with the DBR=2 option there was no indication that the data was not loaded and the calculation proceeded without warning. The easiest way to verify whether a calculation was affected was to rerun with DBR=0, and if the random walk was identical, then the DBRC was not successful. Note that there was no such defect on Linux and Mac systems.

Kinematics data setup

An issue has been fixed in SCALE 6.2.4 where including a thermal moderator nuclide (e.g., H-1) at multiple temperatures in the input was not handled correctly. This issue was introduced in 6.2.2 and affects both TRITON and CSAS calculations which utilize KENO as the transport solver. It was discovered when inconsistent results were observed in TRITON as a function of the addnux parameter. H-1 existed in the moderator (585K) as expected but was also introduced into the fuel at 900K, as part of the automatic depletion setup with the addnux parameter. The bias introduced in eigenvalue is estimated to be less than 200 pcm.

ORIGEN

Large decay steps may lead to certain (alpha-n) sources not being included

An issue has been fixed in SCALE 6.2.4 where in ORIGEN calculation of (alpha,n) sources for 10 million years decay, ORIGEN did not include Am-241 in the results. This issue was due to floating point comparisons applied to the final time isotopics where very little Am-241 was left, leaving out Am-241 in early times. The parameter alphan_cutoff has a default to include all potential sources, so this was unexpected behavior. Although it is recommended to update to SCALE 6.2.4 for ORIGEN users, a workaround for SCALE 6.2.0-6.2.3 users is to use a single case for each decay step, effectively forcing the (alpha,n) source criteria to be applied at each time step.

ORIGAMI

Zero decay length in cycle

An issue has been fixed in SCALE 6.2.4 where ORIGAMI did not allow some valid power histories which occur when one wants to model a fine-grained power history with no intermittent decay as shown below.

```
cycle{ power=30 burn=1 down=0 }
cycle{ power=31 burn=1 down=0 }
```

In SCALE 6.2.3 only, the calculation would end with an error if “down=0” were used. A workaround in that case was to use “down=1e-5”, which will not alter results on the important time scales.

TRITON

Material Swap

An issue with the TRITON swap capability has been fixed in SCALE 6.2.4, where the TRITON swap capability did not function correctly in many scenarios. The extent of the error was not fully categorized but the error is due to incorrect bookkeeping of the volume

of mixtures involved in the swap. All users of the TRION swap capability are encouraged to update to 6.2.4.

MAVRIC

Response generation from CE cross-sections

An issue was fixed in SCALE 6.2.4 where MAVRIC could not perform CE responses for nu-fission. The nu-fission reaction (mt=1452) is useful as a response and is supported for MG simulations. However, this reaction is not present in CE libraries directly; rather it is calculated as a multiplication of nu-bar (mt=452) and σ_f (mt=18) fission cross sections during the response generation. MAVRIC CE responses for the nu-fission reaction are now enabled in 6.2.4.

Although they are not as common as flux-to-dose conversion factors or neutron cross section responses, photon cross section responses may be defined in MAVRIC. However, a defect was identified in 6.2.3 when using macroscopic cross sections for responses with photon cross sections. This issue has been fixed in 6.2.4.

Other Minor Miscellaneous Issues fixed in SCALE 6.2.4

- A minor formatting issue in the MCNP card output of ORIGAMI was fixed. This MCNP card enables users to generate MCNP sources directly in the MCNP format based on ORIGAMI-calculated spent fuel isotopics.
- A minor issue was corrected in SCALE's installation testing. SCALE deploys with a test suite of regression and sample problems designed to verify the installation on a particular computer. Due to small differences in the way different CPUs round and perform basic mathematical operations, the random particle histories of the Monte Carlo transport codes in SCALE cannot be made identical for two different systems. In order to overcome this difficult on installation testing, a fuzzy tolerance is used to check the local machine result (a) versus the deployed baseline result (b). In the case both results have uncertainty, the check was looser than intended doing a simple overlap of the uncertainty bands. The check was updated to $|b-a| \leq N\sqrt{\sigma_a^2+\sigma_b^2}$ where N=3 is typically used and σ is a standard deviation reported by the code. The previous test criteria used $|b-a| \leq N(\sigma_a+\sigma_b)$ with most tests at the N=2 sigma level. With the new, better test criteria but the old N=2, there were a handful of failures on Windows when the baseline was generated on Linux. Given we are running hundreds of tests, this is statistically within expectations. Users should not be concerned that the old testing was incorrect. With either test criteria, a failure indicates either an installation failure or an "unlucky" random walk far outside expectations.
- A minor issue was corrected in Fulcrum where the mesh viewer could fail to remove loaded mesh files, requiring a restart of Fulcrum to deallocate program memory associated with mesh data.
- A minor issue was fixed in MAVRIC where some input blocks required lower case, even though SCALE is case insensitive for keywords.

- A minor issue was fixed in the legacy "solution" composition input where an upper-case composition name failed to be processed. The issue was due to a missing case conversion on the "solution" composition name that was used for the standard composition library composition STDCOMP lookup.
- A minor issue was fixed where CSAS printed the incorrect atomic weight for ^{18}O in the mixing table output when running in MG mode. The correct atomic weight is now printed.
- A minor issue was fixed in ORIGEN when using "previous=0" to load isotopics from a previous "case" in the input.
- A minor issue was fixed in ORIGEN's FIDO interface, in which data file paths were truncated to 80 characters. When reading files in the SCALE installation directory, data directory, or temporary directory plus the file path of more than 80 characters, the code would terminate with a "file not found" error. The only workaround was to move or symbolically link the relevant directories to shorter paths. The paths have been extended to 1,024 characters in 6.2.4.
- A minor issue was fixed in which the ZA column in the CSAS mixing table output edits did not show the correct value for the free gas hydrogen (nuclide ID 8001001), for example. The ZA should have shown 1001, but instead it just repeated the nuclide ID.
- A minor issue was fixed in all MG calculations in which the incorrect atomic weight for ^{18}O was shown in mixing tables as *18.1551* instead of *17.9992*. This cannot affect a calculation because the ^{18}O cross section is zero in ENDF/B-VII.
- A minor issue was fixed in which the CSAS5 mesh tally capability did not function correctly, especially for the grid flux and fission source distribution mesh tallies, if the specified mesh in the grid geometry block covered only a fraction of the global geometry.
- A minor issue was fixed in the AmpxMGConverter utility, which allows SCALE 6.2 MG libraries to be converted to the previous SCALE 6.1 MG format. The conversion of SCALE 6.2 formatted macroscopic MG libraries to SCALE 6.1 formatted MG libraries has not been operational in SCALE 6.2.0-6.2.3. It now works as expected in SCALE 6.2.4.

System Requirements

System architecture:

- Linux 64-bit (RHEL 6 or newer)
- Mac OS X (Darwin) 10.11.6 or newer
- Windows 7, 64-bit or newer

System requirements:

Minimum requirements: 4 GB RAM per CPU, 40 GB of disk space + additional space to store output results

Recommended requirements: 8 GB RAM per CPU, 40 GB of disk space + 100 GB of scratch space + additional space to store output results

Production requirement for large models: 64 GB RAM, 40 GB of disk space + 500 GB of scratch space + additional space to store output results

Java requirements:

Java 1.6 or newer.

Installation Instructions

The SCALE 6.2.4 installation has been divided into three components: 64-bit pre-compiled binaries, source code, and the data. The precompiled binaries are available in platform-familiar installers: NSIS on Windows, Drag-N-Drop bundle on Mac, and Tar GZip on Linux. For deployments that include source code, it is available as a zip file, and the data are available as a self-extracting IzPack installer. Other systems may require a custom build of SCALE from source code using the build instructions provided below.

Pre-Compiled Binaries

Note: **After the Binaries are installed, the nuclear data still must be installed.** After completing the binary installation according to the instructions in this section, please follow the instructions for SCALE 6.2 Data.

Windows

Double-click the Windows installation file "SCALE-6.2.4-setup.exe", agree to the terms, and the following "Welcome" dialog will be shown.

Figure 12. Example Windows installation start screen.

Follow the prompts through the install. There are two user decisions. The first is regarding the install location, as shown below. Generally, the "C:\SCALE-6.2.4" is sufficient. (Do not install SCALE to the "Program Files" directory, as it has insufficient default privileges.)

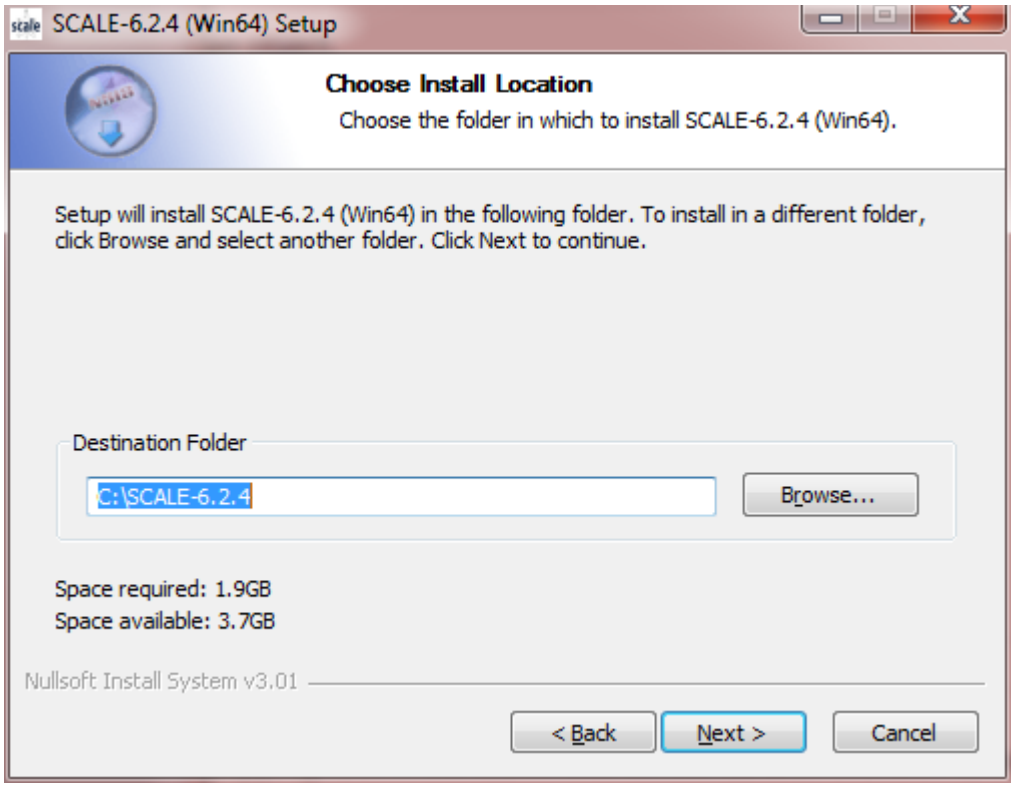

Figure 13. Example Windows install location.

The next user decision is to designate the name of the SCALE 6.2.4 application folder within the Windows start menu. The default is "SCALE 6.2.4 (Win64)"; however, changing this name will not affect the installation in any way.

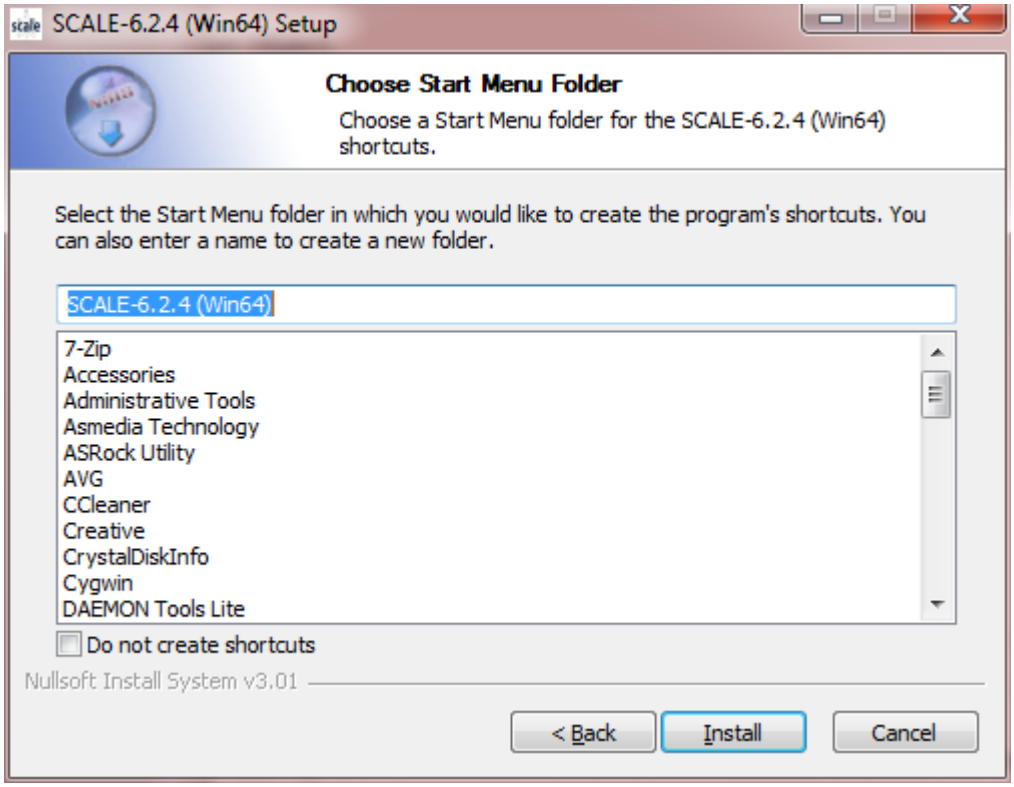

Figure 14. Example Windows start menu folder selection.

The installation can take several minutes. **Note that Norton Antivirus on Windows requires an exception for the SCALE Runtime Environment program, scalerte.exe.** If using Norton Antivirus, please establish this exception prior to testing; otherwise, SCALE 6.2.4 will not be able to execute. **Once installation is complete, follow the instructions given below to install SCALE 6.2 Data**.

Mac OSX

Double click the Mac OSX installation file "SCALE-6.2.4-setup.dmg"; after a few moments, the following screen will open.

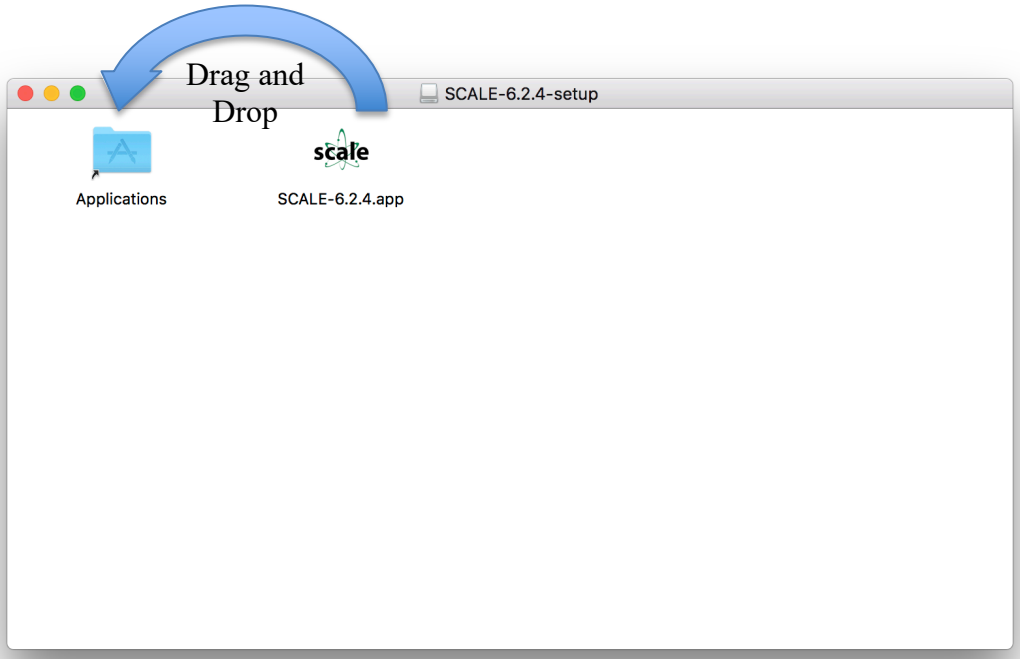

Figure 15. Example Mac OS X bundle contents.

Drag the "SCALE-6.2.4.app" icon onto "Applications" to install SCALE-6.2.4. **Once installation is complete, follow the instructions given below to install SCALE 6.2 Data**.

Linux

Copy the SCALE-6.2.4.tar.gz to the installation directory. Invoke 'tar -xzf SCALE-6.2.4.tar.gz' to create the SCALE-6.2.4 directory.

```
[user]ls
SCALE-6.2.4.tar.gz
[user]tar -xzf SCALE-6.2.4.tar.gz
[user]cd SCALE-6.2.4
[user]ls
Ampx                CentrmOptions.xml  docs                help     Javapeno  MoreOptions.xml  python      ScaleRunResources.xml
AmpxRunResources.xml cmds              etc                 images   lib       ParmOptions.xml  regression  uslstats
bin                 Copyrights.txt     FileNameAliases.txt include  Meshview  plugins          samples     vibe
[user]
```

Figure 16. Example Linux Tar GZip.

Once installation is complete, follow the instructions given below to install SCALE 6.2 Data.

Source Code

If you received the source code version, you can unzip SCALE-6.2.4-Source.zip file to any location on your computer.

For example, on a Windows platform, double click the SCALE-6.2.4-Source.zip file. This will extract the files into the "SCALE-6.2.4-Source" directory.

On Linux and Mac OS X, create a destination directory for the source and copy the SCALE-6.2.4-Source.zip into that directory.

Change to the directory and invoke 'unzip SCALE-6.2.4-Source.zip' to deploy the source code.

SCALE 6.2 Data

Note that if you have SCALE 6.2 data installed from a prior SCALE 6.2 installation, you can copy or link the data into the SCALE 6.2.4 directory. To link preinstalled SCALE 6.2 data, open a command prompt and change the directory to the SCALE 6.2.4 installation directory:

(C:\SCALE-6.2.4, /Applications/SCALE-6.2.4/Contents/Resources, etc.).

On Windows, the following will link the SCALE 6.2 data into the SCALE 6.2.4 installation. (This may require administrative privileges.)

```
mklink /D data C:\SCALE-6.2\data
```

On OS X, the following will link the SCALE 6.2 data into the SCALE 6.2.4 installation:

```
ln -s /Applications/SCALE-6.2.app/Contents/Resources/data data
```

On Linux, the following will link the SCALE 6.2 data into the SCALE 6.2.4 installation:

```
ln -s /scale/scale6.2/data data
```

To begin installation of SCALE 6.2 data**, copy the scale-6.2-data--setup.jar to your local disk. Double-click this jar file. If the installer does not start**, then bring up a command prompt or terminal window and issue the following command: `java -jar scale-6.2-data-setup.jar` in the location where the installer jar file was copied.

After launching the installer, a dialog should appear as shown below.

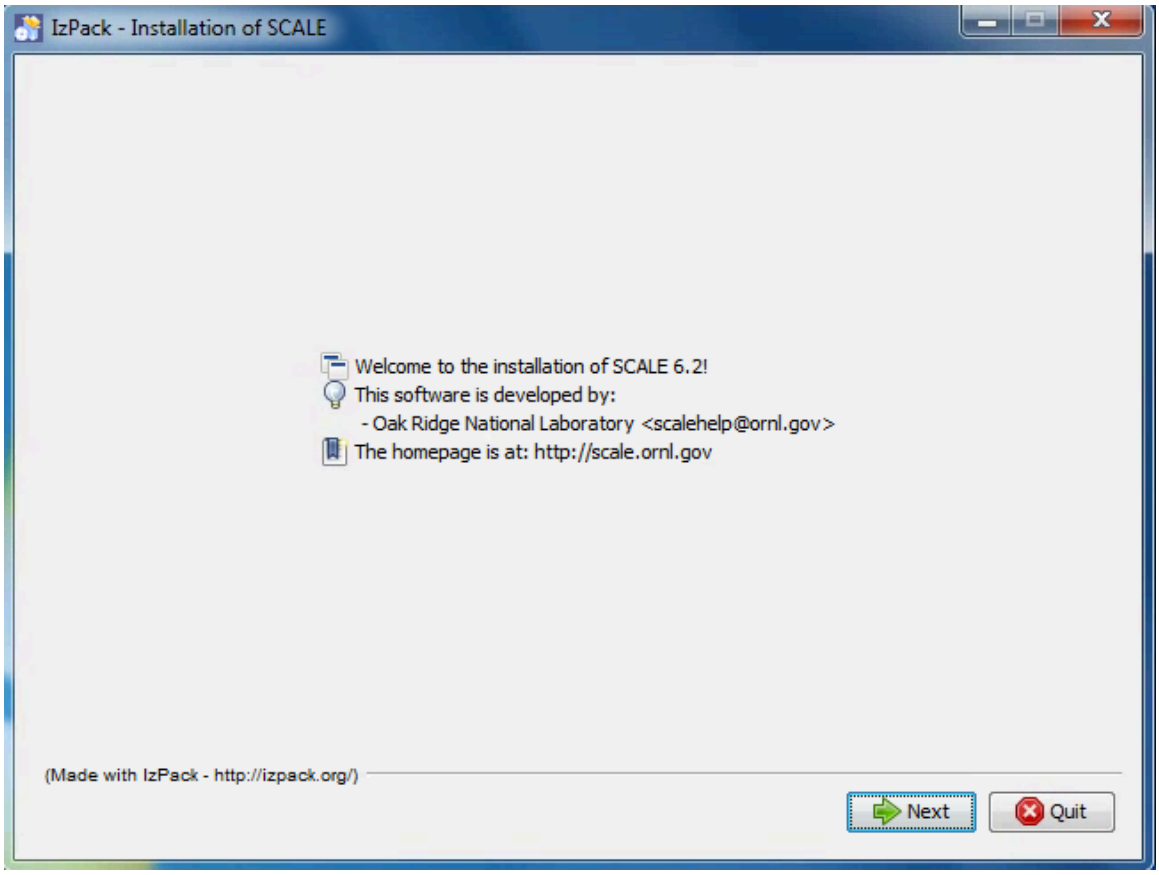

Figure 17. SCALE 6.2 data installer welcome dialog.

Continue by pressing *Next*.

You will be prompted to review and accept the terms of the license agreement.

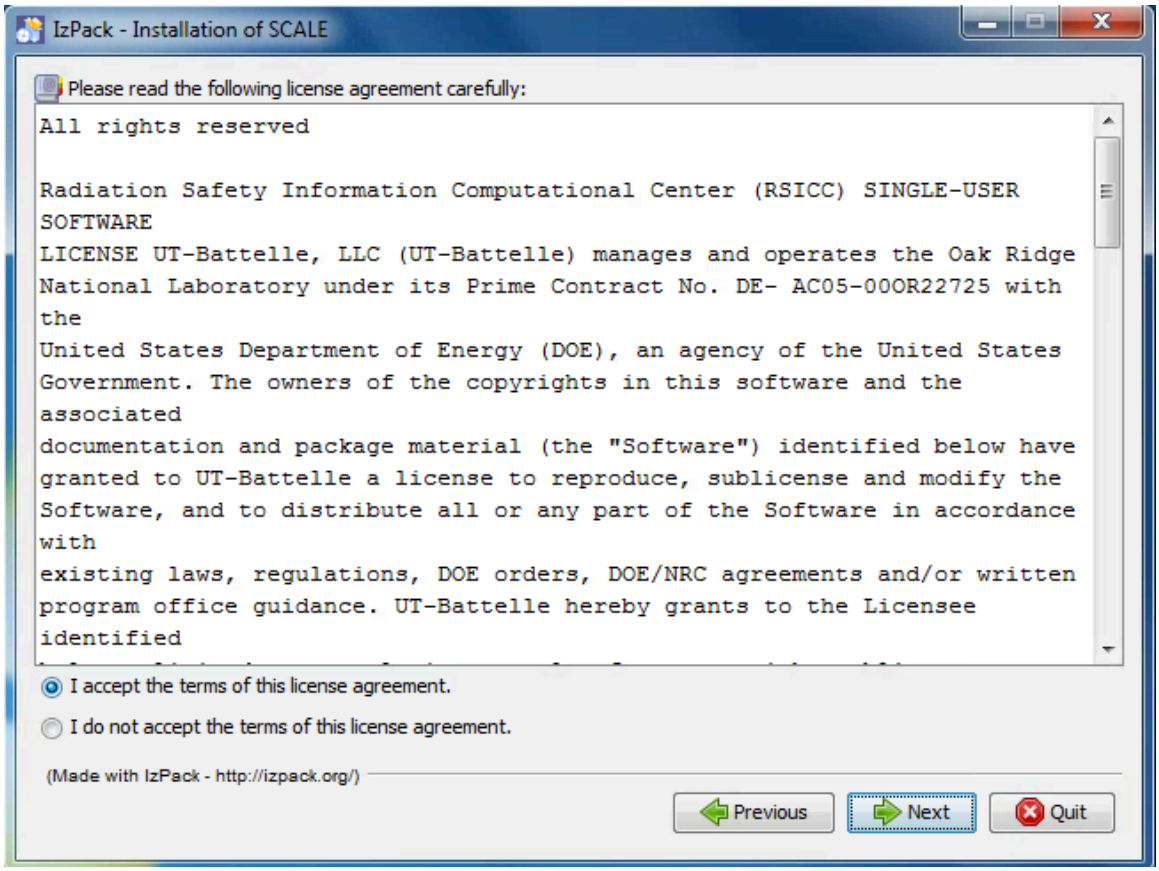

Figure 18. SCALE license agreement.

To proceed, check to indicate your acceptance of the terms, and press next.

You will be prompted to choose the destination of your installation.

For Windows users, the recommended installation path is inside your SCALE-6.2.4 directory:

```
c:\SCALE-6.2.4
```

For Linux, a typical location is:

```
/scale/scale6.2.4
```

For Mac, a typical location is:

```
/Applications/SCALE-6.2.4.app/Contents/Resources
```

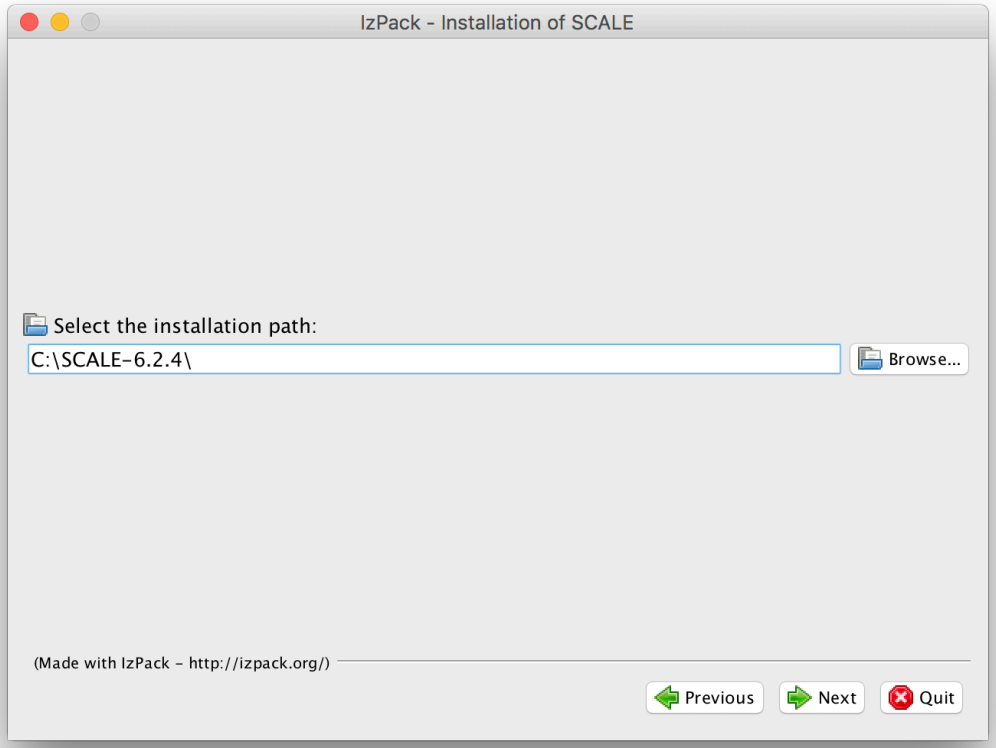

Figure 19. Example setting typical data installation path on Windows.

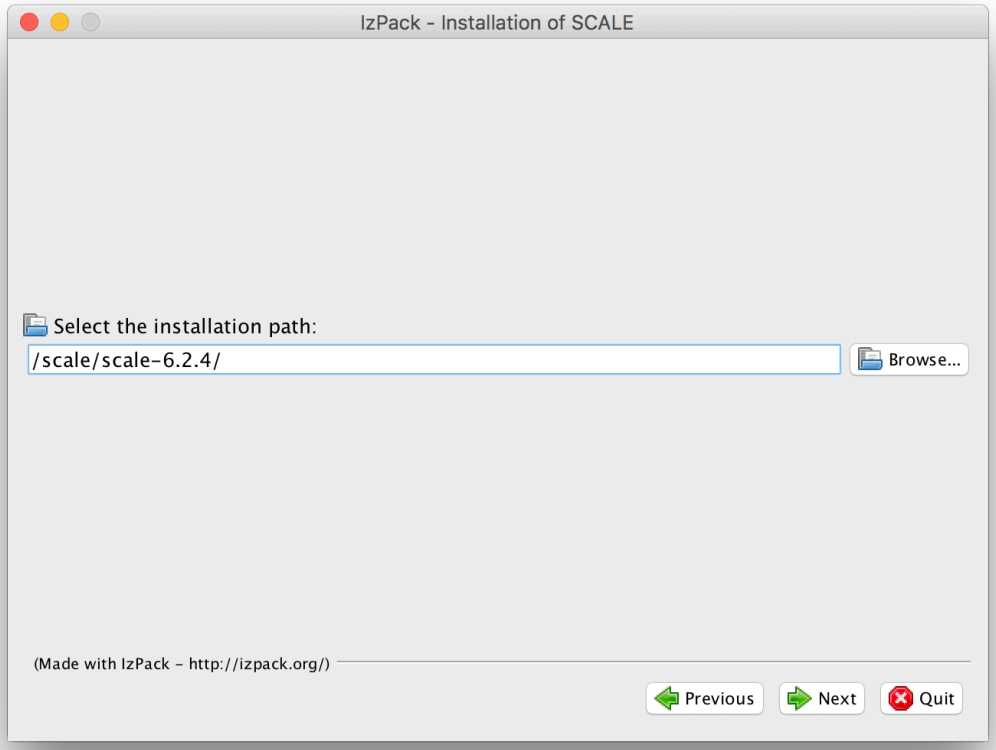

Figure 20. Example setting a typical data installation path on Linux.

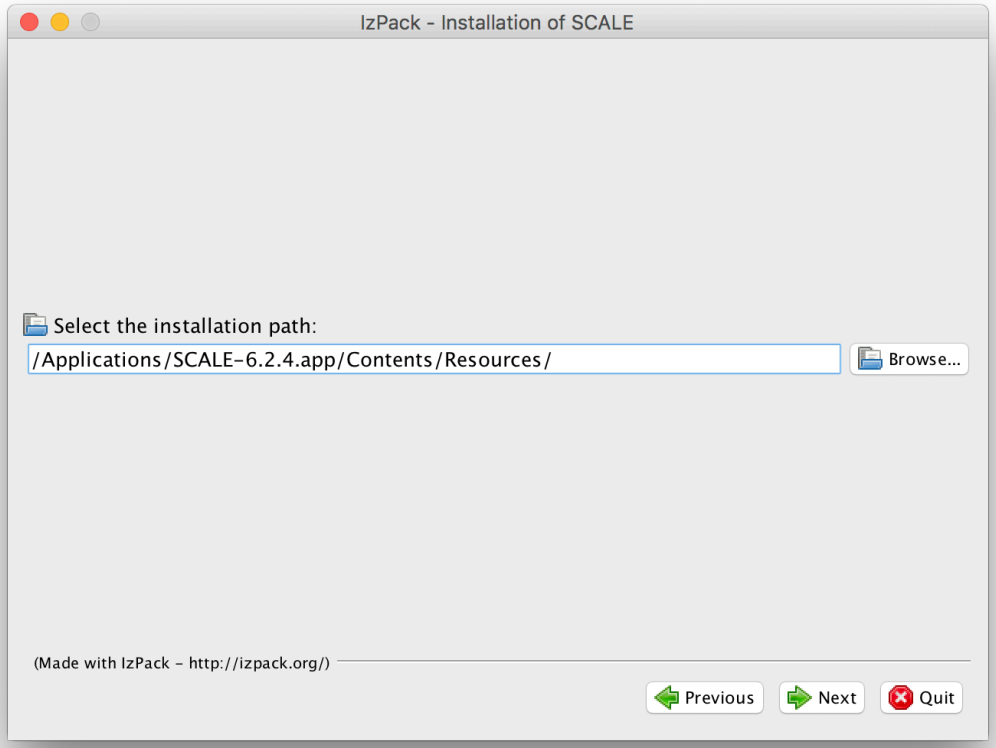

Figure 21. Example setting a typical data installation path on Mac OS X.

For some systems, the installer will not be allowed to create a new directory. If you encounter a message like the one shown below, simply create the directory manually (e.g., using Windows Explorer), and then return to the installer and continue.

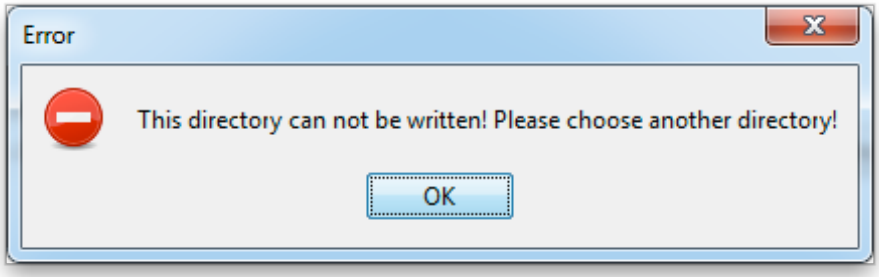

Figure 22. Data installer directory creation error message.

In most cases, the installer will present a prompt to confirm the creation of a new directory; if that target directory is correct, then you can simply press *OK*.

If the directory was manually created, the installer will notify you that it is about to overwrite any previous contents. Press *Yes* to continue.

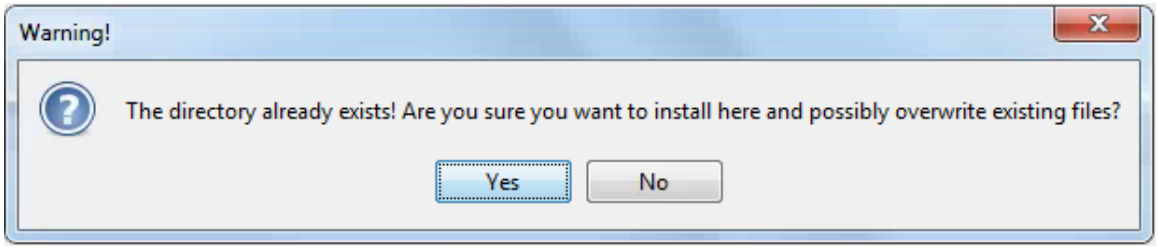

Figure 23. Directory overwrite dialog.

The installer then presents a dialog for available data sets you may wish to install.

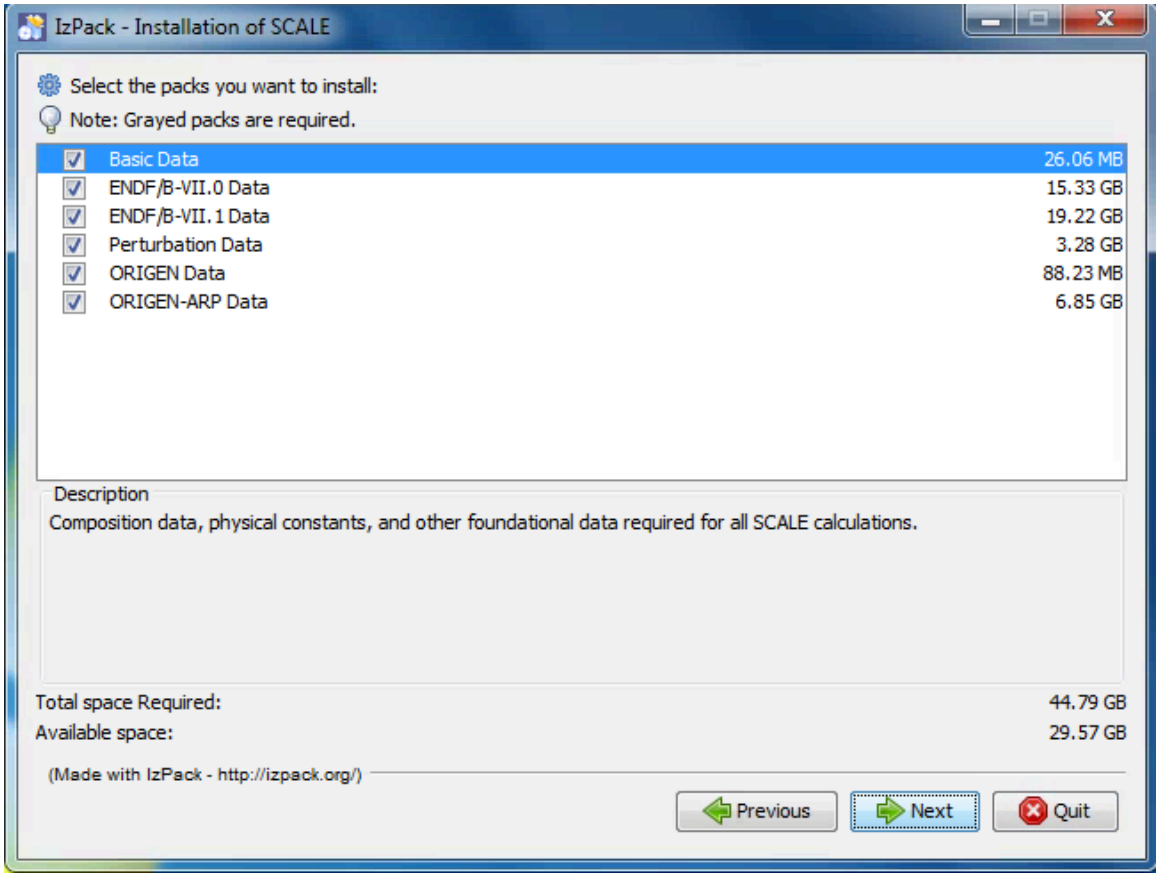

Figure 24. Data selection dialog.

Please select the data needed to perform your desired SCALE calculations.

- Basic Data — Composition data, physical constants, and other foundational data required for all SCALE calculations
- ENDF/B-VII.0 Data — Nuclear Data from ENDF/B-VII.0 for CE and MG calculations, coupled n-gamma data from ENDF/B-VII.0 for MG calculations, and SCALE 6.0/6.1 44-group neutron covariance data (optional for most calculations, but provided for backwards compatibility)
- ENDF/B-VII.1 Data — Nuclear Data from ENDF/B-VII.1 for CE and MG calculations, coupled n-gamma data from ENDF/B-VII.1 for MG calculations, and ENDF/B-VII.1 neutron covariance data (recommended for most calculations; required to run the SCALE sample problems)
- Perturbation data — 1,000 samples of data each for ENDF/B-VII.1 neutron covariance data, SCALE 6.0/6.1 neutron covariance data, fission product yield covariance data, and radioactive decay covariance data (required for Sampler calculations perturbing nuclear data)
- ORIGEN Data — Activation, depletion and decay data from ENDF/B-VII.1 and JEFF 3.0/A (required for activation, depletion and decay calculations)
- ORIGEN reactor libraries — Pre-generated ORIGEN reactor libraries for many fuel types (required for spent fuel characterization and source terms calculations)

Next, the installer may ask for the location of the data *.pak* files that are unpacked during the installation process. Please direct the installer to the location of these data files, which are part of the SCALE distribution and may be on the distribution media or copied to a local directory as shown below.

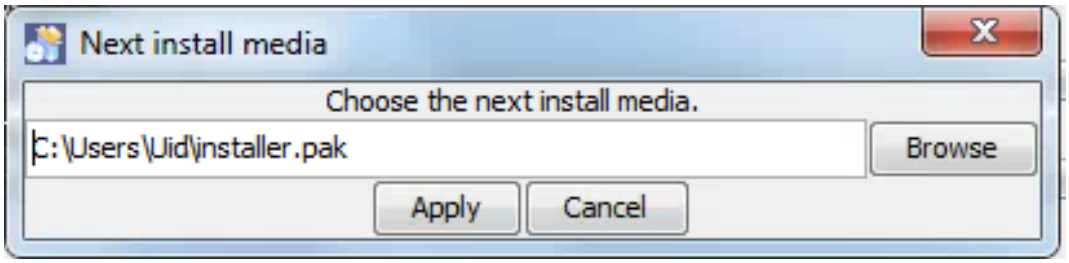

Figure 25. Media selection dialog.

The installer will display the progress of the installation. If installing from a DVD set, part way through the installation, you will be prompted for `installer.pak.1`. Please insert the PAK.1 disk and click *Apply*.

The installation from PAK.1 will complete and prompt for `installer.pak.2`. Please insert the PAK.2 disk and click *Apply*.

PAK.2 will finish. Proceed with all DVDs or files in the delivery until you have completed your installation of SCALE 6.2 data.

Running SCALE

SCALE is run by using the Fulcrum user interface or by invoking the SCALE Runtime Environment, *scalerte*, from the command line. Note that this release does not include the previous interfaces GeeWiz or OrigenArp for running SCALE on Windows, as Fulcrum should be used instead. Additionally, previous shortcuts like *runscale* are not implemented.

Running SCALE from Fulcrum

The most convenient way to run SCALE from a desktop is by launching Fulcrum. The Fulcrum executable is provided in the *bin* directory where SCALE was installed (e.g., C:*SCALE-6.2.4**bin**Fulcrum.exe*). Fulcrum includes an online help document to assist users with its many features, and it includes links to the user manual and primers.

Windows

For a Windows installation, launch Fulcrum from either the start menu or the shortcut provided in the *SCALE-6.2.4* folder on the desktop.

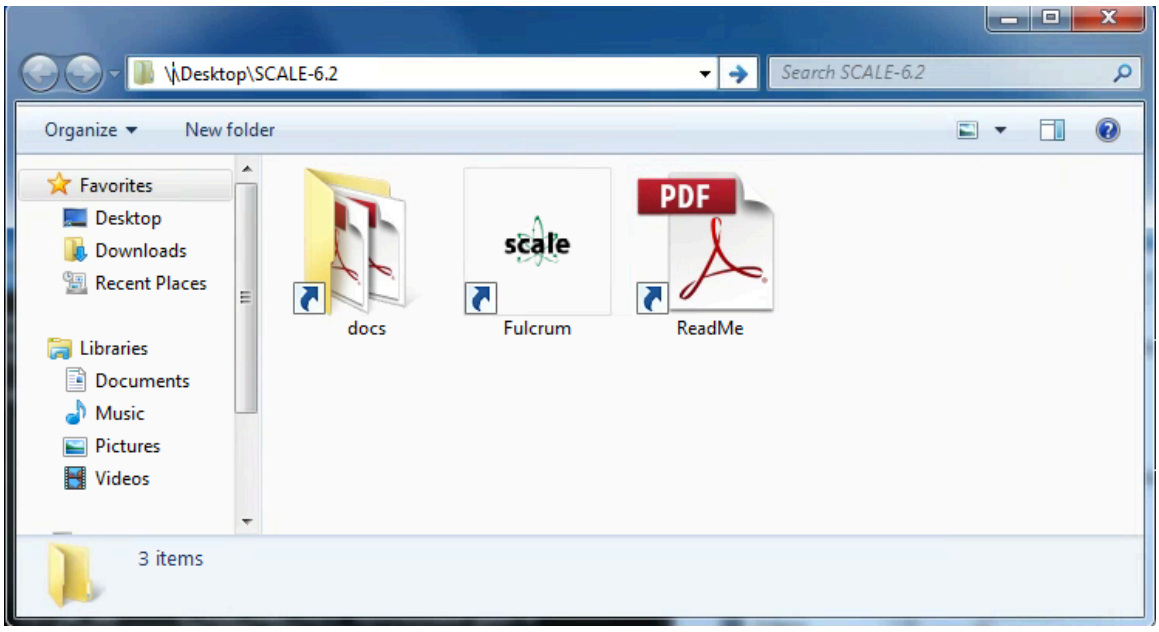

Figure 26. Example Windows desktop SCALE shortcuts folder.

Linux

For a Linux installation, launch Fulcrum directly from the bin directory of the SCALE installation (e.g., */scale/scale6.2.4/bin/Fulcrum*).

Mac OS X

For a Mac installation, launch Fulcrum by executing the *SCALE-6.2.4* app in the Applications directory.

Running SCALE from the Command Line

Using the command line, SCALE can be executed using the *scalerte* command from the *bin* directory inside the SCALE installation. Paths for each platform are shown below based on recommended installation directories. Your directory may differ based on the installation.

Windows

C:*SCALE-6.2.4**bin**scalerte.exe*

*Note that Norton Antivirus may require an exception for scalerte.exe on Windows to prevent the executable from being quarantined.

Linux

/scale/scale6.2.4/bin/scalerte

Mac

/*Applications/SCALE-6.2.4.app/Contents/Resources/bin/scalerte*

The SCALE runtime environment provides several command line options. The usage is as follows.

`scalerte [options] inputfile(s) [options] [inputfile(s)]`

Where `inputfile(s)` are one or more files or file patterns (*test.inp*, or *test*.inp*, etc.).

Where *options* are:

`-a`: Specify alias file.

```
-a path/to/aliasesfile
```

`-f`: Add hostname to output filename. Produces inputfile.hostname.out

`-h`: Print this information as a help message.

`-I`: Number of threads to use for MPI/OpenMP directives. `-I 4`

`-m`: Print information messages as SCALE executes.

`-M`: Specify a machine names file for SCALE parallel capabilities.

```
-M /path/to/machine/names/file
```

`-n`: Nice level on Nix systems, ignored on Windows. Default: `-n 2`

`-N`: Number of MPI processes to run. `-N 20`

`-o`: Overrides the default *inputfile.out* output name. The *.out* extension is appended by scalerte, so there is no need to specify the extension.

```
-o path/to/outputfile
```

NOTE: If the *path/to/outputfile* already exists, it will be deleted. If this option is specified while in stack mode (multiple input files), the value provided is prepended to the inputfile's basename.

`scalerte triton* -o myout` results in output names `myout.triton*.out`

`-r`: Keep the temporary working directory after execution.

`-t`: No new temporary working directory. Uses last temporary working directory, `-r` is implied.

`-T`: Specify temporary working directory.

```
-T directory/path
```

NOTE: If `-T` is specified while in stack mode (multiple input files) the value provided is appended with the index of the file.

```
scalerte t0.inp t1.inp t2.inp -T mytmp
```

results in *mytmp*, *mytmp1*, and *mytmp2* temporary directories.

`-v`: Turn on verbose activity printing for scalerte.

`-V`: Print the scalerte version date.

`-x`: Do not return XSDRNPM output in a *.xsdrnfiles* directory.

`-z`: Add date to the output filenames.

Produces output files in the form of
inputfile.yyyy.MM.ddThh.mm.ss.out

inputfile.yyyy.MM.ddThh.mm.ss.msg

inputfile.yyyy.MM.ddThh.mm.ss.etc

Where:

- `yyyy- is the year of execution.`
- `MM- is the month of execution.`
- `dd- is the day of execution.`

- hh- is the hour of execution.
- mm- is the minute of execution.
- ss- is the second of execution.

Example Invocation

For users familiar with previous invocations of the SCALE batch script, this usage is no longer valid. The only valid entry point is scalerte. Scalerte can be executed from anywhere with a fully qualified path such as `c:\SCALE-6.2.4\bin\scalerte` or `/scale/scale6.2.4/bin/scalerte`, for example.

Invoke SCALE on a single input file named *HelloWorld.inp.*

```
scalerte HelloWorld
```

or

```
scalerte HelloWorld.inp
```

Invoke SCALE on all input files patterned *HelloWorld*.inp.*

```
scalerte HelloWorld*.inp
```

Invoke SCALE on all input files patterned *HelloWorld*.inp* and print runtime messages to the console.

```
scalerte HelloWorld*.inp –m
```

Invoke SCALE on all input files patterned *HelloWorld*.inp* and include hostname and date/time in the output file's name.

```
scalerte HelloWorld*.inp –fz
```

or

```
scalerte HelloWorld*.inp –f –z
```

Invoke SCALE on *HelloWorld.inp* and rename output to be *MyHello.out.*

```
scalerte HelloWorld –o MyHello
```

or

```
scalerte HelloWorld.inp –o MyHello
```

Invoke SCALE on all files patterned *HelloWorld*.inp* and rename output to be *MyHelloWorld*.out*.

NOTE: When SCALE is run in stack mode (multiple inputs), the output override is prepended to the input file's name.

```
scalerte HelloWorld*.inp –o My
```

Invoke SCALE on *HelloWorld.inp* and keep the working directory.

```
scalerte HelloWorld.inp –r
```

Invoke SCALE on *HelloWorld.inp* and override and keep the working directory.

```
scalerte HelloWorld.inp –r –T myHelloWorldTempDir
```

Invoke SCALE on *HelloWorld.inp* and specify the number of threads to be 4.

```
scalerte HelloWorld.inp –I 4
```

SCALE Variables

This section describes the environment variable used within *scalerte*. These variables can be accessed through SCALE's *shell* module to populate the working directory and/or to return SCALE-generated files that were not returned by *scalerte*.

Shell is used to perform system commands inside a problem before, after, or between explicitly called modules. It is usually used in SCALE to link a file from one name and place to another name and place, to delete files or directories, and to move or copy files. The use of shell in an input has the following form:

```
=shell

 *** System Commands ***

end
```

where *System Commands* are any UNIX or DOS command(s). This is particularly useful in tandem with the following environment variables when files not automatically returned are desired. The following example shell command copies the x16 file back alongside the output file.

```
=shell

cp x16 ${OUTBASENAME}.x16

end
```

Please note the syntax of Nix and Windows environment variables, ${VAR} and %VAR% respectively, are interchangeable, as *scalerte* and *shell* understand both.

Below are the seven primary locations known by *scalerte*:

- The user's home directory, HOME

    *Nix systems, ${HOME}, /home/uid

*Windows, %HOME%, C:\Users\uid

- The directory of SCALE, SCALE

*Nix systems, ${SCALE}, location of user's installation—typically /scale/scale#

*Windows, %SCALE%, location of user's installation—typically C:\SCALE#

- The directory of the input file, INPDIR

*Nix systems, ${INPDIR}

*Windows, %INPDIR%

- The directory of the output file, OUTDIR, which by default is the same as INPDIR, because the output file is written next to the input file

*Nix systems, ${OUTDIR}

*Windows, %OUTDIR%

- The directory from which SCALE was invoked, the return directory, RTNDIR, which is the directory your console will return to upon completion

*Nix systems, ${RTNDIR}

*Windows, %RTNDIR%

- The directory that contains the SCALE data, DATA

*Nix systems, ${DATA}

*Windows, %DATA%

- The working directory for a given input file, TMPDIR, or shorthand TMP

*Nix systems, ${TMPDIR}, ${TMP}

*Windows, %TMPDIR%, %TMP%

There are several secondary locations in the SCALE directory tree. These are as follows:

- The directory containing the platform-specific compiled programs, PGMDIR, or legacy PGM_DIR:

*Nix systems, ${PGMDIR}, ${PGM_DIR}

*Windows, %PGMDIR%, %PGM_DIR%

Lastly, there are several environment variables provided for convenience and/or that are associated with output data that can be useful.

- The directory containing the ORIGEN data files, ORIGENDIR

*Nix systems, ${ORIGENDIR}

*Windows, %ORIGENDIR%

- The base name of the input file, BASENAME, which is the name of the input file without both absolute path and extension

*Nix systems, ${BASENAME}, or ${CASE_NAME}

*Windows, %BASENAME%, or %CASE_NAME%

- The base name of the output file, OUTBASENAME, or legacy CASE_NAME, which is the name of the output file without both absolute path and extension

*Nix systems, ${OUTBASENAME}, or ${CASE_NAME}

*Windows, %OUTBASENAME%, or %CASE_NAME%

- The base name of the output file, OUTBASE, which is the absolute name of the output file without file extension

*Nix systems, ${OUTBASE}

*Windows, %OUTBASE%

- The absolute path to the input file, INPUTFILE

*Nix systems, ${INPUTFILE}

*Windows, %INPUTFILE%.

- The absolute path to the output file, OUTFILE.

*Nix systems, ${OUTFILE}

*Windows, %OUTFILE%

- The directory containing USLSTATS output, USLDIR (If USLSTATS data were output, then these data would be located in OUTDIR\OUTBASENAME.uslstats directory.)

*Nix systems, ${USLDIR}

*Windows, %USLDIR%

- The directory containing CENTRM output, CENTRMDIR (If CENTRM data were output, then these data would be located in OUTDIR\OUTBASENAME.centrmfiles directory.)

*Nix systems, $CENTRMDIR

*Windows, %CENTRMDIR%

- The directory containing XSDRNPM output, XSDRNDIR (If XSDRNPM data were output, then these data would be located in OUTDIR\OUTBASENAME.xsdrnfiles directory.)

    *Nix systems, $XSDRNDIR

    *Windows, %XSDRNDIR%

- The platform-specific file separator, FS, which is either backslash (\) on Windows, or forward slash (/) on Nix systems

    *Nix systems, ${FS}

    *Windows, %FS%

Parallel Execution Capability

SCALE 6.2 contains four modules and sequences that have distributed memory (MPI) parallelism: KENO V.a, KENO-VI, Sampler, and ORIGAMI. However, the binary executable files distributed with SCALE do not have MPI enabled. To run one of these codes in parallel, the user must first build SCALE with MPI enabled (see build instructions in this guide). Control modules like CSAS6, T6-DEPL, and TSUNAMI-3D-K6 automatically initiate the parallel version of KENO–VI in a parallel SCALE build if the user provides the required arguments as summarized below. When running a standalone code in parallel (such as KENO-VI), a "%" prefix is required on the sequence specification record in the input file (e.g., =%keno-vi). Parallel code execution is available on Linux and Mac systems but is not available on Windows PCs.

The executable binary code distributed with SCALE only enables serial calculations. If MPI parallelism is desired, then the source code must be compiled with MPI support enabled for the platform and configuration where the code will be executed in parallel. The SCALE build configuration sets some variables (*SCALEMPI*, *SCALECMDS*, and *MPIRUN*), depending on the third-party MPI package for the SCALE driver, which prepares two different execution environments with these variable sets for both serial and parallel code execution.

Executing SCALE in parallel is initiated by *scalerte* when the user provides the necessary MPI command line arguments with the two options, *–N* and *–M*, which specify the number of MPI processes and machine names, respectively. To run an input called `HelloWorld.inp` from an MPI build on SCALE on two nodes specified in the machine file *mach*, use the following command:

```
scalerte –N 2 –M mach HelloWorld.inp
```

With these options, *scalerte* sets *NTASKS* and *MACHINEFILE* variables, depending on the user request, and passes them to the SCALE driver. During the parallel code execution process, the driver invokes the MPIRUN wrapper to run the parallel functional module across MPI processes. An environment variable *MPIARGS* is available for the driver to pass some user-defined MPI options to MPIRUN wrapper.

SCALE Sample Problems

The SCALE sample problems are designed by the SCALE developers to verify the installation and functionality of SCALE relative to the expected results. Users are urged to run the sample problems to verify the proper installation of SCALE. ORNL has provided a set of reference results from each sample problem against which the results of each installation can be compared.

The sample problems are most easily run through Fulcrum by selecting *Run SCALE Verification* from the *Run* menu on the main menu bar. This will run all of the sample problems sequentially and will present any differences from the ORNL-generated results.

The SCALE runtime environment, *scalerte*, which is described in the subsequent section, has a built-in scripting interface to allow for invocation of several groupings of sample problems, including individual problems, problems for a specific module, subsets of modules, or all samples. The sample problems will print a message indicating the sample problem currently running, followed by the differences between ORNL-generated results and the newly generated results for the sample problem(s). Note that there may be up to an hour's delay before messages are printed to the console. The final message will indicate that the "Process finished with a 0 return code . . . ." If no differences or minimal differences are noted for a particular sample problem, then SCALE has been properly installed for the tested functionality.

The set of sample problems is located in the samples directory of the SCALE installation.

To run all sample problems, execute the following command:

```
scalerte @samples/samples
```

To invoke sample problems for a particular module or sequence, use

```
scalerte @samples/samples modulename
```

where *modulename* is the name of the module or sequence to test, e.g., *centrm*.

To invoke a single sample problem, do the following.

```
scalerte @samples/samples problemname
```

where *problemname* is the name of the specific sample problem to test, e.g., *centrm-pwr.inp*.

The above *modulename* and *problemname* examples can be combined and repeated to exercise sets of sample problems of interest. For example, run *csas* and *origen* sequence sample problems in addition to the *centrm-pwr.inp* sample.

```
scalerte @samples/samples csas centrm-pwr.inp origen
```

As the sample problems execute, feedback will be provided to the screen such as that shown in the example below. If no differences or only small differences are reported between the ORNL results and the currently generated results for each sample, then SCALE has been properly installed and configured for the tested functionality.

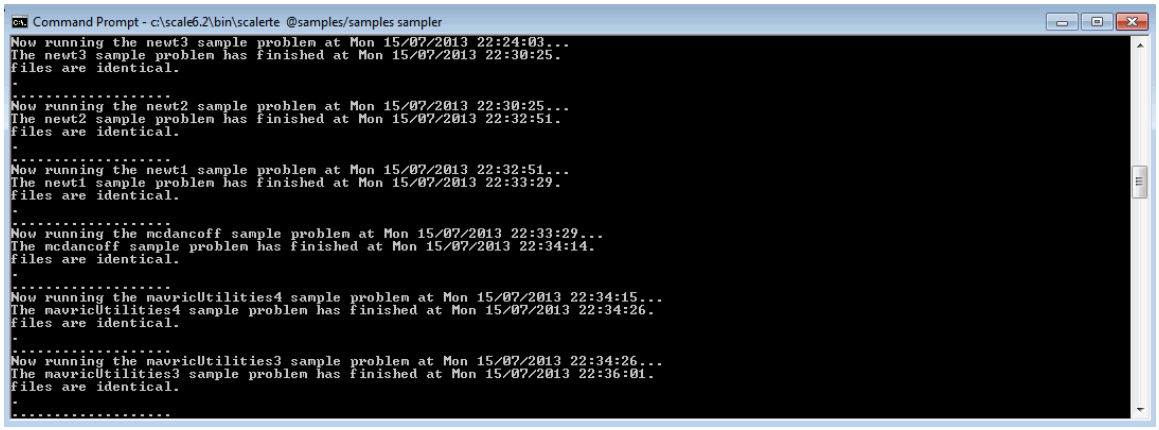

Figure 27. Sample problem output messages.

For any problems or questions, please contact scalehelp@ornl.gov.

Build Instructions

These instructions are only for those who wish to recompile their SCALE binaries. If you are running SCALE using the precompiled binary executable files distributed with SCALE, then please disregard this section.

For SCALE 6.2 and subsequent updates, the build configuration has been completely renewed relative to all previous versions. The SCALE build is now based on CMake from KitWare, which supports a consistent experience on Linux, Mac, and Windows.

Overview

There are four main steps to create and install SCALE binaries

1. Install compilers and third-party libraries (TPLs).
2. Configure CMake to generate a native build tree.
3. Compile all executables and libraries.
4. Install to deploy all executables into a configuration ready for execution.

Required Resources

SCALE requires the following programs in order to compile:

1. Fortran Compiler
    i. Windows – Intel Fortran compiler 15.0
    ii. Linux - Intel Fortran compiler 14.1+/GNU gfortran 4.8.3+ compiler
    iii. Mac OS – GNU gfortran 4.8.5+ compiler
2. C/C++ Compiler
    i. Windows – Intel C/C++ compiler 15.0.=
    ii. Linux – Intel C/C++ compiler 14.1+ / GNU g++/gcc 4.8.3+ compiler
    iii. Mac OS – GNU g++/gcc 4.8.5+ compiler
3. CMake 3.13+ - Platform independent build configuration for Linux, Darwin, and Windows

SCALE requires the following libraries, which are not distributed with SCALE:

LAPACK libraries:module
    a. lapack
    b. blas

You must modify the LAPACK variable in configure_scale_gnu.sh to point to your installation of LAPACK prior to configuration.

The following optional package is required by SCALE if MPI support is desired:

OpenMPI-1.8.1+ - Optional for SCALE build with MPI support on Linux and Mac OS (currently, SCALE does not support MPI for Windows)

Mac OSX Resources

Mac OSX does not come preloaded with the necessary resources for compiling SCALE. Macports provides a simple mechanism for retrieving almost all of the required resources necessary to compile SCALE on a Mac. This process has only been tested on Mac OSX 10.11.6.

You can download the latest macports from http://www.macports.org/. You will need XCode (free from the App Store) with commandline tools installed for macports to work.

You will need administrative privileges to install macports and the necessary resources.

Please see macports instructions for xcode installation/requirements.
http://guide.macports.org/#installing.xcode

After installing these resources, a new shell session is necessary to access the new tools.

NOTE if your rsync port is blocked by the firewall (as is the case at ORNL), you may synchronize over http by updating your */opt/local/etc/macports/sources.conf* file to change the line:

```
rsync://rsync.macports.org/release/tarballs/ports.tar [default]
```

to

```
http://www.macports.org/files/ports.tar.gz [default]
```

The following commands will install all necessary resources.

If the rsync port is blocked, use

```
$> sudo port -d sync
```

If the rsync port is open, use

```
$>sudo port selfupdate
```

Regardless of rsync status, execute the following commands:

```
$>sudo port install gcc48

$>sudo port select gcc mp-gcc48

$>sudo port install qt4-mac
```

These commands upgrade the default compilers from gcc-4.2.2 to gcc-4.8.3, and they install qt4.8.6.

CMake Configuration

CMakeLists.txt files can be found throughout SCALE. From the SCALE root directory, these CMakeLists.txt files create a tree of included directories called the SOURCE TREE. Namely, the source directories are

`packages/AmpxLib`

`XSProc`

`ScaleLib`

`etc.`

To configure a build, call cmake on the root CMakeLists.txt file, namely `scale_dir/CMakeLists.txt`. CMake takes your source tree and creates a BUILD TREE. The build tree contains or will contain the build configuration, the Make or NMake files, and all compilation output: object files, archive libraries, and binary executables.

SCALE requires several TPLs, specifically, QT and Lapack. These TPLs must be specified at the time of configuration. For ease of use, configuration scripts for every supported platform are available in the scripts directory of the source code. These scripts describe the necessary variables to define. A user's modifications to these scripts should be limited to the path to the root directories for the TPLs.

Recommended Configuration Procedure

After unpacking the source code, navigate to the root scale directory (<SCALE_SRC_ROOT>. You will see CMakeLists.txt, PackagesList.cmake, and CTestConfig.cmake. This is the root of the source tree, to which you will point CMake. This example demonstrates creating build trees for multiple configurations for your working copy.

Linux and Mac Configuration

- **Make Build Directory**

  `mkdir build`

  `mkdir -p build/intel` **this could be any directory

  or

  `mkdir -p build/gcc`

- **CMake Initialization**

  Copy the cmake script from the scripts directory to your build directory. Update the cmake script with your TPL specifications.

- Serial SCALE (without MPI support)

```
cp     <SCALE_SRC_ROOT>/script/configure_scale_gnu.sh
build/gcc

chmod u+x build/gcc/configure_scale_gnu.sh
```

- Parallel SCALE (with MPI support)

```
cp script/configure_scale_mpi.sh build/gcc

chmod u+x build/gcc/configure_scale_mpi.sh
```

- **Create Your Configuration**

  Create your configuration by pointing this script at the source tree root

```
cd build/gcc

Edit the  CMakelists.txt file in
<SCALE_SRC_ROOT>/Trilinos/packages/anasazi/src/ so as
to comment out the following lines:

ASSERT_DEFINED(Anasazi_ENABLE_ThyraEpetraAdapters)

ASSERT_DEFINED(Anasazi_ENABLE_ThyraCore)

ASSERT_DEFINED(Anasazi_ENABLE_Tpetra)
```

  Serial SCALE (without MPI support)

```
./configure_scale_gnu.sh ../..
```

  - Parallel SCALE (with MPI support)

```
./configure_scale_mpi.sh ../..
```

  /*** Configuration Output.... ***/

  **If you add or remove source files from the source tree, CMake will NOT see these modifications unless a CMake file is modified (`CMakeLists.txt`,`PackagesList.cmake`,`etc...`).

  CMake will re-evaluate the entire source tree when any CMake file has been modified. If CMake does not pick up the addition/removal of sources files, then the easiest way to update the build tree is to "touch" any CMake file in the source tree.

Windows Configuration

Instructions are not documented here. Please contact scalehelp@ornl.gov for assistance.

Compilation

Every library and executable is a TARGET. Calling make on Linux and Mac and nmake on Windows from the root of your build tree (<SCALE_SRC_ROOT>/`build/gcc` from the previous example) will build ALL targets. There are two options when building specific targets. For example, MavricUtilities contains a number of executables: mtadder, mtaverager, and so on.

You may invoke make mtadder to build mtadder alone. Alternatively, you can build it from `build/gcc`, `cd packages/MavricUtilities` and `make` to compile ALL targets in mavricUtilities.

Compilation Flags

You may modify `CMAKE_Fortran_FLAGS`, `CMAKE_C_FLAGS`, and `CMAKE_CXX_FLAGS` on the cmake command invocation line.

Installation

CMake provides the install target, which installs all binaries from the current directory down. For example, `make install`' from `build/gcc` will install any targets, which would install aim, mavric, mtadder, mtaverager, etc., while `cd packages/Mavric` and `make install` will only install targets declared in the Mavric directory.

***Note that `make install` re-evaluates the build for all dependencies. For example, package A depends on packages B and D. Package D depends on package E. Therefore, `make install` for package A would result in packages E, D, and B being re-evaluated and rebuilt if necessary. Thus, if you know you want to build and install, you can save time building by simply doing a `make install`. An alternative is make install/fast, which will skip the dependency checking and will only execute the install operations.

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