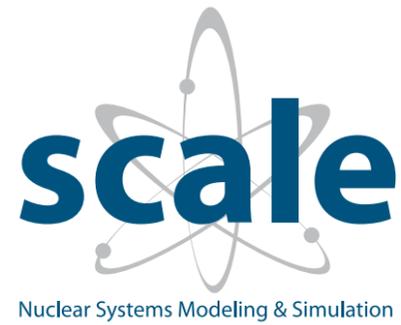


Nuclear Systems Modeling & Simulation

FISCAL YEAR 2016 REPORT ON SCALE
MAINTENANCE AND DEVELOPMENT



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MISSION STATEMENT

Develop, deploy, and support a quality-assured computational toolkit that advances the state of the art and exemplifies ease of use in a scalable architecture beginning with fundamental physical data and providing research, production, and licensing calculations for current and emerging nuclear modeling and simulation needs.



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MANAGER STATEMENT

The SCALE team is pleased to present this annual report documenting the development, maintenance, distribution, and training accomplishments from fiscal year 2016 (FY16). This year brought the release of SCALE 6.2, an important milestone in the evolution from the established infrastructure of SCALE 6.1 to an integrated, efficient infrastructure that will move SCALE into the future to the fully modernized, parallelized SCALE 7.

SCALE 6.2 is the culmination of a 5-year \$20 million investment. In this work, the SCALE team looked holistically at all aspects of the code system, ranging from the fundamental nuclear data to the interactive user interfaces. For the first time in SCALE's 40-year development history, the internal workings of the computational sequences and the fundamental binary data formats were reworked. The success of this major initiative depended on the creation of an automated development and testing system in which the impacts on trusted results from the massive internal updates to all aspects of the code could be quantified on an hourly basis on all supported platforms.

Having a sound testing infrastructure and modernized foundational components to improve efficiency and minimize redundancy enabled the team to introduce the wide variety of innovative features listed later in this report. Some highlights include the Polaris tool for simple and efficient light water reactor (LWR) lattice physics analysis, the Sampler tool for stochastic uncertainty quantification, the ORIGAMI tool for 2D and 3D spent fuel source term generation, parallel computing capabilities in KENO, and greatly enhanced continuous energy (CE) Monte Carlo features including criticality safety, radiation shielding, sensitivity/uncertainty analysis, and depletion, all with user-specified temperature corrections generated at runtime. SCALE 6.2 also includes the AMPX tools to generate multigroup (MG) and CE cross section libraries, the first release of AMPX since 1992.

In addition to integrating these innovative features, a deep review was performed on many existing features to improve their accuracy, efficiency, and usability. Some highlights of these improvements include minimizing of historical biases for MG calculations for LWR systems; holistic review of continuous-energy physics and nuclear data with substantial gains in accuracy and efficiency over SCALE 6.1; faster lattice physics calculations with TRITON, realizing an average speedup of 4x, and in with some cases running 30x faster than SCALE 6.1; extension of the maximum number of materials in a model from ~2,000 to ~2 billion; as well as many more enhancements too numerous to list here.

In a bold step to enhance the SCALE user experience, eight user interfaces from SCALE 6.1 were replaced with the new Fulcrum user interface. Fulcrum introduces several new concepts as an integrated user interface for nuclear analysis, building on decades of experience from thousands of users. Fulcrum is a cross-platform graphical user interface (GUI) designed to create, edit, validate, and visualize input, output, and data files. While the transition away from the familiar GeeWiz interface may seem like a significant change, the experiences with Fulcrum have been far superior for users in training classes and tutorial sessions.

The entire SCALE team is pleased to present SCALE 6.2, which we hope you will find to be innovative, accurate, efficient, and easy to use.

Sincerely,

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Consortium for the Advanced Simulation of LWRs



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Shanghai Institute of Applied Physics, Chinese Academy of Sciences

ACRONYMS

- 1D = one-dimensional
- 2D = two-dimensional
- 3D = three-dimensional
- AEC = US Atomic Energy Commission
- API = application programming interface
- ASME = American Society of Mechanical Engineers
- CADIS = Consistent Adjoint Driven Importance Sampling
- CAS = Chinese Academy of Sciences
- CASL = Consortium for Advanced Simulation of Light Water Reactors
- CE = continuous energy
- CSAS = criticality safety analysis sequence
- DOE = US Department of Energy
- DSA = Division of Systems Analysis
- DSFM = Division of Spent Fuel Management
- ENDF = evaluated nuclear data file
- ESC = extended step characteristic
- ExSITE = Extensible SCALE Intelligent Text Editor
- FHR = fluoride salt-cooled high-temperature reactor
- FSCB = Fuel and Source Term Code Development Branch
- FW-CADIS = Forwarded-Weighted CADIS
- FY16 = fiscal year 2016
- GLLS = generalized linear least-squares
- GUI = graphical user interface
- HIVE = Hierarchical Input Validation Engine
- JEFF = joint evaluated fission and fusion file
- KMART = KENO Module for Activity-Reaction Rate Tabulation
- LDRD = Laboratory Directed Research and Development
- LWR = light water reactor
- MAVRIC = Monaco with Automated Variance Reduction Using Importance Calculations
- MCDancoff = Monte Carlo Dancoff
- MCNP = Monte Carlo N-Particle
- MEPhI = Moscow Engineering Physics Institute
- MG = multigroup
- MSR = molten salt reactor
- NA-22 = Office of Defense Nuclear Nonproliferation
- NCSP = Nuclear Criticality Safety Program
- NE = Office of Nuclear Energy
- NEA = Nuclear Energy Agency
- NEAMS = Nuclear Energy Advanced Modeling and Simulation
- NEWT = New ESC-Based Weighting Transport
- NNSA = National Nuclear Security Administration
- NRC = US Nuclear Regulatory Commission
- OECD = Organisation for Economic Cooperation and Development
- ORIGAMI = ORIGEN Assembly Isotopics
- ORIGEN = Oak Ridge Isotope Generation
- ORNL = Oak Ridge National Laboratory
- PCP = packaging certification program
- QA = quality assurance
- RES = Office of Nuclear Regulatory Research
- RIST = Research Organization for Information
- RNSD = Reactor and Nuclear Systems Division Science and Technology
- RSICC = Radiation Safety Information Computational Center
- SAMS = Sensitivity Analysis Module for SCALE
- SCALE = Standardized Computer Analyses for Licensing Evaluation
- SDF = sensitivity data file
- SFR = sodium-cooled fast reactor
- SINAP = Shanghai Institute of Applied Physics
- STARBUCS = Standardized Analysis of Reactivity for Burnup Credit Using SCALE
- S/U = sensitivity and uncertainty
- TCF = Technology Commercialization Fund
- TRITON = Transport Rigor Implemented with Time-Dependent Operation for Neutronic Depletion
- TSAR = Tool for Sensitivity Analysis of Reactivity Responses
- TSUNAMI-IP = TSUNAMI Indices and Parameters
- TSURFER = Tool for S/U Analysis of Response Functions Using Experimental Results
- USLSTATS = Upper Subcritical Limit Statistical Software
- VIBE = Validation, Interpretation, and Bias Estimation
- XSPProc = cross section processing



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 the 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 three deterministic solvers and three Monte Carlo radiation transport solvers selected based on the user's 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 GUIs assist with accurate system modeling and convenient access to desired results.

This report summarizes the capabilities of SCALE 6.2, as well as the maintenance and development activities performed during fiscal year 2016 (FY16). The current public version of SCALE is 6.2.1, which was released in July 2016, following the release of SCALE 6.2 in April 2016.

BACKGROUND

The history of the SCALE code system dates to 1969, when ORNL began providing the transportation package certification staff at the US Atomic Energy Commission (AEC) with computational support in the use of the new KENO code. KENO was used to perform criticality safety assessments with the statistical Monte Carlo method. From 1969 to 1976, the AEC certification staff relied on ORNL personnel to assist them in the correct use of codes and data for criticality, shielding, and heat transfer analysis of transportation packages. However, the certification staff learned that users had difficulty in becoming proficient in performing the calculations often needed for an independent safety review. Thus, shortly after the certification staff was moved to the US Nuclear Regulatory Commission (NRC), the NRC proposed development of an easy-to-use analysis system that provided the technical capabilities of the individual modules with which they were familiar. With this proposal, the concept of SCALE as a comprehensive modeling and simulation suite for nuclear safety analysis and design was born.

The NRC staff provided ORNL with some general development criteria for SCALE: (1) focus on applications related to nuclear fuel facilities and package designs, (2) use well-established computer codes and data libraries, (3) design an input format for the occasional or novice user, (4) prepare standard analysis sequences (control modules) to automate the use of multiple codes (functional modules) and data to perform a system analysis, and (5) provide complete documentation and public availability. With these criteria, the ORNL staff laid out the framework for the SCALE system and began development efforts. The initial version of SCALE (Version 0) was distributed in July 1980. Although the capabilities of the system continue to evolve, the philosophy established with the initial release still serves as the foundation of this year's SCALE 6.2 release, more than 35 years later.

SCALE RELEASES

Year	Version	RSICC ID	Year	Version	RSICC ID
1980	0	CCC-288	1998	4.4	CCC-545
1981	1	CCC-424	2000	4.4a	CCC-545
1983	2	CCC-450	2004	5	CCC-725
1985	3	CCC-466	2006	5.1	CCC-732
1990	4	CCC 545	2009	6	CCC-750
1992	4.1	CCC-545	2011	6.1	CCC-785
1994	4.2	CCC-545	2016	6.2	CCC-834
1996	4.3	CCC-545			



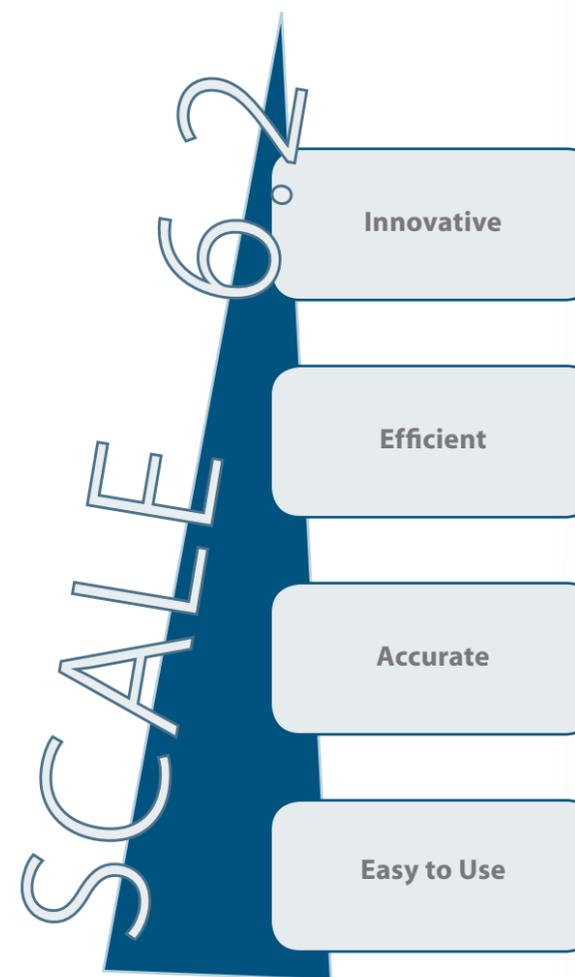
SCALE 6.2

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:

- ENDF/B-VII.1 nuclear data libraries CE and MG with enhanced group structures
- Neutron covariance data based on evaluated nuclear data file (ENDF)/B-VII.1 and supplemented with ORNL data
- Covariance data for fission product yields and decay constants
- Stochastic uncertainty and correlation quantification for any SCALE sequence with Sampler
- Parallel calculations with KENO
- Problem-dependent temperature corrections for CE calculations
- CE shielding and criticality accident alarm system analysis with Monaco with Automated Variance Reduction Using Importance Calculations (MAVRIC)
- CE Monte Carlo depletion with Transport Rigor Implemented with Time-Dependent Operation for Neutronic Depletion (TRITON)
- CE sensitivity/uncertainty analysis with TSUNAMI-3D
- Simplified and efficient LWR lattice physics with Polaris
- Simplified spent fuel characterization with Oak Ridge Isotope Generation (ORIGEN) Assembly Isotopics (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
- 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 cross section processing (XSProc) integrated into most sequences
- Accelerated calculations with TRITON (generally 4x 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
- Numerous other enhancements for improved usability and stability

The user documentation for SCALE has also been substantially updated and reorganized around capabilities instead of being divided into function modules, control modules, etc.



CAPABILITIES OF SCALE

A primary goal of SCALE is to provide robust calculations while reducing requirements for user input and knowledge of the intricacies of the underlying code and data architecture. SCALE provides standardized sequences to integrate many modern, advanced capabilities into a seamless calculation that the user controls from a single input file. Additional utility modules are provided primarily for post processing data generated from the analysis sequences for advanced studies. Input for SCALE sequences is provided in the form of text files using free-form input with extensive use of keywords and engineering-type input requirements. A GUI is provided to assist in the creation of input files, visualization of geometry and nuclear data, execution of calculations, viewing output, and visualization of results. An overview of the major SCALE capabilities and the analysis areas they serve is provided in Table 1, with additional descriptions provided below.

Table 1. Summary of major SCALE capabilities

Analysis area	Modules/libraries	Analysis function(s)
Criticality safety	Criticality Safety Analysis Sequence (CSAS)5/CSAS6	Three-dimensional (3D) MG and CE eigenvalue Monte Carlo analysis and criticality search capability
	Standardized Analysis of Reactivity for Burnup Credit Using SCALE (STARBUCS)	Burnup credit analysis using 3D Monte Carlo
	Sourcerer	Hybrid 3D deterministic/Monte Carlo analysis with optimized fission source distribution
Reactor physics	TRITON	One-dimensional (1D) and two-dimensional (2D) general purpose lattice physics depletion calculations and generation of few-group cross section data for use in nodal core simulators 3D MG and CE Monte Carlo depletion analysis 2D eigenvalue and reaction rate sensitivity analysis
	Polaris	2D streamlined LWR lattice physics depletion calculations and generation of few-group cross section data for use in nodal core simulators
Radiation shielding	MAVRIC	3D CE and MG fixed-source Monte Carlo analysis with automated variance reduction
Activation, depletion and decay	ORIGEN	General purpose point depletion and decay code to calculate isotopic concentrations, decay heat, radiation source terms, and curie levels
	ORIGAMI	Simulated 2D and 3D analysis for LWR spent fuel assemblies (isotopic activation, depletion, and decay for LWR fuel assemblies)
	ORIGEN reactor libraries	Pregenerated burnup libraries for a variety of fuel assemblies for commercial and research reactors
Sensitivity and uncertainty analysis	TSUNAMI	1D and 2D MG eigenvalue and reaction rate sensitivity analysis 3D MG and CE eigenvalue and reaction rate sensitivity analysis Determination of experiment applicability and biases for use in code and data validation
	Sampler	Stochastic uncertainty quantification in results based on uncertainties in nuclear data and input parameters

Analysis area	Modules/libraries	Analysis function(s)
Material specification and cross section processing	XSPROC	Temperature correction, resonance self-shielding, and flux weighting to provide problem-dependent microscopic and macroscopic MG cross section data integrated with computational sequences; also available for stand-alone analysis
	Standard composition library	Library used throughout SCALE that provides individual nuclides; elements with tabulated natural abundances; compounds, alloys, mixtures, and fissile solutions commonly encountered in engineering practice
	Monte Carlo Dancoff (MCDancoff)	3D Monte Carlo calculation of Dancoff factors
Monte Carlo transport	KENO V.a/ KENO-VI	Eigenvalue Monte Carlo codes applied in many computational sequences for MG and CE neutronics analysis
	Monaco	Fixed source Monte Carlo code applied in the MAVRIC sequence for MG and CE analysis
Deterministic transport	XSDRNPM	1D discrete ordinates transport applied for neutron, gamma, and coupled neutron/gamma analysis
	New ESC-Based Weighting Transport (NEWT)	2D extended step characteristic (ESC) transport with flexible geometry applied to neutronics analysis, especially within the TRITON sequences
	Denovo	3D Cartesian geometry discrete ordinates transport applied for neutron, gamma, and coupled neutron/gamma analysis, especially to generate biasing parameters within the MAVRIC and Sourcerer sequences (not generally run as stand-alone code in SCALE)
Nuclear Data	Cross section data	Recent neutron, gamma and coupled neutron/gamma nuclear data libraries in CE and several MG structures for use in all transport modules
	ORIGEN data	Recent nuclear decay data, neutron reaction cross sections, energy-dependent neutron-induced fission product yields, delayed gamma ray emission data, neutron emission data, and photon yield data
	Covariance data	Recent uncertainties in nuclear data for neutron interaction, fission product yields, and decay data for use in TSUNAMI tools and Sampler
Utilities	Various	Numerous pre- and post-processing utilities for data introspection and format conversion

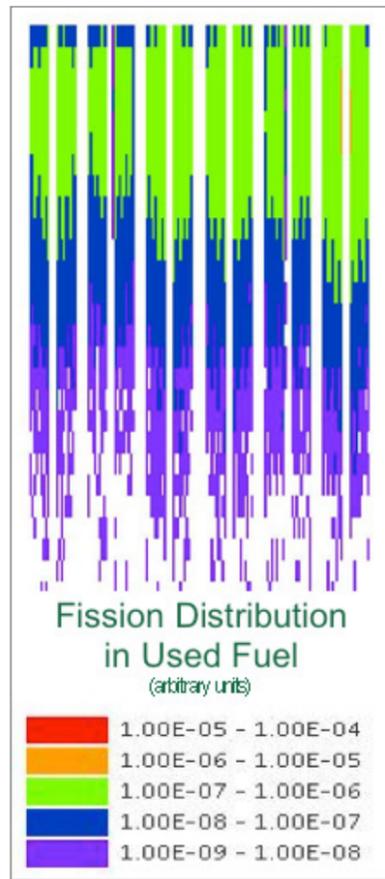
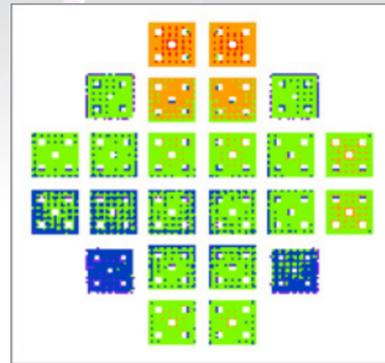


Fig. 1. As-loaded used fuel cask.

Criticality Safety

SCALE provides a suite of computational tools for criticality safety analysis that is primarily based on the KENO Monte Carlo codes for eigenvalue neutronics calculations. Two variants of KENO provide identical solution capabilities with different geometry packages. KENO V.a uses a simple, efficient geometry package sufficient for modeling many systems of interest to criticality safety and reactor physics analysts. KENO-VI uses the SCALE Generalized Geometry Package, which provides a quadratic-based geometry system with much greater flexibility in problem modeling but with slower runtimes. Both versions of KENO perform eigenvalue calculations for neutron transport primarily to calculate multiplication factors (k_{eff}) and flux distributions of fissile systems in CE and MG modes and are typically accessed through Criticality Safety Analysis Sequence with KENO V.a (CSAS5) and Criticality Safety Analysis Sequence with KENO-VI (CSAS6). The CSAS sequences implement XSPROC to process material input, and they provide a temperature- and resonance-corrected cross section library based on the physical characteristics of the problem being analyzed. If a CE cross section library is specified, no resonance processing is needed, and the CE cross sections are used directly in KENO, with temperature corrections provided as the cross sections are loaded.

A search capability is available with CSAS5 to find desired values of k_{eff} as a function of dimensions or densities. The two basic search options offered are (1) an optimum search seeking a maximum or minimum value of k_{eff} and (2) a critical search seeking a fixed value of k_{eff} . For CE calculations, reaction rate tallies can be requested within the CSAS input, and for MG calculations, reaction rate calculations are performed using the KENO Module for Activity-Reaction Rate Tabulation (KMART) post-processing tools. A conversion tool is provided to up-convert KENO V.a input to KENO-VI either as a direct KENO input K5toK6, or more commonly, as a CSAS sequence C5toC6.

STARBUCS performs criticality calculations for spent fuel systems employing burnup credit. STARBUCS automates the criticality safety analysis of spent fuel configurations by coupling the depletion and criticality aspects of the analysis, thereby eliminating the need to manually process the spent fuel nuclide compositions into a format compatible with criticality safety codes. For burnup loading curve iterative calculations, STARBUCS employs the search algorithm from CSAS5 to determine initial fuel enrichments that satisfy a convergence criterion for the calculated k_{eff} value of the spent fuel configuration.

The Sourcerer sequence applies the Denovo discrete ordinates code to generate the starting fission source distribution (Fig. 1) in a KENO Monte Carlo calculation. This sequence is especially applied to burnup credit transportation and storage analysis of as-loaded canister of used fuel (Fig. 2).



Fig. 2. Used fuel storage/ transportation cask.

Reactor Physics

The TRITON control module provides flexible capabilities to meet the challenges of modern reactor designs by providing 1D pin-cell depletion capabilities using XSDRNP, 2D lattice physics capabilities using the NEWT flexible mesh discrete ordinates code, or 3D Monte Carlo depletion using KENO V.a or KENO-VI, including CE treatment with problem-dependent temperature corrections (Fig. 3). For MG analysis, TRITON implements XSPROC to process material input and to provide a temperature- and resonance-corrected cross section library. TRITON allows users to enter Dancoff factors to account for nonuniform lattices. In all cases, ORIGEN is implemented for depletion and decay calculations. Additionally, TRITON can produce assembly-averaged few group cross sections for use in core simulators.

Polaris is an optimized tool that produces assembly-averaged few group cross sections for LWR analysis with core simulators. Polaris provides simplified input; only a few lines are required to describe the entire model. Polaris uses an MG self-shielding method called the Embedded Self-Shielding Method (ESSM) and a Method-of-Characteristics (MoC) transport solver. The ESSM approach computes MG self-shielded cross sections using Bondarenko interpolation. The background cross section used in the interpolation is determined by a series of 2D MoC fixed-source calculations similar to the subgroup method that does not require explicit unit cell input data. Additionally, heterogeneous lattices are explicitly treated without the need to externally compute Dancoff factors. Like TRITON, Polaris implements ORIGEN for depletion and decay calculations (Fig. 4).

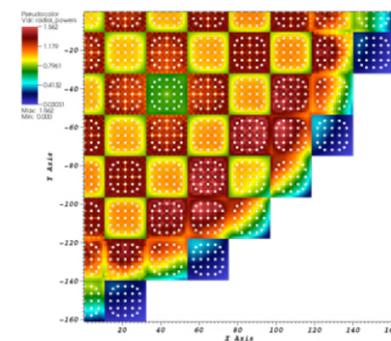
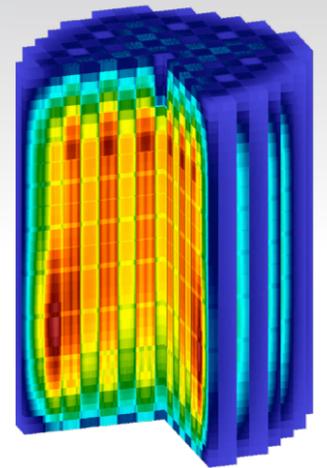


Fig. 3. Reference CE Monte Carlo power distribution for AP-1000 reactor.

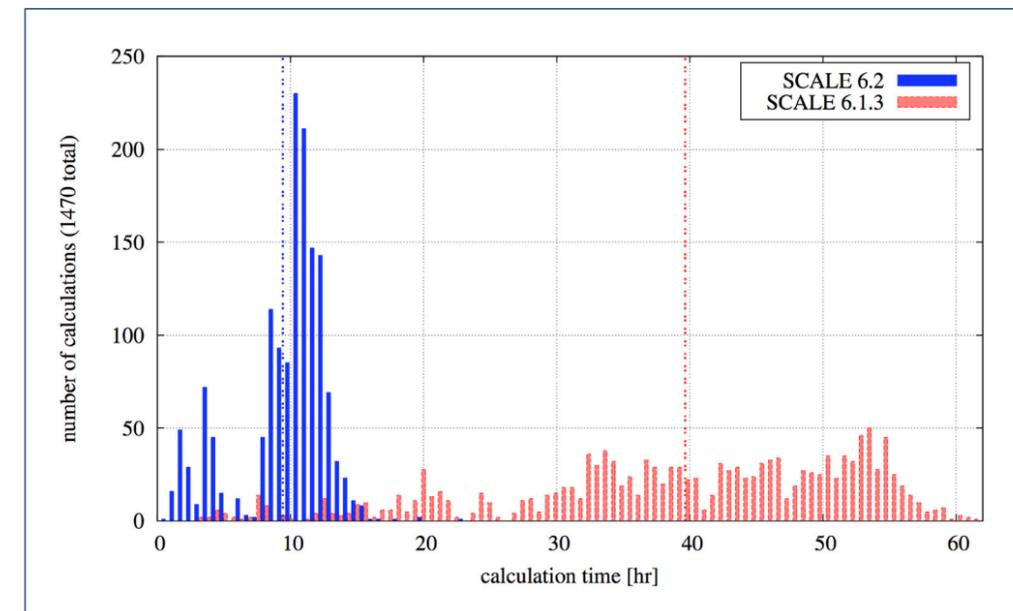


Fig. 4. TRITON runtimes for 1,470 depletion calculations.

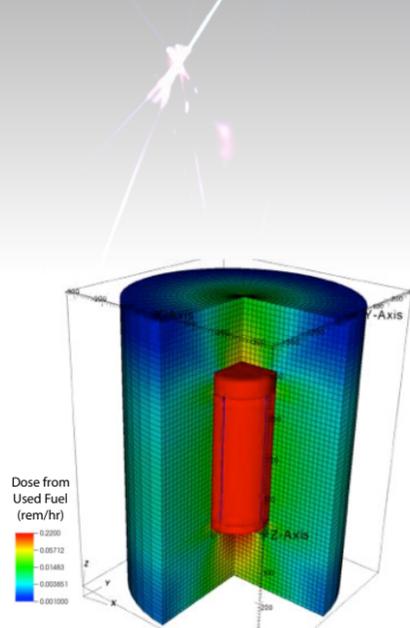


Fig. 5. Dose rate for spent nuclear fuel transportation package.

Radiation Shielding

The MAVRIC fixed-source radiation transport sequence is designed to apply the MG and CE fixed-source Monte Carlo code, Monaco, to solve problems too challenging for standard, unbiased Monte Carlo methods. The intention of the sequence is to calculate fluxes and dose rates with low uncertainties in reasonable times, even for deep penetration problems (Fig. 5). MAVRIC is based on the Consistent Adjoint Driven Importance Sampling (CADIS) methodology, which uses an importance map and a biased source that are derived to work together. MAVRIC generates problem-dependent cross section data, and then it automatically performs a coarse mesh 3D discrete ordinates transport calculation using Denovo to determine the adjoint flux as a function of position and energy and to apply the information to optimize the shielding calculation in Monaco. In the Forward-Weighted CADIS (FW-CADIS) methodology, an additional Denovo calculation is performed to further optimize the Monaco model to obtain uniform uncertainties for multiple tally locations. Several utility modules are also provided for data introspection and conversion.

Activation, Depletion, and Decay

The ORIGEN code calculates time-dependent concentrations, activities, and radiation source terms for a large number of isotopes simultaneously generated or depleted by neutron transmutation, fission, and radioactive decay. Provisions are made to include continuous nuclide feed rates and continuous chemical removal rates that can be described with rate constants for application to reprocessing or other systems that involve nuclide removal or feed. ORIGEN has the ability to use MG cross sections processed from standard ENDF/B evaluations. Within SCALE, transport codes can be used to model user-defined systems, and the COUPLE code can be applied to calculate problem-dependent neutron-spectrum-weighted cross sections representative of conditions within any given reactor or fuel assembly. COUPLE then converts these cross sections into a library to be used by ORIGEN. Time-dependent cross section libraries can be produced to reflect fuel composition variations during irradiation. An alternative sequence for depletion/decay calculations is ORIGEN-ARP, which interpolates pregenerated ORIGEN cross section libraries versus enrichment, burnup, and moderator density.

ORIGAMI computes detailed isotopic compositions for LWR assemblies containing UO_2 fuel by using the ORIGEN code with pregenerated ORIGEN libraries for a specified assembly power distribution. The assembly may be represented by a single lumped model with only an axial power distribution or by a square array of fuel pins with variable pin powers, as well as an axial distribution. Multiple cycles with varying burn times and down times may be used. ORIGAMI produces files containing SCALE and Monte Carlo N-Particle (MCNP) composition input for material in the burnup distribution, files containing decay heat for use in thermal analysis, and an energy-dependent radioactive source for use in shielding calculations (Fig. 6).

A series of pregenerated burnup libraries for use in ORIGEN and ORIGAMI are provided with SCALE for 61 different fuel assembly designs for commercial and research reactors.

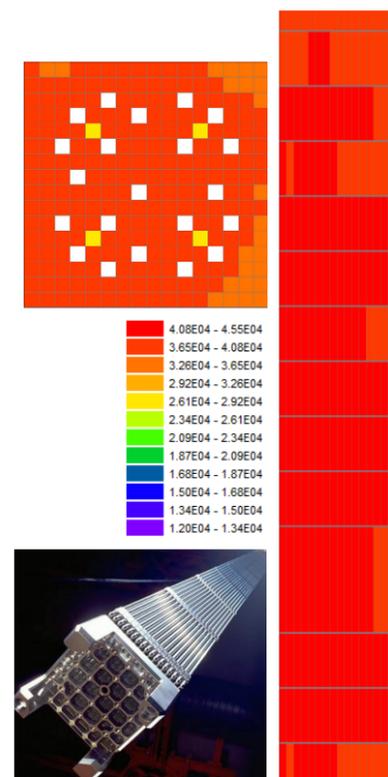


Fig. 6. Pin-by-pin burnup and radioactive source terms.

Sensitivity and Uncertainty Analysis

SCALE provides a suite of computational tools for sensitivity and uncertainty analysis to (1) identify important processes in safety analysis and design, (2) provide a quantifiable basis for neutronics validation for criticality safety and reactor physics analysis based on similarity assessment, and (3) quantify the effects of uncertainties in nuclear data and physical parameters for safety analysis.

The TSUNAMI-1D, TSUNAMI-2D and TSUNAMI-3D analysis sequences compute the sensitivity of k_{eff} and reaction rates to energy-dependent cross section data for each reaction of each nuclide in a system model (Fig. 7). The 1D transport calculations are performed with XSDRNPM, the 2D transport calculations are performed using NEWT, and the 3D calculations are performed with KENO V.a or KENO-VI. The Monte Carlo capabilities of TSUNAMI-3D provide for sensitivity and uncertainty (S/U) analysis from either CE or MG neutron transport, where the deterministic capabilities of TSUNAMI-1D and TSUNAMI-2D only operate in MG mode. The Sensitivity Analysis Module for SCALE (SAMS) is applied within each analysis sequence to provide the requested S/U data. Whether performing a CE or MG calculation, energy-dependent sensitivity data are stored in group form in a sensitivity data file (SDF) for subsequent analysis. These sequences use the energy-dependent cross section covariance data to compute the uncertainty in the response value due to the cross section covariance data.

The Tool for Sensitivity Analysis of Reactivity Responses (TSAR) computes the sensitivity of the reactivity change between two k_{eff} calculations using SDFs from TSUNAMI-1D, TSUNAMI-2D, and/or TSUNAMI-3D. TSAR also computes the uncertainty in the reactivity difference due to the cross section covariance data.

TSUNAMI Indices and Parameters (TSUNAMI-IP) computes correlation coefficients that determine the amount of shared uncertainty between each target application and each benchmark experiment considered in the analysis (Fig. 8). TSUNAMI-IP offers a wide range of options for more detailed assessment of system-to-system similarity. TSUNAMI-IP can generate input for the Upper Subcritical Limit Statistical Software (USLSTATS) trending analysis and can compute a penalty or the additional margin needed for the gap analysis.

Tool for S/U Analysis of Response Functions Using Experimental Results (TSURFER) is a bias and bias uncertainty prediction tool that implements the generalized linear least-squares (GLLS) approach to data assimilation and cross section data adjustment that also uses the SDFs generated from TSUNAMI-1D, -2D, -3D, or TSAR. The data adjustments produced by TSURFER are not used to produce adjusted cross section data libraries for subsequent use; rather, they are used only to predict biases in application systems.

The GUI Extensible SCALE Intelligent Text Editor (ExSITE) facilitates analysis with TSUNAMI-IP, TSURFER, TSAR, and USLSTATS. The Validation, Interpretation, and Bias Estimation (VIBE) interface is applied to examine SDF files, create sets of benchmark experiments for subsequent analysis, and gather additional information about each benchmark experiment.

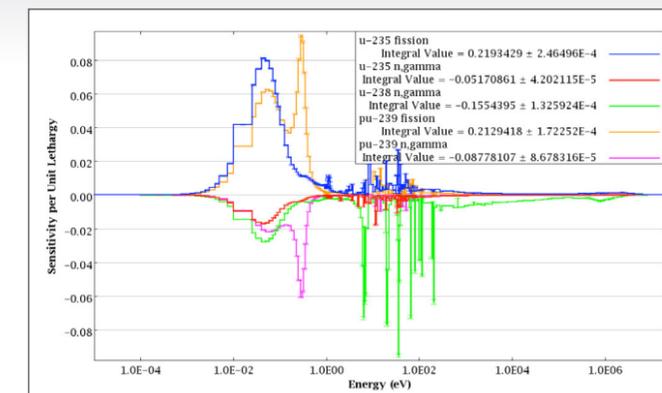


Fig. 7. Sensitivity of k_{eff} to cross section data.

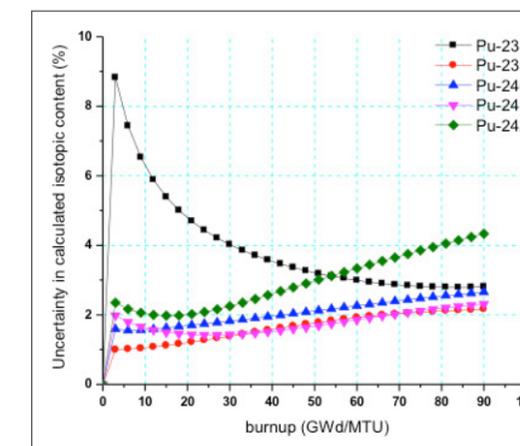


Fig. 8. Uncertainty in plutonium isotopes in LWR in depletion.

Sampler is a super-sequence that performs general uncertainty analysis by stochastically sampling uncertain parameters that can be applied to any type of SCALE calculation, propagating uncertainties throughout a computational sequence. Sampler treats uncertainties from two sources: (1) nuclear data and (2) input parameters. Sampler generates the uncertainty in any result generated by any computational sequence through stochastic means by repeating numerous passes through the computational sequence, each with a randomly perturbed sample of the requested uncertain quantities.

Material Specification and Cross Section Processing

Cross section Processing (XSProc) provides material input and MG cross section preparation for most SCALE sequences. XSProc allows users to specify problem materials using easily remembered, easily recognizable keywords associated with mixtures, elements, nuclides, and fissile solutions provided in the SCALE Standard Composition Library. For MG calculations, XSProc provides cross section temperature correction and resonance self-shielding, as well as energy group collapse and spatial homogenization for systems that can be represented in unit cell input data as infinite media, finite 1D systems, or repeating structures of 1D systems such as uniform arrays of fuel units. Improved resonance self-shielding treatment for nonuniform lattices can be achieved through the use the MCDancoff code that generates Dancoff factors for generalized 3D geometries for subsequent use in XSProc. Cross sections are generated on a microscopic and/or macroscopic basis as needed. Although XSProc is most often used as part of an integrated sequence, it can be run without subsequent calculations to generate problem-dependent MG data for use in other tools.

Nuclear Data

The cross section data provided with SCALE include comprehensive CE neutron and coupled neutron-gamma data based on ENDF/B-VII.0 and ENDF/B-VII.1. These data have been generated with the AMPX codes (Fig. 9). The MG data are provided in several energy-group structures optimized for different application areas, including criticality safety, lattice physics, and shielding analysis. The comprehensive ORIGEN data libraries are based on ENDF/B-VII.1 and recent joint evaluated fission and fusion file (JEFF) evaluations, and they include nuclear decay data, neutron reaction cross sections, neutron-induced fission product yields, delayed gamma ray emission data, and neutron emission data for over 2,200 nuclides. The photon yield data libraries are based on the most recent ENDF nuclear structure evaluations. The libraries used by ORIGEN can be coupled directly with detailed, problem-dependent physics calculations to obtain self-shielded, problem-dependent cross sections based on the most recent evaluations. There are no limitations with regard to compositions or energy spectra. SCALE also contains a comprehensive library of neutron cross section covariance data for neutron interactions, fission product yields, and decay data for use in sensitivity and uncertainty analysis with the TSUNAMI codes and Sampler.

The full suite of AMPX codes for generating MG and CE neutron, gamma, and coupled neutron/gamma libraries and covariance data are also included in the SCALE distribution, allowing users to create their own nuclear data libraries using differing sources of data and energy group structures than those provided with SCALE.

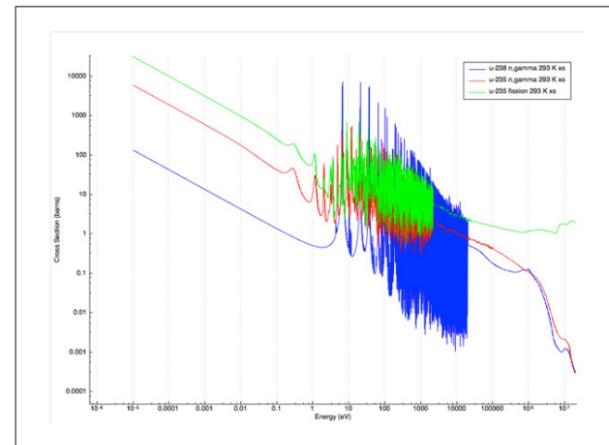


Fig. 9. Nuclear data generated with AMPX.

Graphical User Interfaces

Fulcrum is a cross platform GUI designed to create, edit, validate and visualize SCALE input, output, and data files (Fig. 10). SCALE has provided several special purpose GUIs which operate only on specific platforms and are loosely integrated with SCALE's computational and data components. Fulcrum 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.

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 data plotting from most SCALE file formats. An error checking parser interactively identifies poorly constructed input with spelling errors or data entry omissions for all SCALE sequences. The Hierarchical Input Validation Engine (HIVE) will identify allowed data ranges and interdependencies in the input and report inconsistencies to the user. Fulcrum will interactively process standard composition data to produce a mixing table, list expanded input aliases for review, provide an internal list of input as is required for Sampler material and geometry perturbation analysis, and launch the SCALE sample problems. The layout of panels in Fulcrum is highly configurable to accommodate user preferences.

ORIGAMI Automator, a GUI integrated with Fulcrum, facilitates the quantification of isotopics as a function of time for a large set of fuel assemblies, such as the complete inventory of a spent fuel pool. This tool was developed to support the NRC in severe accident analyses, but it can be adapted to many other uses.

Additional user interfaces include the KENO3D interactive visualization program for Windows for solid-body rendering of KENO geometry models, as well as the previously mentioned ExSITE and VIBE interfaces for sensitivity and uncertainty analysis. Several codes provide HTML-formatted output, in addition to the standard text output, to allow for convenient navigation using most common web browsers through the computed results with interactive color-coded output and integrated data visualization tools.

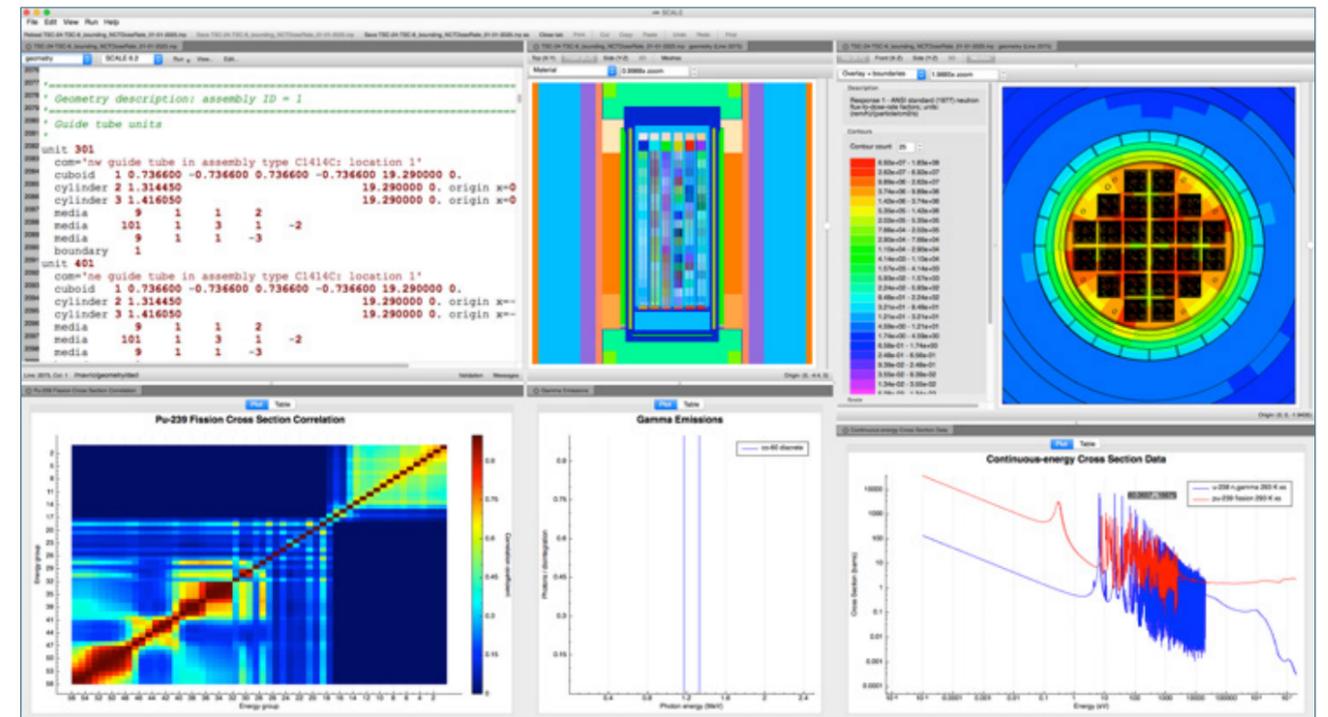


Fig. 10. Fulcrum GUI.

DISTRIBUTION

The SCALE code system continues to provide capabilities for the analysis needs of the multi-agency programs that support SCALE. Additionally, the system continues to grow in popularity with domestic and international users with nearly 4,500 licenses issued for SCALE 6.1 through September 2016, with over 3,600 of the licenses issued to new users who had not previously licensed any version of SCALE, marking considerable growth for this tool (Fig. 11). SCALE 6.2 was released in April 2016. Through September 2016, the end of this reporting period, over 900 licenses were issued, including nearly 300 to users who had never licensed any version of SCALE before. At the end of FY16, there are over 7,500 individuals in 56 nations licensed for one or more versions of SCALE (Fig. 12).

The distribution of SCALE to end-users is subject to US export control regulations, and each user must be individually licensed through an authorized distribution center. SCALE licenses are primarily issued through the Radiation Safety Information Computational Center (RSICC) at ORNL, with mirrors at the Organisation for Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA) Data Bank in France and the Research Organization for Information Science and Technology (RIST) in Japan. Any license fees collected for the distribution of SCALE are retained by these organizations to offset the costs of background checks and media duplication, and no part of the license revenue is used to support SCALE activities. RSICC's current license recovery fee is \$150, or \$650 per user, depending on the level of export control review required. The fee is waived for all requests from US universities. The fee is waived for users supported by the Nuclear Criticality Safety Program (NCSP) or users who are performing nuclear criticality safety work with SCALE.

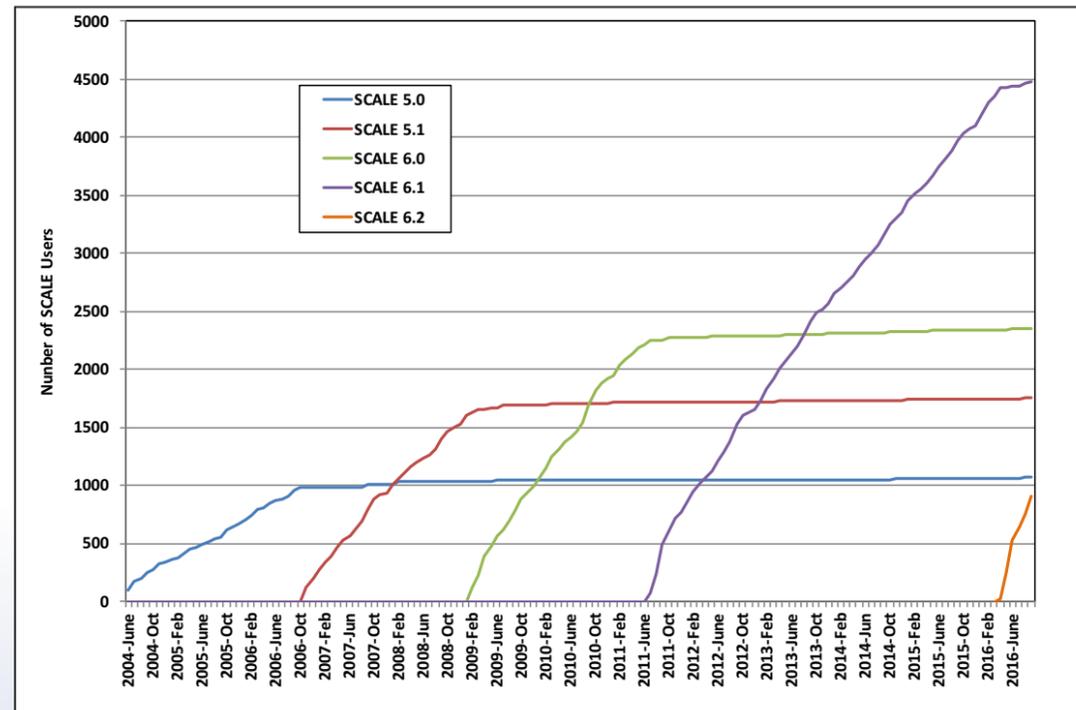


Fig. 11. Number of SCALE licenses issued for SCALE 5.0–6.2.

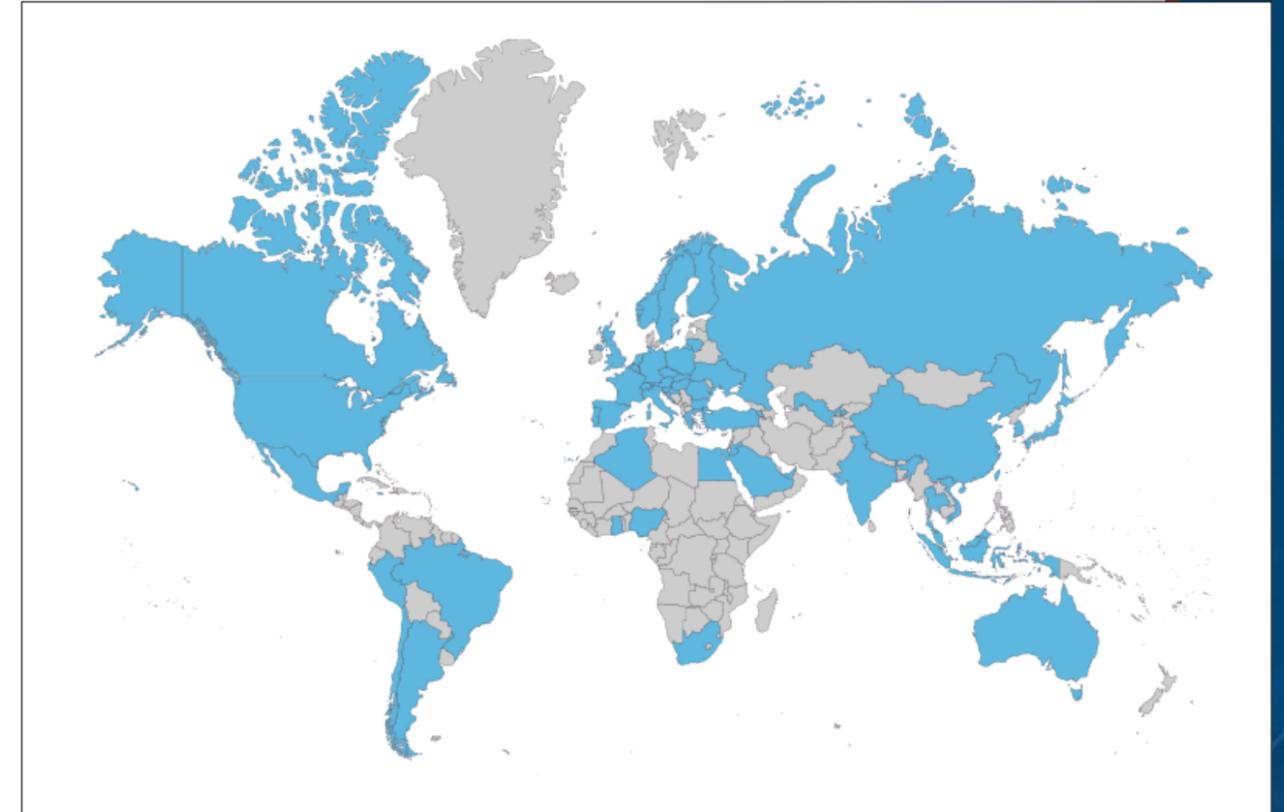


Fig. 12. Nations with licensed SCALE users.

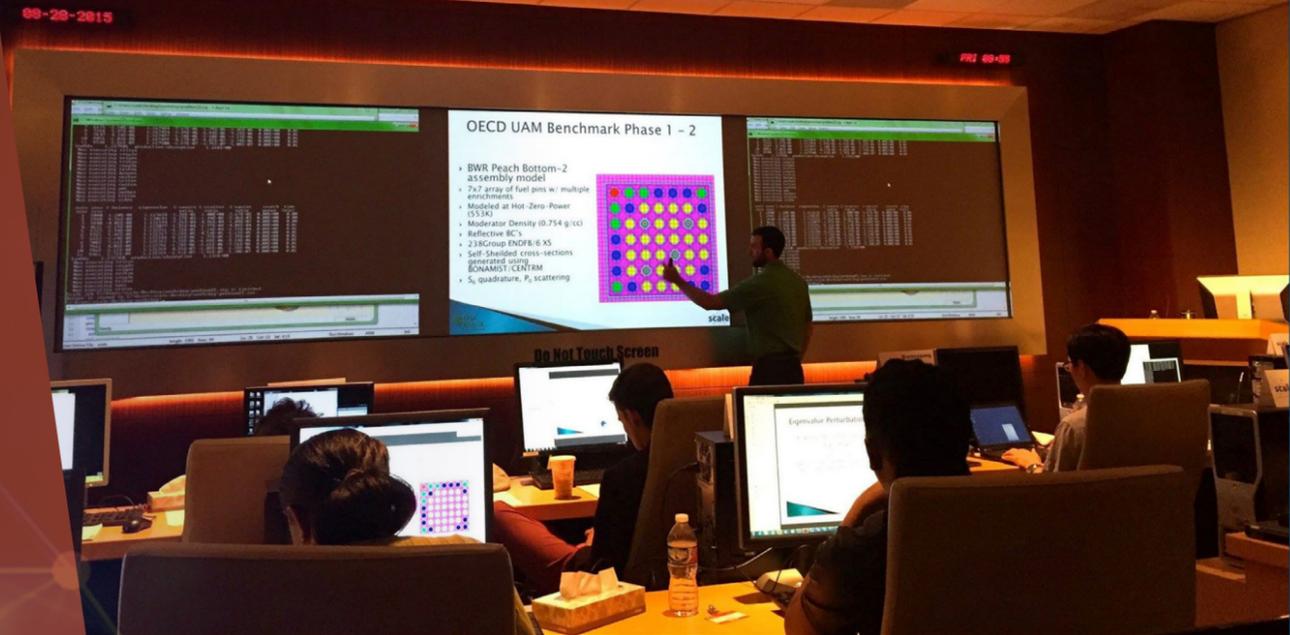


Fig. 13. ORNL training facility.

TRAINING COURSES AND WORKSHOPS

SCALE training courses and workshops continue to be popular with users. Training is provided by developers and expert users from the SCALE team. Courses provide a review of theory, descriptions of the capabilities and limitations of the software, and hands-on experience running problems of varying levels of complexity. In FY16, a total of 12 week-long courses were presented at ORNL (Fig 13), the OECD/NEA Data Bank, NRC headquarters, and user facilities. Two new opportunities were provided to coordinate with the International Atomic Energy Agency and the National Nuclear Security Administration (NNSA) to present a training class at the Institute of Nuclear Physics in Tashkent, Uzbekistan (Fig. 14), and to coordinate through the OECD/NEA to present a course at the National Research Nuclear University Moscow Engineering Physics Institute (MEPhI) in Moscow, Russia (Fig. 15). A conference workshop was also presented (Fig. 16). In total, SCALE training was presented to more than 150 participants from 15 nations. The training courses are funded through user registration fees and are self sustaining.



Fig. 14. Tashkent, Uzbekistan, SCALE training class.



Fig. 15. Moscow, Russia, SCALE training class.



Fig. 16. Conference workshop.



MAINTENANCE AND DEVELOPMENT ACTIVITIES

The primary goal of the SCALE maintenance and development activities is to ensure that the SCALE code system continues to meet the needs of sponsors and users by providing verified and validated results and remaining current with state-of-the-art computing technology (Fig. 17).

SCALE maintenance activities provide an essential foundation for all activities related to reliable development and use of SCALE. Maintenance activities include quality assurance (QA), development coordination, building and testing infrastructure, and support for all existing capabilities and features. Recently, the SCALE team has focused efforts on infrastructure modernization by reviewing and incrementally updating the components and procedures, which had evolved over a 40-year period, with modern software development practices and QA standards. An essential component of this ongoing activity is the development of a modern framework for SCALE analysis, which enables rapid development of advanced methods, parallel operation, and easy integration of SCALE tools with other analysis packages.

Development activities involve major enhancements and introduction of advanced methods to existing modules, as well as development of new modules, data libraries, and user interfaces. These activities employ current computing and programming techniques, building upon the modernized framework of the overall SCALE code system.

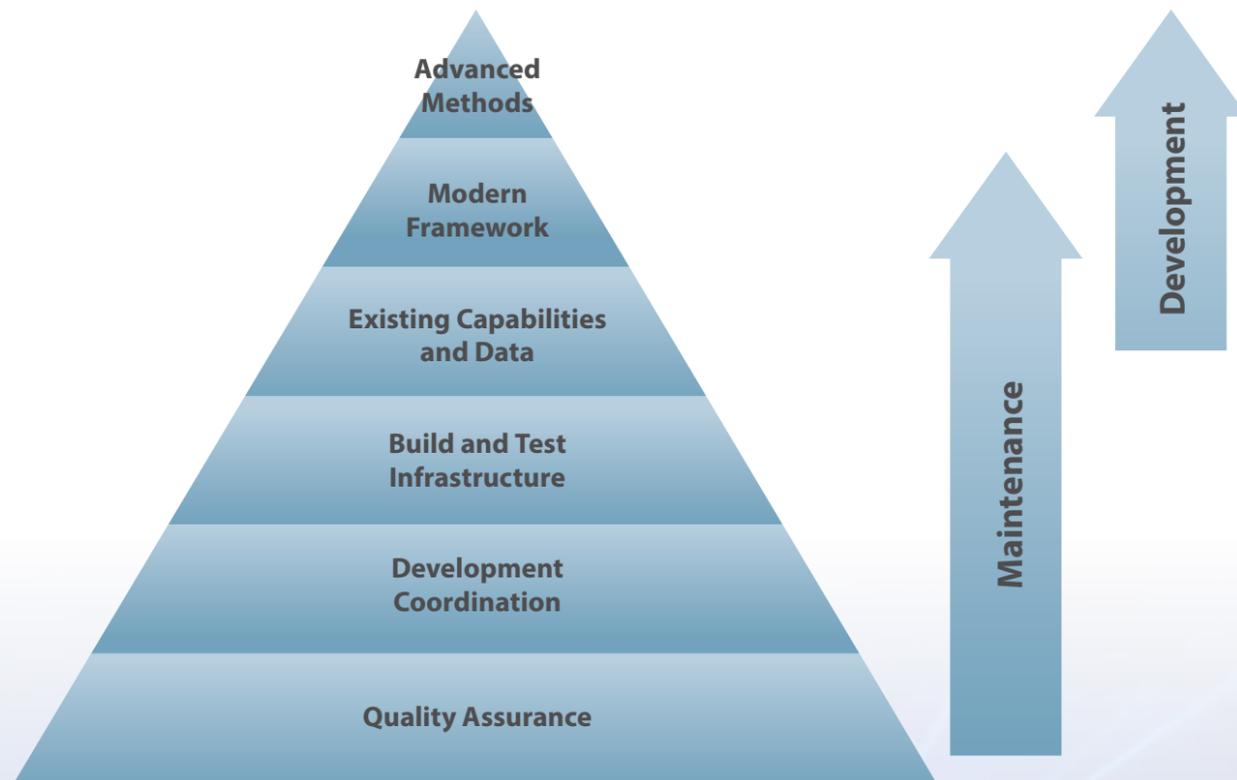


Fig. 17. SCALE activities diagram.

Quality Assurance

Activities classified as maintenance begin with the establishment of the QA framework applied to all SCALE codes and data (Fig. 18). The SCALE QA program is kept current with international consensus standards (ISO-9001-2008, American Society of Mechanical Engineers [ASME] NQA-1), US Department of Energy (DOE) orders (DOE 414.1D), NRC guidelines (NUREG/BR-0167) and the ORNL Standards-Based Management System. A review of the SCALE QA plan is performed annually by the ORNL RNSD Software QA Board. The SCALE QA plan continues to be viewed as a model plan both inside and outside ORNL.

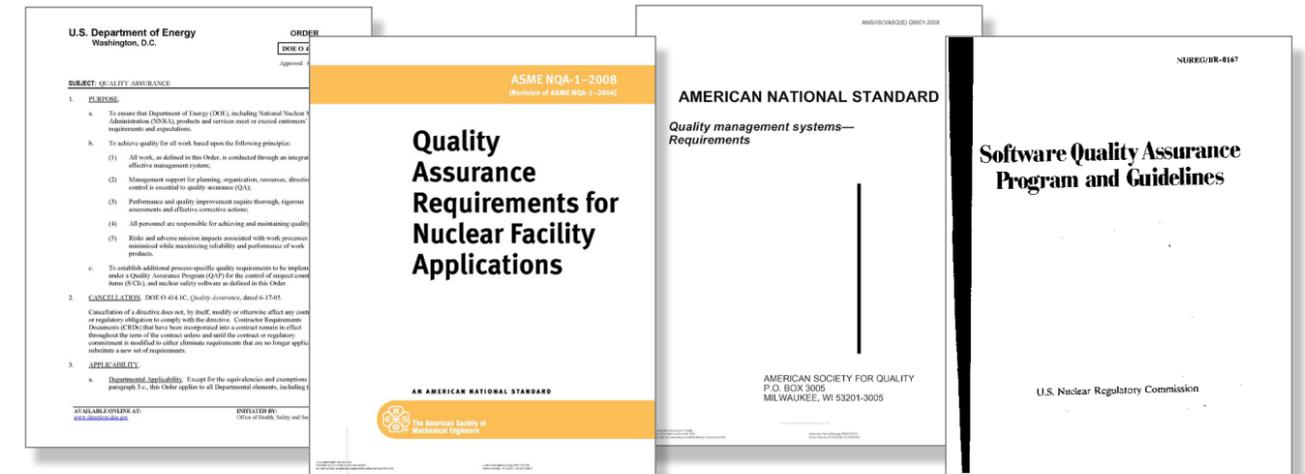


Fig. 18. Reference documents for SCALE QA plan.

Development Coordination

The SCALE code system is developed, deployed, and supported by dozens of staff members throughout ORNL/RNSD. All SCALE activities are coordinated to facilitate consistency throughout the project, especially in the implementation of QA, development practices, and testing strategies. The SCALE Leadership Team consists of the SCALE manager, line managers, program managers, and developers, as designated by the SCALE manager. The Leadership Team meets regularly to discuss the current status and to make programmatic and management decisions regarding SCALE.

SCALE teams are organized to coordinate work activities within given areas. Each team meets independently to plan and coordinate work activities. The teams are organized so that members from different work areas are included on multiple teams to improve communication and coordination across the entire team. Although the activities of most teams are supported by targeted development tasks, coordination of the teams and review of their work is supported as a maintenance activity. A weekly forum for developers and users is conducted to maintain a productive dialogue and collaboration among developers, users, and managers within ORNL.

SCALE TEAM STRUCTURE

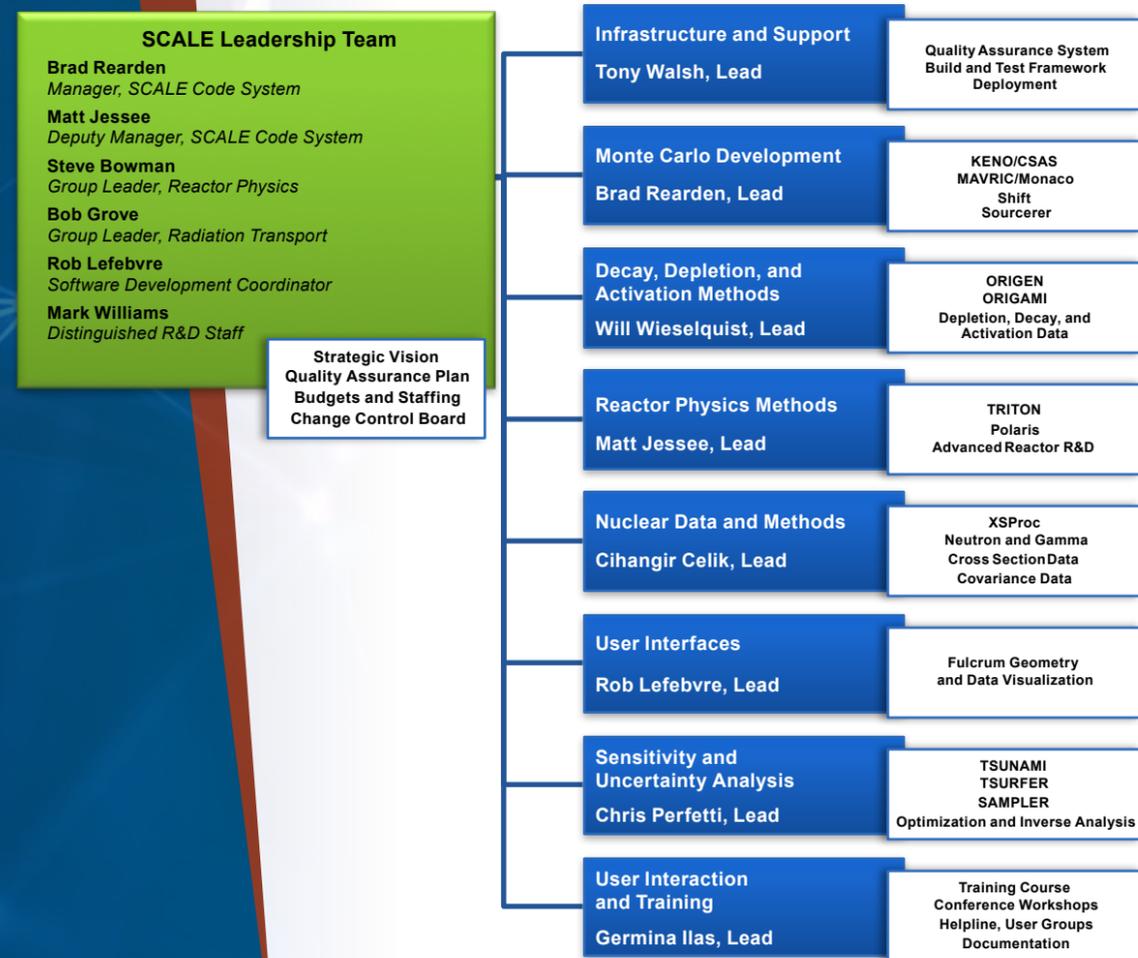


Fig. 19. SCALE team structure.

In addition to the Leadership Team and team leads shown above (Fig. 19), the 49 other RNSD staff members who contributed to the release of SCALE 6.2 are shown in Table 2 and the RSICC staff who were instrumental in the release of SCALE 6.2 are shown in Table 3. The SCALE 6.2 team is pictured in Fig. 20.



Fig. 20. SCALE 6.2 Team – May 2016.

(Left to right) Ahmed Ibrahim, Germina Ilas, Brandon Langley, Andrew Holcomb, Shane Hart, Cihangir Celik, Seth Johnson, Matt Jessee, Kevin Clarno, Adam Thompson, Bob Grove, Rob Lefebvre, Greg Davidson, Charles Daily, Alan Icenhour, Barbara Snow, Brian Ade, Brad Rearden, Ben Betzler, B. J. Marshall, Kursat Bekar, Will Wieselquist, Mark Baird, Mark Williams, Georgeta Radulescu, Ron Ellis, Thomas Miller, Dan Ilas, Elizabeth Jones, Cecil Parks, Sheila Walker, Teresa Moore, Marsha Henley, Sandra Poarch, Lester Petrie

Table 2. SCALE team members

• Brian J. Ade	• Ian C. Gauld	• Kang Seog Kim	• Georgeta Radulescu
• Lindsey D. Aloisi	• Cole A. Gentry	• Brandon R. Langley	• Rose B. Raney
• Goran Arbanas	• Andrew T. Godfrey	• Jordan P. Lefebvre	• Joel M. Risner
• Kaushik Banerjee	• Steven P. Hamilton	• William J. Marshall	• Diane J. Sams
• Kursat B. Bekar	• Shane W. Hart	• Ugur Mertuyrek	• John M. Scaglione
• Benjamin R. Betzler	• Andrew M. Holcomb	• Thomas Martin Miller	• Steven E. Skutnik
• Keith C. Bledsoe	• Jianwei Hu	• Donald E. Mueller	• Vladimir Sobes
• Justin B. Clarity	• Ahmad M. Ibrahim	• Tara M. Pandya	• Adam B. Thompson
• Charles R. Daily	• Germina Ilas	• Douglas E. Peplow	• Sheila Y. Walker
• Gregory G. Davidson	• Dan Ilas	• Joshua L. Peterson	• Dorothea Wiarda
• Kristin Gunter Ellestad	• Joshua J. Jarrell	• Lester M. Petrie, Jr.	
• Ronald J. Ellis	• Seth R. Johnson	• Marco T. Pigni	
• Thomas M. Evans	• Elizabeth L. Jones	• Sandra J. Poarch	

Table 3. RSICC staff

• Timothy E. Valentine, Director, RSICC	• Mark L. Baird	• Marsha D. Henley	• Teresa G. Moore
	• Barbara J. Snow	• Sheila Y. Walker	

Build and Test System

The success of any ongoing software project depends on the team’s ability to routinely compile and test the software and data and to provide continual support to the latest hardware and compilers. For SCALE, this foundation is implemented as a maintenance activity.

After each incremental update to the source code, a suite of over 2,000 test cases is run on each of dozens of computer platform configurations, including Linux, Mac, and Windows, with different compilers and compiler options. This rigorous testing is performed dozens of times each day, resulting in the quantification of performance with approximately 150,000 tests per day. Test results and the associated changes are reported to an internal website known as the SCALE Dashboard. All developers can review the Dashboard to monitor the performance of numerous SCALE features on different platforms with different compilers using a pass/fail metric, thus eliminating the need for users to configure and run all tests themselves. In FY16, the number of systems that are continually building and testing SCALE was increased to obtain even finer quantification of the impacts of individual changes. The hardware shown in Table 4, which consists of 288 processors and 872 GB RAM, is dedicated to running automated SCALE testing 24 hours a day, 7 days a week.

Table 4. SCALE continuous integration hardware

Platform	Hardware
Linux	<ul style="list-style-type: none"> 8 cluster nodes each with 8 processors and 32 GB RAM 1 dedicated computer with 64 cores and 256 GB RAM
Mac	<ul style="list-style-type: none"> 3 Mac Pro computers each with 16 processors and 20 GB RAM 2 Mac Pro computers each with 24 processors and 64 GB RAM
Windows	<ul style="list-style-type: none"> 2 Windows 7 computers each with 8 processors and 16 GB RAM 1 Windows 7 computer with 16 processors and 12 GB RAM 1 Windows 2012 Server with 32 processors and 128 GB RAM

All changes to SCALE source code are recorded and versioned in a repository system. This system streamlines the development process, facilitates easier collaboration between developers, and provides easier quantification of changes to improve the QA review process.

Existing Capabilities and Data

SCALE 6.2 consists of approximately 2,000,000 lines of source code for 77 executable modules, 43 GB of nuclear data in approximately 9,000 files, and more than 2,700 pages of user documentation. With 7,500 licensed users of SCALE 5.0–6.1 in 56 nations, extensive communication is required. In FY16, the SCALE team provided ongoing support to users by addressing approximately 700 inquiries through scalehelp@ornl.gov email. Additionally, an online discussion forum is available for SCALE users to post and review issues as a community (<https://groups.google.com/forum/#!forum/scale-users-group>). User communication in the form of website postings and newsletters is also provided.

Targeted development tasks generate dozens of new capabilities each year, and as each development task is completed, enhancements and user support for these features, additional testing and bug fixes, and integration of new features with existing features are supported as maintenance activities.

Modern Framework

In the SCALE 6.1 framework, a calculation involved a subset of the 89 independent computational modules, each executing in serial through progressive sequences where data are passed between modules through the computationally expensive process of reading and writing to the hard disk through file input/output (I/O). The vision set forth in the SCALE Modernization Plan calls for a modern framework in which the majority of data transfers occurs in-memory, and many of SCALE’s computational components will be able to operate on parallel computers ranging from multi-core desktop machines to Linux clusters to the leadership class supercomputers. The development of components within the modern SCALE framework is supported as ongoing maintenance and modernization of existing features. When a particular component requires updating, the best practices of modern software development are employed to ensure minimal development and maintenance costs in the future. The majority of FY16 SCALE maintenance support from all sponsors was focused on a modernization effort to realize substantial gains for SCALE 6.2.

The foundation of modern SCALE is a modular C++ software framework for efficient operation that also enables parallel computations. Individual computational components communicate through an efficient in-memory Application Programming Interface (API) instead of slow file I/O to the hard disk. Using APIs for communication between components also allows for clear requirements on the data I/O of each modular component. Each capability that provides an API is referred to as a *module*. When internal tests are applied to ensure that data passed through the API meet all requirements of the module, linkages with other modules can be efficiently modified without disrupting any part of the overall system. The concept of individual functional modules as standalone executable programs will diminish as individual physics capabilities are consolidated into a unified executable program capable of performing all SCALE functionality within an efficient parallel infrastructure. Additionally, the modern API-based framework enables the development of a modern GUI that implements the same modules used for computational analysis, removing the need to develop and maintain a feature twice, once for computational use, and again for the GUI.

Advanced Methods

Advanced methods are developed as targeted tasks unless an incremental advancement is required to correct a discrepancy or to enhance an existing feature for compatibility with a new feature. However, once an advanced method is completed, there are often QA and maintenance activities required to continue to provide support for it. Thus, as new features are integrated into SCALE, the amount of maintenance required is incrementally increased pending removal of outmoded features. While many advanced methods were introduced to SCALE 6.2, the SCALE modernization plan details additional advancements that will culminate in the fully modernized SCALE 7. A key aspect of SCALE 7 will be the replacement of the KENO and Monaco Monte Carlo codes with the advanced, integrated Shift Monte Carlo code. A prototype integration of Shift is planned for initial deployment with SCALE 6.3.

SPONSORED ACTIVITIES

The maintenance and development of SCALE and AMPX are supported by several sustaining sponsors (Table 5), who have provided support over many years, as well collaborating sponsors, who interact with the SCALE team for particular enhancements important to their mission. Since 1976, NRC has been the lead sponsor in the development of SCALE, with additional support provided by both the Office of Nuclear Material Safety and Safeguards (NMSS) and the Office of Nuclear Regulatory Research (RES). SCALE maintenance and development activities have been co-sponsored since 1987 by DOE and NNSA.

Table 5. Sponsor information

Sponsor		Description
Sustaining Sponsors	NRC/NMSS/Division of Spent Fuel Management (DSFM)	Criticality, shielding, source terms, and validation methods for spent nuclear fuel licensing
	NRC/RES/Division of Systems Analysis (DSA)/Fuel and Source Term Code Development Branch (FSCB)	Nuclear data, lattice physics, criticality safety, depletion, shielding, source terms, and validation for current and advanced reactor licensing
	NNSA/NCSP	Criticality safety analysis, validation methods, criticality accident alarm system analysis, and nuclear data processing
	DOE/Packaging Certification Program (PCP)	Shielding and source terms for radioactive material packaging
Collaborating Sponsors	DOE/Office of Nuclear Energy (NE)/Nuclear Energy Advanced Modeling and Simulation (NEAMS)	Depletion and decay methods, nuclear data, and integration with other NEAMS tools
	DOE/NE/Consortium for Advanced Simulation of Light Water Reactors (CASL)	Cross section data and methods integrated with CASL tools
	DOE/Technology Commercialization Fund (TCF)	Enhancements for molten salt reactors (MSRs)
	Chinese Academy of Sciences (CAS)/Shanghai Institute of Applied Physics (SINAP)	Enhancements for fluoride salt-cooled high temperature reactors (FHRs)
	ORNL/Laboratory Directed Research and Development (LDRD)	Sensitivity/uncertainty methods for isotope production
	NNSA/Office of Defense Nuclear Nonproliferation (NA-22)	Enhancements for nonproliferation analysis

FUTURE DEVELOPMENT

The SCALE team is dedicated to supporting the advanced features provided in SCALE 6.2 and is working to extend these capabilities for additional types of analysis such as: very large and complex interim storage sites for used fuel; analysis of advanced reactors including MSRs, FHRs, and sodium-cooled fast reactors (SFRs); analysis of accident-tolerant fuels; and advanced validation approaches for new or challenging systems (Figs. 21, 22, and 23). Existing capabilities will continue to be improved through additional efficiency and accuracy gains, as well as additional enhancements to the user interface. The development of many of these capabilities is in progress now to be available with SCALE 6.3. The nuclear data generated by the AMPX tools for all SCALE CE, MG, activation/decay, and covariance libraries will continue to be improved through an iterative development cycle that includes increased testing under the QA plan and timely deployment of the most current nuclear data libraries. Modernization plans for SCALE and AMPX include increased synchronization of development activities and shared resources between these two projects.

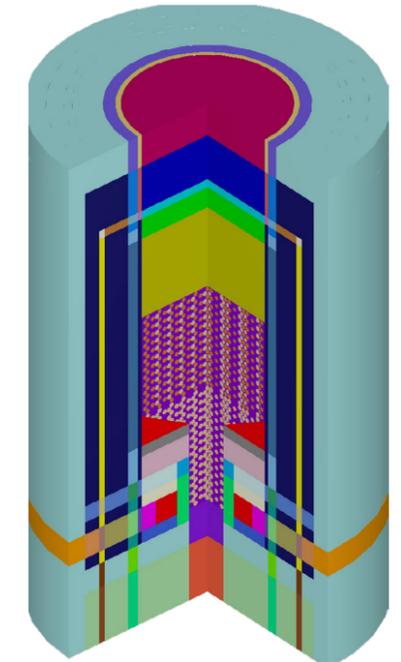


Fig. 21. SCALE model of an high-temperature gas cooled reactor (HTGR).

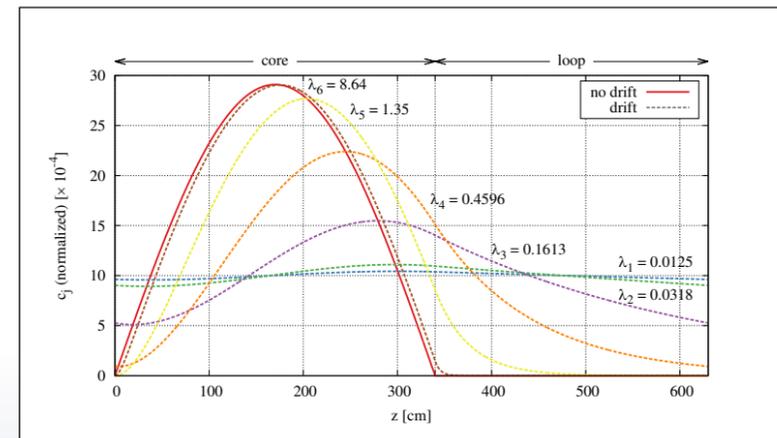


Fig. 22. MSR delayed neutron precursor drift modeling.

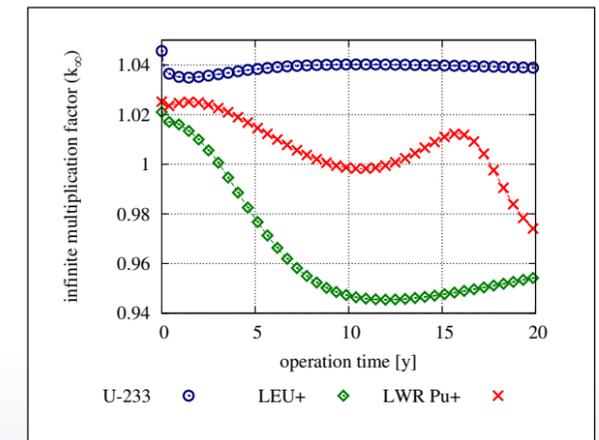


Fig. 23. Time-dependent MSR modeling.

SCALE is being positioned for the future, with an extensive reprogramming of existing capabilities to improve run-time performance and solution fidelity. The most significant changes planned include the ability to execute SCALE in parallel on multiple CPUs – whether on desktops, workstation clusters, or high-performance supercomputers. This strategy includes the development of a new Monte Carlo code capable of excellent parallel scaling on leadership class computing architectures such as ORNL's TITAN machine, with approximately 300,000 processors. The Shift Monte Carlo code (Fig. 24) leverages many SCALE modernization capabilities, including input generation, nuclear data resources, and modules for CE and MG physics, modular geometry, sensitivity/uncertainty analysis, and depletion. The staged migration and testing of individual SCALE capabilities in the modern framework ensures robust development, testing, and deployment of this new tool. The long-term modernization plan includes full modularity and parallelization in SCALE 7, including the integration of the Shift Monte Carlo code.

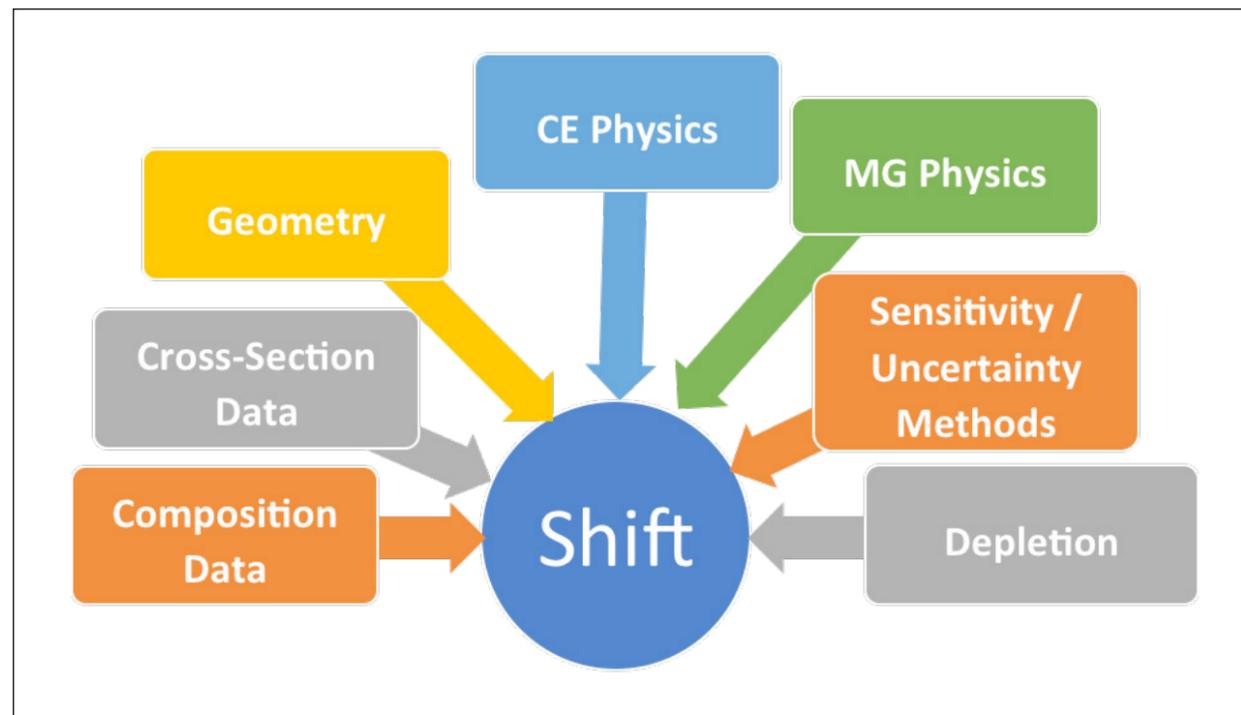
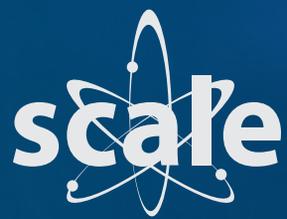


Fig. 24. Advanced Monte Carlo methods with Shift.



Nuclear Systems Modeling & Simulation