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SCALE Newsletter

William A. Wieselquist
SCALE Director

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Oak Ridge National Laboratory
P.O. Box 2008, Bldg. 5700 MS-6170
Oak Ridge, TN 37831

Email: scalehelp@ornl.gov
https://www.ornl.gov/scale

The last SCALE newsletter was published just before I became director of the code system in August 2018, so after all this time, we have plenty of news! The last two years have certainly been exciting and challenging for the SCALE Team, with twists and turns that no one could have expected. Some of our great ones have retired or passed on, which has been very sad, but we have also gained some new great-ones-to-be, and we have introduced new roles and experimented with new responsibilities. Nuclear is quite exciting now, with uncharted territory in innovative new systems such as tristructural-isotropic fuels and heat-pipe reactors. Proposed enhancements to conventional systems include development of small modular reactors and advancements in extended enrichment and burnup. Our work for the US Nuclear Regulatory Commission (NRC) is refocusing to support potential applications across this space, with multiyear projects in severe accident analysis for non-light-water reactors (LWRs), high-assay low-enriched uranium, high burnup fuel, and accident-tolerant fuel (ATF) for LWRs throughout the fuel cycle, not to mention nuclear data gap analyses and improvements. Our work for the US Department of Energy (DOE) Nuclear Criticality Safety Program (NCSP) continues to advance innovations in sensitivity and uncertainty quantification and code validation.

We have finished the final maintenance update to the SCALE 6.2 series, v6.2.4. Please find more information about this update in the section entitled "SCALE 6.2.4 Update." We are implementing a new policy to only fix issues in maintenance releases. In the past, we have allowed the release of some sneak preview capabilities, but no longer. This ensures that users can have confidence in upgrading to the most current maintenance release: a correct answer should not change from v6.2.3 to v6.2.4. Users who want new features should look to the beta releases, which are now released every six weeks.

We are revamping the SCALE website to include landing pages for each code release and a current list of known issues found in the latest version. In the section entitled "SCALE 6.3 Preview," I share some of the new capabilities in the SCALE 6.3 series, and v6.3.0 will be available near the end of December 2020. We are still happy to engage 6.3 beta users, so please email scalehelp@ornl.gov for details. The new website will also include detailed descriptions of beta content, so stay tuned!

Figure 1. William A. Wieselquist, SCALE Director.

SCALE Version Support

More than 9,000 SCALE users in 62 nations are using several major versions of SCALE across multiple operating system versions of Windows, Mac, and Linux. These benefit from the ScaleHelp system (scalehelp@ornl.gov), a Google forum (https://groups.google.com/forum/#!forum/scale-users-group), 12+ training classes (https://www.ornl.gov/scale/scale-training), and the annual SCALE Users' Group meeting (https://scalemeetings.ornl.gov). These resources provide expertise and assistance for all applications.

In response to recent inquiries about software support for various SCALE versions, the SCALE Code System's software lifecycle and maintenance schedule is detailed here.

In an effort to improve the user's experience and make maintenance operations more efficient, we formed the SCALE Training and User Interaction Team, which is responsible for scheduling and coordinating training and the annual SCALE Users' Group meeting and for curating the ScaleHelp system and Google forum. The ScaleHelp system has received approximately 3 inquires per day for the last 8 years of recordkeeping (Figure 2). Each inquiry is assigned a case number under which all inquiry correspondence is tracked. The SCALE User Support and Development Teams work to answer these inquires as expeditiously as possible, often in their own free time.

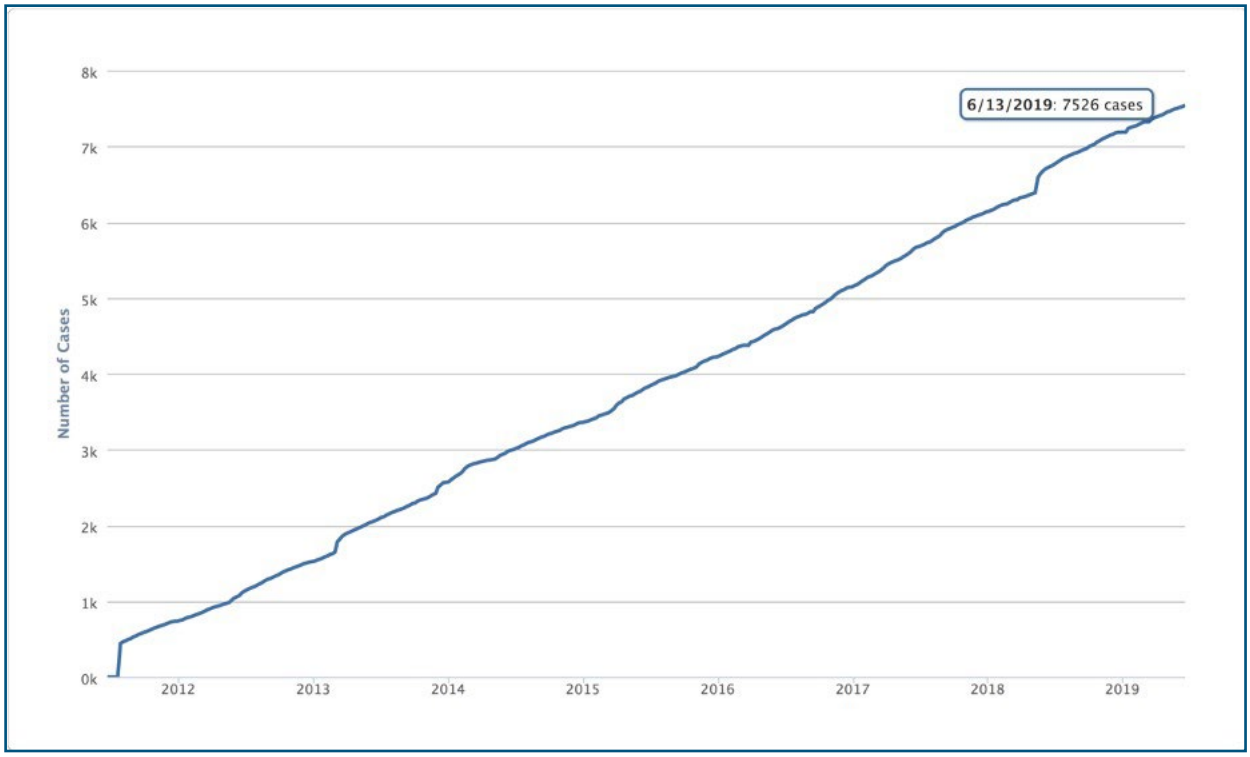


Figure 2. ScaleHelp cases over time.

There are two main categories of SCALE software maintenance: *customer support*, which includes assistance with the installation of prebuilt binaries, training, and troubleshooting, and *technical support*, which assists with code compilation, provides maintenance releases, and supports feature development.

As shown in Table 1, SCALE leadership has established tentative end-of-life dates for each of these activities to enhance the team's focus on research and development activities and to limit costly maintenance activities.

Table 1. SCALE version support and end-of-life dates

Version	0,1,2,3,4…4.4a	5.0	5.1	6.0	6.1	6.2	6.3
Customer support	No	No	Limited	Limited	Limited	Yes	Yes
Technical support	No	No	No	No	No	Yes	Yes
Release date	2000	2004	2006	2009	2011	2016	~2020
End-of-life date	NA	NA	2019	2019	2020	~2023	~2026

The limited customer support for SCALE versions 5.1, 6.0, and 6.1 is most notable. With the significant modernization effort undertaken in the release of SCALE 6.2, the SCALE build system was upgraded to reduce maintenance needs and to increase longevity. This factor, along with staff focus on new research and development, has eliminated the SCALE Team's ability to provide technical support for these versions. Additionally, in the 14, 11, and 9 respective years since these versions were released, the changes in operating systems and compilers and the changes in ORNL's software security posture have limited new installations, a critical factor when providing complete customer support. This has led to reduced customer support for SCALE 5.1, 6.0, and 6.1, so only limited support is available for installation and troubleshooting.

Customer support for SCALE 5.1 and 6.0 ended at the conclusion of 2019. Customer support for SCALE 6.1 will no longer be provided at the conclusion of 2020, so *users are highly encouraged to upgrade to SCALE 6.2.*

SCALE leadership is constantly working to balance the requests of users from university, industry, and regulatory sectors, to streamline maintenance operations, and to reduce cost. Software release and end-of-life cadence is under review, and your input is welcome. Tentative plans are to perform a major software release (6.3, 6.4, etc.) every 3 years, and support will be provided for the current release and one prior release. For example, a new release will have 3 years of support provided while it is the current release, followed by 3 more years of support as the prior release, for a total of 6 years of support.

We look forward to supporting your needs as SCALE evolves to provide ever expanding capabilities in comprehensive modeling and simulation for nuclear safety analysis and design.

SCALE 6.2.4 Update

In the SCALE versioning scheme, 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 was followed with maintenance releases 6.2.1, 6.2.2, 6.2.3, and now, 6.2.4. The maintenance releases only fix issues found by the user community while the next feature release is being developed. This article describes the fixes that have been made in 6.2.4.

Licensed users of SCALE 6.2 can request the 6.2.4 update by sending an email to scalehelp@ornl.gov, with "SCALE 6.2.4 update" as the subject line. The update will be provided via a download link. The 6.2.4 update includes all previous updates and can be applied directly to any SCALE 6.2 release.

The 6.2.4 updates described below are organized by major sequence/module.

STDCOMP: Missing Element Isotopic Distribution Check

The Standard Composition Library (STDCOMP) and related functions did not include an input check to ensure that certain elements have user-defined isotopics. The elements listed in Table 7.2.2 of the SCALE manual have natural abundances that define a default isotopic distribution. Elements not listed in the 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 material's production source and decay time, so users are 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 input check was not operating as intended, but the issue has been fixed in SCALE 6.2.4.

This issue was elevated to a high-priority fix because 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 nonconservative result in versions 6.2.0–6.2.3.

KENO

Doppler broadening rejection correction on Windows

Doppler broadening rejection correction (DBRC) data were not being correctly loaded on Windows installs of SCALE version 6.2.3, and with the DBR=2 option, there was no indication that the data were not loaded. Therefore, the calculation proceeded without warning. To verify whether a calculation had been affected, users could rerun the calculation with DBR=0, and if the random walk were identical, then the DBRC was not successful. There was no such issue on Linux and Mac systems. This issue has been fixed in SCALE 6.2.4.

Kinematics data setup

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

ORIGEN: Large Decay Steps May Lead to Omission of Certain (Alpha,n) Sources

In an ORIGEN calculation of (alpha,n) sources for 10 million years of decay, it was found that ORIGEN did not include ^{241}Am in the results. This issue was due to floating point comparisons applied to the final decay time step isotopics in which very little ^{241}Am was left, resulting in the omission of ^{241}Am in earlier time steps. The parameter alphan_cutoff has a default to include all potential sources, so this was unexpected behavior. Although it is recommended that ORIGEN users update to SCALE 6.2.4, a workaround for users of SCALE 6.2.0–6.2.3 is to use in the input a single case for each decay

step, effectively forcing the (alpha,n) source criterion to be applied at each time step. This issue has been fixed in SCALE 6.2.4.

ORIGAMI: Zero Decay Length in Cycle

ORIGAMI did not allow some valid power histories that could occur when a fine-grained power history with no intermittent decay is being modeled, 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 was to use "down=1e-5" so that results were not altered on the important timescales. This issue has been fixed in SCALE 6.2.4.

TRITON: Material Swap

The TRITON swap capability did not function correctly in many scenarios. The extent of the issue was not fully categorized, but it was determined to be due to incorrect bookkeeping of the volume of mixtures involved in the swap. All users of the TRITON swap capability are encouraged to update to SCALE 6.2.4, in which the issue has been fixed.

MAVRIC: Response Generation from CE Cross Sections

MAVRIC could not perform continuous energy (CE) responses for nu-fission. The nu-fission reaction (mt=1452) is useful as a response and is supported for multigroup (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 fission cross section (mt=18) during the response generation. MAVRIC CE responses for the nu-fission reaction are now enabled in SCALE 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, an issue was identified in SCALE 6.2.3 when using macroscopic cross sections for responses with photon cross sections. This issue has been fixed in SCALE 6.2.4.

Other Minor Miscellaneous Issues Fixed in SCALE 6.2.4

1. A minor formatting issue in the Monte Carlo N-Particle Transport Code (MCNP) card output of ORIGAMI was found. This MCNP card enables users to generate MCNP sources directly in the MCNP format based on ORIGAMI-calculated spent fuel isotopics. This issue has been fixed in SCALE 6.2.4.
2. A minor issue was discovered 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 central processing units 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. To overcome this problem on installation testing, a fuzzy tolerance is used to check the local machine result, a, vs. the deployed baseline result, b. If both results had uncertainty, then the check was looser than intended, resulting in 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 $|b-a| \leq (\sigma a+\sigma b)$, with most tests at the N=2 sigma level. With the new improved test criteria and the old N=2, a handful of failures occurred on Windows when the baseline was generated on Linux. Since hundreds of tests are being run, this is statistically within expectations. Users should not be concerned that the old testing process was incorrect. With either test criterion, a failure message would indicate either an installation failure or an "unlucky" random walk that is far outside expectations. This issue has been corrected.
3. A minor issue was found in Fulcrum in which the mesh viewer could fail to remove loaded mesh files, requiring a restart of Fulcrum to deallocate the program memory associated with mesh data. This issue has been corrected.

4. A minor issue was discovered in MAVRIC in which some input blocks required lowercase text, even though SCALE is case insensitive for keywords. When lowercase text was used in these input blocks, the 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 STDCOMP lookup. This issue has now been fixed.
5. A minor issue was found in which 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.
6. A minor issue was seen in ORIGEN that occurred when using "previous=0" to load isotopics from a previous "case" in the input. This issue has now been fixed.
7. A minor issue was found 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, and when the file path included 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 file path character allowance has been extended to 1,024 characters in SCALE 6.2.4; this issue has been fixed.
8. A minor issue was discovered 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. This issue has been addressed so that the correct values are shown.
9. A minor issue was found 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 Evaluated Nuclear Data File (ENDF)/B-VII. This issue has been fixed.
10. A minor issue was found 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. This issue has been corrected.
11. A minor issue was found 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.

SCALE 6.3 Preview

The capabilities described in this section are based on the closed resolved quality assurance cases as of SCALE 6.3 Beta 11, released in May 2020. The capabilities are organized according to end-user SCALE products. Beta releases occur every 6 weeks. Email scalehelp@ornl.gov to request access to beta releases.

ORIGEN Library Generation in Polaris

Polaris now generates a system-average ORIGEN library as `${BASENAME}.f33` in all depletion calculations. This library was compared with the library obtained with the TRITON version, and excellent agreement has been observed. Polaris uses a slightly more rigorous formulation than TRITON. In the Polaris formulation, reaction rates are consistently collapsed from all regions of the problem, whereas in the TRITON approach, a system-average flux is calculated and then used to collapse MG cross sections. The main use-case for ORIGEN libraries is to enable fast spent fuel calculations.

New ATF Compositions in Polaris

In this enhancement, new compositions were added to support additional compositions used for ATF concepts, including chromia (Cr_2O_3), alumina (Al_2O_3), and beryllia (BeO). In addition to the uranium oxide (UOX) comp card option, the USi and UN comp options were added for silicide (U_3Si_2) and nitride fuels (UN), respectively. The UN comp option allows users to specify the ^{15}N enrichment if needed. Moreover, fuel material specifications support dopant properties, allowing users to add dopant quantities of alumina, chromia, and beryllia.

Coupled Neutron/Gamma Calculations in Polaris

Polaris now supports a gamma calculation that can perform detector response modeling as necessary to approximate boiling water reactor (BWR) detection systems. Users can specify a physical detector zone or a "virtual" detector using a specific cross section—or a combination of cross sections folded with a specific zone flux—without including the physical material in the geometry. The capability requires coupled neutron and photon libraries, which are included in the new SCALE 6.3 data directory.

New Shift Monte Carlo Solver Integrations

The Shift Monte Carlo solver has been integrated as an option in all three Monte Carlo sequences: CSAS, MAVRIC, and TRITON. The default solver is still KENO in CSAS and TRITON. For example, "=csas6" will run KENO-VI, and "=csas6-shift" will run Shift, and the default solver in MAVRIC is still Monaco. For the SCALE 6.3 release, it is intended that the same capabilities in CSAS-KENO and MAVRIC-Monaco will be available with Shift, with the added benefit of increased parallelism. The most important update is that in previous releases, MAVRIC was a serial code that was unable to take advantage directly of available additional processors. MAVRIC-Shift offers near-perfect speedup: a 4-core calculation will run in ¼ of the time. Shift was designed so that this parallelism extends up to hundreds of thousands of cores. For TRITON-Shift, new capabilities are available in SCALE 6.3 related to the so-called *nodal data generation*, as described below.

Nodal Data Generation in TRITON-Shift

TRITON-Shift contains the majority of TRITON-KENO's capabilities, as well as new nodal data options enabled by the "fgxs" block. Currently, TRITON-Shift allows nodal data generation on cuboid and rhexprism domains (i.e., the global unit is a cuboid or rhexprism) and cuboid and rhexprism meshes. This significantly expands TRITON's ability to provide few-group cross sections for downstream core simulators such as PARCS. The following input block example enables a 4-group tally on a hexagonal mesh centered at (0,0) with a single axial zone.

```
read fgxs
  shape global id=10
  energy  id=10  1.0E-05 1.506540e+04 1.110900e+05
8.208500e+05 2.0E+07 end
  mesh hexagonal id=10 hpitch=8.12355 origin x=0 y=0
dz 1.0 end
  tallyset t16 id=10
end fgxs
```

Figure 3. Example of a few-group cross section block in TRITON-Shift.

Multiple tallies may be provided in a single input. Each zone produces a single TRITON "T16" file that can be processed into nodal data for a core simulator. With PARCS, this is accomplished through the processor GenPMAXS.

Fulcrum 3D Visualization

A new capability was added to Fulcrum for 3D visualization, including capabilities for rotation, zooming, panning, transparency, and cut planes. Fulcrum now uses the same ray-tracing engine developed for the Shift Monte Carlo code (Figures 4 and 5). This capability is intended to replace the Windows-only KENO3D rendering graphical user interface. Future work will improve the speed and robustness of the visualization capability and will address issues with the user interface based on user feedback.

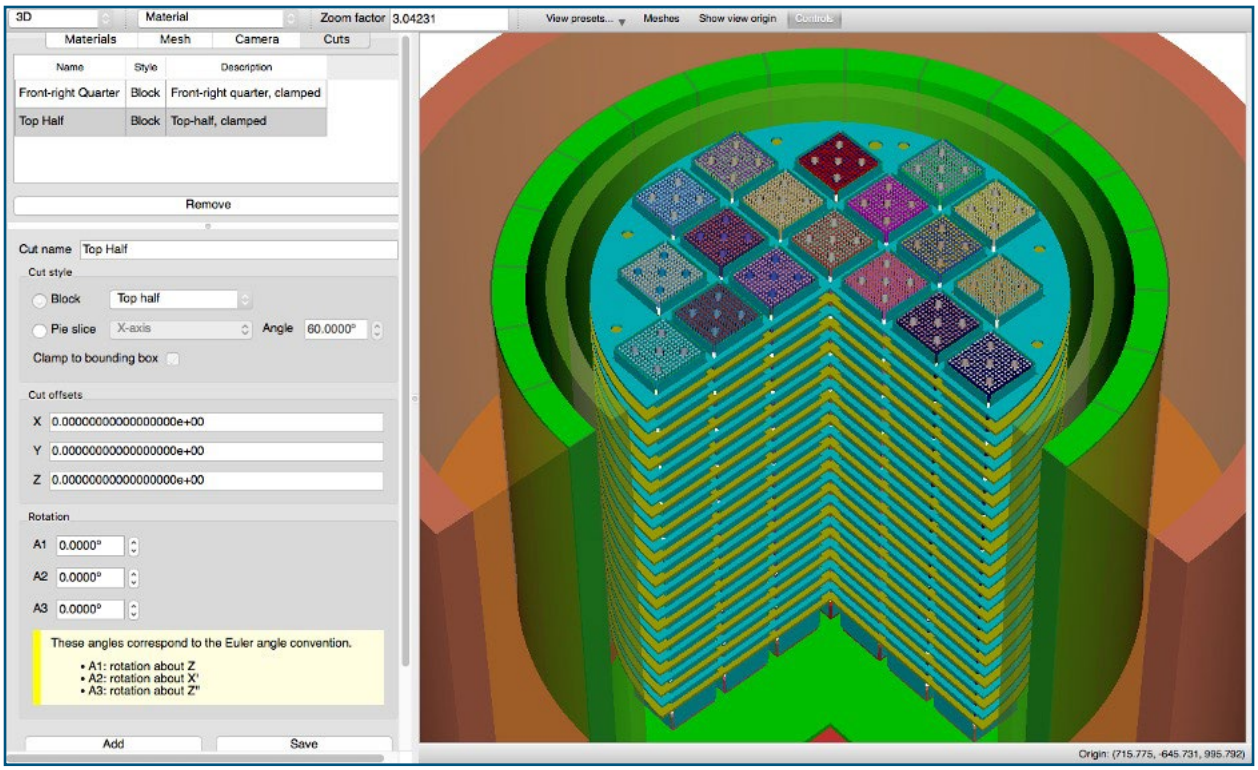


Figure 4. Example of a 3D visualization of geometry through Fulcrum.

Fulcrum 3D Mesh Overlay

Monte Carlo codes in CSAS and TRITON can produce flux and fission rate solutions on a mesh, and MAVRIC may produce nearly any tally on a mesh. However, previous versions of Fulcrum only allowed these data to be viewed in cut planes. New mesh data overlay and overlay + boundaries have been added to the 3D geometry view within Fulcrum.

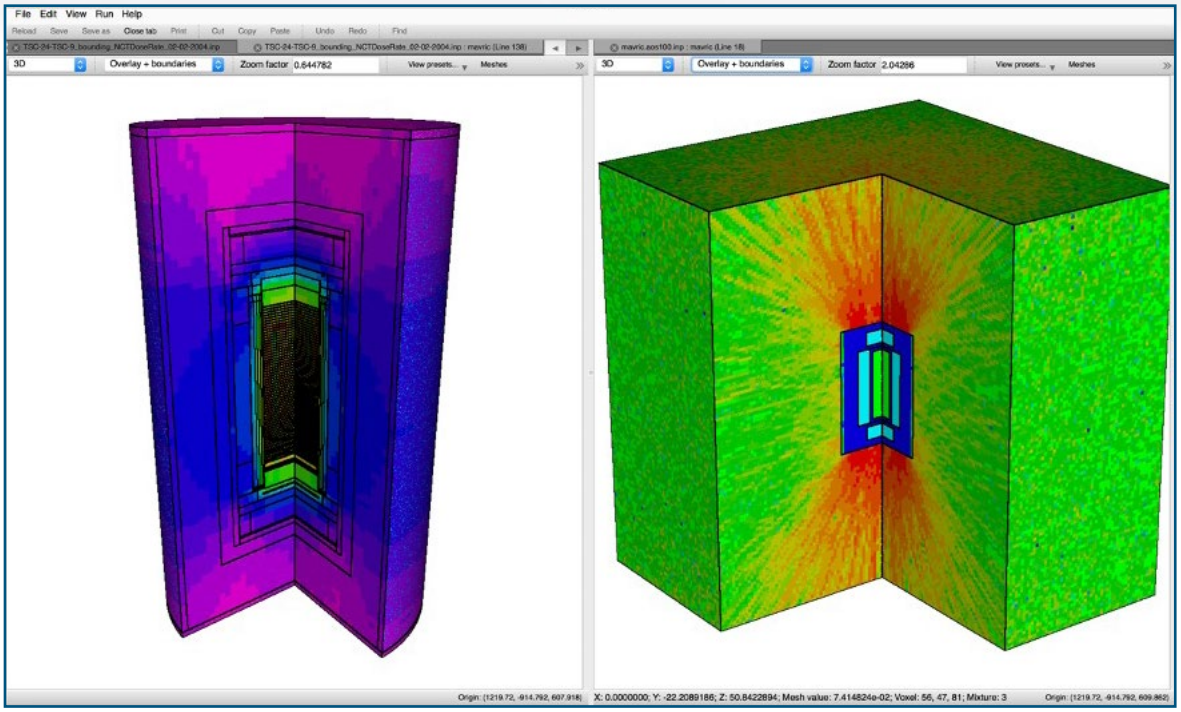


Figure 5. Example of a 3D mesh overlay of a dose tally through Fulcrum.

New SCALE Data Libraries

New data resources were added to the SCALE data to improve capabilities and efficiency and to support non-light water reactor (LWR) calculations.

- Two ENDF/B-VII.1-based coupled MG libraries were added to support coupled (n,γ) reactor physics calculations with Polaris.
- ENDF/B-VII.1 CE libraries were updated with new unresolved resonance region (URR) probability tables to resolve biases in fast system calculations.
- A new 302-group library was added for the analysis of sodium-cooled fast reactor (SFR) systems. The 302-group structure was developed based on group structures optimized for fast spectrum systems used in the DOE Office of Nuclear Energy Advanced Reactor Technologies (ART) program.
- ENDF/B-VIII.0 CE libraries for incident neutron and gamma data were deployed in HDF5 format rather than the legacy binary format. The new HDF5 directory file for the CE libraries follows the usual SCALE convention: ***ce_v8.0_endf***.
- ENDF/B-VIII.0 composition names for ice, reactor grade graphite, silicon carbide, and yttrium-hydride were added.
- Cross section covariance data for ENDF/B-VIII.0 was updated to provide more robust uncertainty estimates.

AMPX GNDS Support and Other Modernization

SCALE's nuclear data processing code, AMPX, has been updated to process the Generalized Nuclear Data Structure (GNDS) file format, which has been designated as the future file format for all nuclear data updates. Additionally, AMPX has been improved to operate as robustly on Windows as on Linux or Mac platforms. The modules POLIDENT and CADILLAC have been modernized with new input interfaces.

More Robust Self-Shielding for Non-LWR Systems in XSProc

XSProc was improved to address higher-than-expected biases observed in MG calculations of non-LWR systems such as the high-temperature gas reactor (HTGR) compared with biases observed in high-fidelity SCALE CE methods. One of the main XSProc updates was to disable a special scattering and lumping treatment, which was designed to speed up LWR calculations with minimal effect on accuracy. Additionally, options in XSProc and AMPX were added to support higher thermal scattering cutoffs in MG libraries beyond 5 eV, which might be necessary for highly scattering graphite systems.

Iterated Fission Probability Sensitivity Methods with Shift

The capability for CE Monte Carlo sensitivity methods was introduced in SCALE 6.2 with the iterated fission probability (IFP) method, as well as the and contribution-linked eigenvalue sensitivity/uncertainty estimation via track length importance characterization (CLUTCH) method. For SCALE 6.3, given the desire to perform future Monte Carlo development only in Shift, the IFP method was reimplemented and reevaluated. The new Shift-based implementation reduced the run time and memory footprints by a factor of 4–8, and it allowed calculations to be distributed to multiple processors. A simple sensitivity input is shown in Figure 6.

Sensitivity Metrics from Sampler

Sampler is the uncertainty propagation application introduced in SCALE 6.2. One key improvement of the sampling-based uncertainty propagation was implemented so that users can determine which uncertainty inputs or nuclear data are causing the uncertainty in an output of interest (Figure 7). In SCALE 6.3, numerous special sensitivity metrics were added in Sampler, such as the correlation coefficients R^2 and SPC^2, to provide additional information on which nuclear data are driving the uncertainty. When Sampler was compared with other sensitivity methods, such as perturbation theory–based analysis with sensitivity coefficients, it was found that approximately five top contributors can be identified using 200–1,000 realizations with Sampler.

```
=tsunami-3d-k5-shift
HEU-MET-FAST-001-001 Solid Godiva (input imported
from SCALE VALID suit)
ce_v7.1_endf
read composition
 u-234 1 0  4.9184e-4 300 end
 u-235 1 0  4.4994e-2 300 end
 u-238 1 0  2.4984e-3 300 end
end composition
read param
 gen=10150 npg=15000 nsk=150
 htm=no
' Sets the sensitivity method (cet=2 --> IFP)
 cet=2
' Sets the number of latent generations used by IFP
 cfp=3
end param
read geometry
global unit 1
 sphere 1 1   8.7407
end geometry
end data
end
```

Figure 6. Example of a TSUNAMI-Shift input using the IFP method.

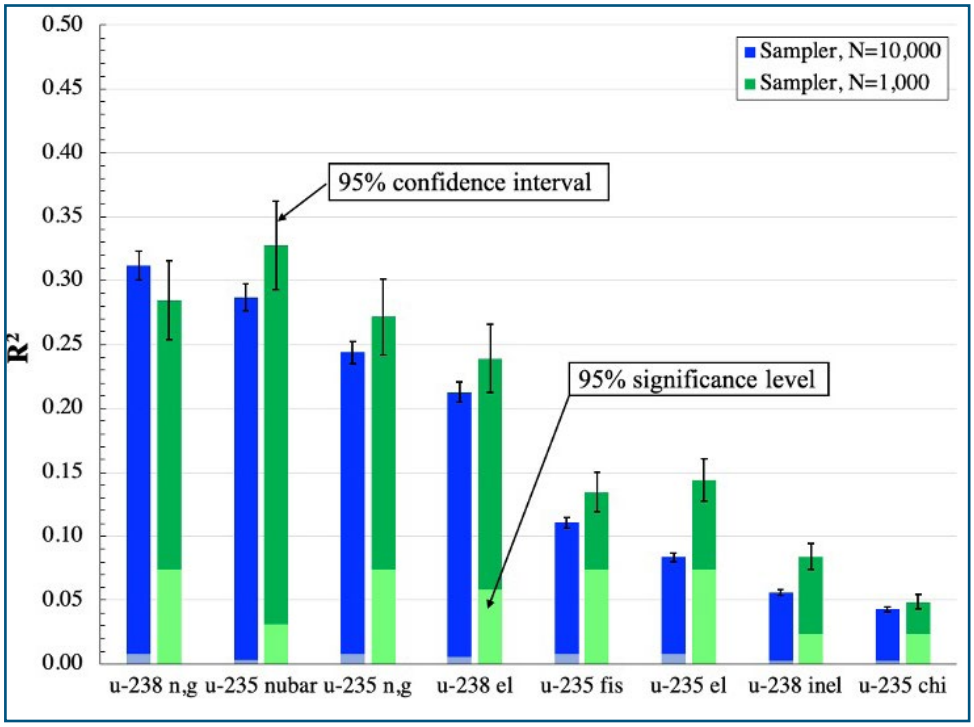


Figure 7. Example of the top eight contributors to k_{eff} uncertainty based on the R^2 sensitivity index, with confidence interval and significance levels for N=1,000 and N=10,000 realizations.

ENDF/B-VIII.0 Data in SCALE 6.3

ENDF/B-VIII.0 SCALE Data

In 2018, ENDF/B-VIII.0, a new revision of the ENDF/B library was released. This release includes many updates to the ENDF/B-VII.1 nuclear data that can significantly change the computational results. These data updates can have a significant impact, especially for advanced reactor concepts using materials that are significantly different than those used in the historically well-investigated LWR systems. For example, significant differences between ENDF/B-VII.1 and VIII.0 include fission and capture cross sections of ^{235}U, ^{238}U, and ^{239}Pu, as well as the neutron multiplicities () of ^{235}U and ^{239}Pu (see Figure 8 for comparisons of ^{239}Pu). The scattering and capture cross sections of ^{1}H, ^{16}O, and ^{56}Fe also are significantly different. The AMPX/SCALE 252-, 1597-, and 302-group and CE cross section libraries were processed based on ENDF/B-VII.1 and VIII.0, in which the 1597- and 302-group structures were newly developed for various advanced reactor analyses in SCALE 6.3. Various benchmark calculations were performed using SCALE with the ENDF/B-VII.1 and VIII.0 AMPX libraries, and the computational results were compared.

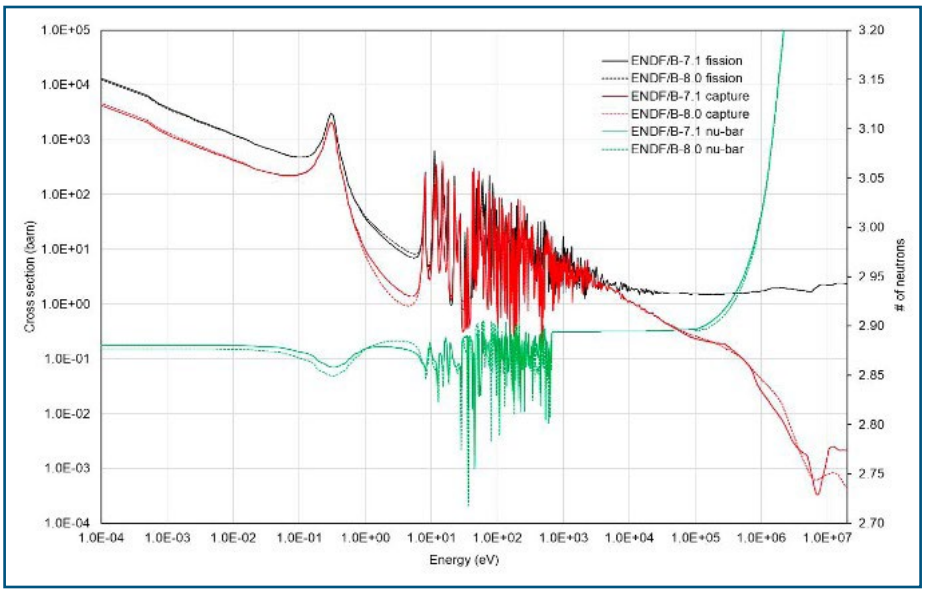


Figure 8. Comparison of the ENDF/B-VII.1 and VIII.0 ^{239}Pu cross sections.

[1]D. A. Brown et al. 2018. "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-Project Cross Sections, New Standards and Thermal Scattering Data," Nuclear Data Sheets **148**, pp. 1–142.

[2]M. B. Chadwick et al. 2011. "ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data," Nuclear Data Sheets **112**, Issue 12, pp. 2887–2996.

Numerical Benchmark Calculations

A suite of benchmark problems for single fuel pins and assemblies was developed for LWR and various advanced reactor fuels, including oxide and metal fuel–based SFR systems, thermal and fast molten salt reactors (MSRs), and pebble and prismatic HTGRs. The ENDF/B-VII.1 and VIII.0 benchmark results were compared for various conditions, such as different moderator densities, burnups, and temperatures. Although the eigenvalues of the pressurized water reactor and thermal MSR systems show only a small difference between the two ENDF/B libraries, the eigenvalues for BWR fuel calculations differ by up to 500 pcm, depending on the void fraction. For low void fractions, the eigenvalue is a few hundred pcm smaller for ENDF/B-VIII.0, whereas it is larger for high void fractions. The eigenvalues for EBR-II SFR with highly enriched uranium are up to 500 pcm smaller when using ENDF/B-VIII.0 compared with ENDF/B-VII.1. The SFR systems with metal and oxide fuel and the fast-spectrum MSR system show larger eigenvalues with ENDF/B-VIII.0, in the range 300–1,200 pcm, depending on the temperature and coolant density. The largest outlier is observed in the results for the metallic fuel SFR system, which is characterized by a harder neutron spectrum compared with the other systems.

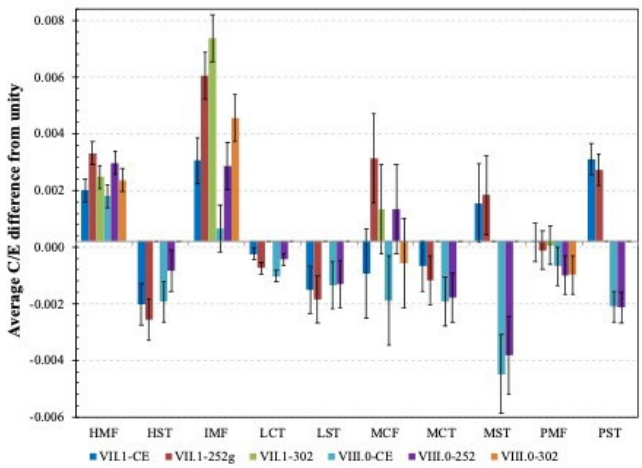
VALID Benchmark Calculations

Benchmark calculations were performed using the SCALE Monte Carlo codes KENO-V.a and KENO-VI, with ENDF/B-VII.0 and VIII.0 CE data and 252-group data, for over 600 critical experiments. These experiments are included in the Verified, Archived Library of Inputs and Data (VALID), covering various fissile materials, physical forms of the fissile material, and neutron flux spectra. The benchmark results are reported in terms of the calculated-to-experimental (C/E) ratio. Figure 9 shows the average C/E difference from unity for various categories of experiments. (Note that 302-group results are only reported for fast spectrum systems).

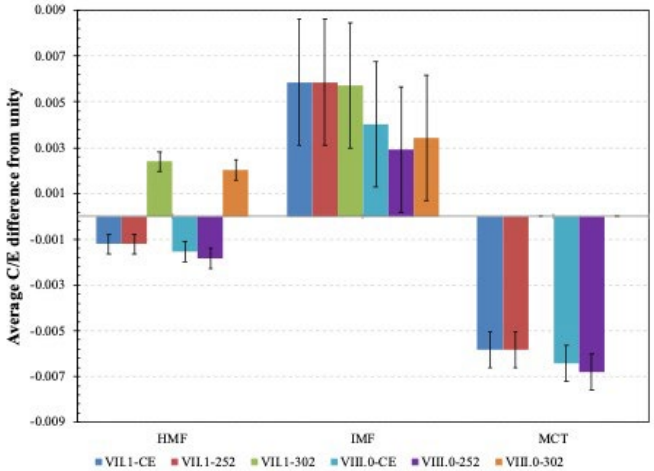
For the thermal systems, the CE and 252-group bias is significantly different between the ENDF/B-VII.1 and VIII.0 calculations of the mixed U and Pu solution thermal spectrum (MST) and Pu solution thermal spectrum categories. For the MET-SOL-THERM experiments, a slight overestimation of the benchmark results with ENDF/B-VII.1 becomes an underestimation of ~0.4% with the ENDF/B-VIII.0 results. For the PU-SOL-THERM results, a positive bias of ~0.3% with the ENDF/B-VII.1 data becomes an underestimation of the same magnitude with the ENDF/B-VIII.0 data. This is most likely the result of the updated ^{239}Pu cross sections, as shown in Figure 8. For some of the fast systems, the eigenvalues of the ENDF/B-VIII.0 calculations were significantly reduced compared with the corresponding ENDF/B-VII.1 eigenvalues, leading to smaller biases for intermediate-enriched U metal fast spectrum systems, but slightly larger biases for mixed compound fast spectrum and Pu metal fast spectrum systems.

[3]Nuclear Energy Agency. 2010. *International Handbook of Evaluated Criticality Safety Benchmark Experiments.* NEA/NSC/DOC(95)03, Nuclear Energy Agency/Organization for Economic Cooperation and Development.

[4]E. M. Saylor, W. J. Marshall, J. B. Clarity, Z. J. Clifton, and B. T. Rearden. 2018. "Criticality Safety Validation of SCALE 6.2.2." ORNL/TM-2018/884, Oak Ridge National Laboratory.



[KENO-V.a]



[KENO-VI]

Figure 9. Absolute bias for the category of experiments.

Employee Spotlight: Dr. Kursat Bekar

Position: Research and Development Staff, Radiation Transport Group, SCALE CSAS Product Owner

Focus Areas: Radiation transport, nuclear criticality safety, reactor physics, radiation shielding design and dosimetry analysis

Most Memorable Projects

Since joining ORNL in 2008, Dr. Kursat Bekar has been involved in a wide variety of projects, including code development and modernization activities in SCALE. One of his most memorable endeavors was to implement parallel execution capabilities to the KENO legacy Monte Carlo transport code in SCALE. He describes it as an exciting opportunity for him since parallelizing KENO was one of his dreams as a master's student in Turkey years ago. This new implementation was just as challenging as it was exciting since KENO had many ancient components and traces of different code development aspects that had evolved since the 1970s, when the first version of the code was released. Ultimately, addressing all these challenges and developing a new parallel framework were a great opportunity for Dr. Bekar to gain more knowledge and expertise in code design. This effort prepared him for the next phase in SCALE modernization activities. He was proud to see that implementing parallel KENO as part of SCALE allowed for faster calculations in very complex models that previously took days to several months to complete.

Life outside of Work

Kursat enjoys spending time with his wife and daughter. He loves cooking, and his family life is centered on it. When at home, he often tries to make time for experimenting with new recipes. Kursat also enjoys spending his spare time outdoors with his family. Hiking and trout fishing are his favorite activities in the East Tennessee wilderness.

Figure 10. Dr. Kursat Bekar.

Employee Spotlight: Dr. Andrew M. Holcomb

Position: Research and Development Staff Member, Nuclear Data and Criticality Safety

SCALE Data Product Owner

Focus Areas: Nuclear data evaluation, processing, advanced representations, testing, validation, and covariances; MG self-shielding methods

Developer: SCALE, AMPX, SAMMY

Most Memorable Projects

During his first year as a postdoctoral researcher in the Nuclear Data and Criticality Safety Group, Dr. Andrew Holcomb was tasked with identifying and resolving a deficiency in the URR energy treatment (probability tables), which only manifested itself in certain fast-spectrum systems with particular subsets of actinides. Dr. Holcomb spent several months working with ORNL staff and external collaborators to track down the root problem, all while gaining valuable knowledge about the inner workings of AMPX and SCALE. He eventually identified and patched the underlying issue, and the new data and improved results are incorporated into the SCALE 6.3 release of the ENDF-7.1 and ENDF-8.0 data libraries.

Dr. Holcomb also worked on implementing a new AMPX module to generate a Windowed Multipole Library Format for use in the Shift Monte Carlo radiation transport code. The new method will allow on-the-fly temperature dependence in continuous-energy neutron cross sections for use on accelerated hardware, greatly reducing the memory footprint. The library is targeted to recreate the temperature-broadened *1D* CE neutron cross sections to within 0.5% at every point on the energy grid for all isotopes. This new library will be used as part of the DOE Exascale Computing Project (ECP) ExaSMR to allow for a rigorous representation of SMR temperature gradients and depletion steps.

Figure 11. Andrew and Marissa's couple's costume for 2018, the frog and the princess.

Currently, Dr. Holcomb is finalizing a new package, *epic*, which couples the US Nuclear Regulatory Commission (NRC) FAST (Fuel Analysis under Steady-state and Transients) fuel performance code to SCALE MG neutronics. FAST will provide model parameters to *epic*, which will automatically generate and run a corresponding t6-depl input. The output from *epic* will provide updated power profiles back to FAST. Dr. Holcomb is also excited about his upcoming work with the SCALE covariance data and implementing/refactoring self-shielding methods into XSProc and Polaris.

Life outside of Work

When the weather is nice, Dr. Holcomb enjoys hiking and gardening with his wife. During the fall, you will find him cheering for/commiserating about the University of Florida football team. Dr. Holcomb also enjoys one-on-one book clubs, and he enjoys trading book recommendations with close friends to find interesting topics and spark fun discussions.

Recent SCALE Publications

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SCALE Direction Team

The SCALE code system is developed, deployed, and supported by dozens of staff members throughout the Reactor and Nuclear System Division at ORNL. All SCALE activities are coordinated to facilitate consistency throughout the project, especially in the application of quality assurance, development practices, and testing strategies. The development process was overhauled in 2019, and new members were added to the SCALE Direction Team in coordination, sponsor support, and line management roles. The Direction Team meets regularly to discuss the current status and to make programmatic and managerial decisions regarding SCALE.

Figure 12. SCALE Direction Team (left to right):
Matt Jessee, NRC Sponsor Representative; B.J. Marshall, NCSP Sponsor Representative; Will Wieselquist, Director; Germina Ilas, User Support and Training Coordinator; Rob Lefebvre, Production Coordinator; Marsha Henley, Quality Coordinator; Bob Grove, Group Leader, Radiation Transport; and Doug Bowen, Group Leader, Nuclear Data & Criticality Safety (not pictured: Seth Johnson, Technology Coordinator).

Upcoming SCALE Training Courses

Training courses are presented by developers and expert users from the SCALE Team. These courses include reviews of theory, as well as descriptions of capabilities and software limitations. Hands-on exercises at varying levels of complexity are included.

All SCALE training course attendees must be licensed users of SCALE 6.2, which is available from ORNL/Radiation Safety Information Computational Center (RSICC) (https://rsicc.ornl.gov/Login.aspx?p=po) in the United States, the Organisation for Economic Cooperation and Development (OECD) OECD/ Nuclear Energy Agency (NEA) Data Bank (http://www.oecd-nea.org/databank) in France, and RIST (http://www.oecd-nea.org/dbcps) in Japan.

The next SCALE training series at ORNL will be held October 5–30, 2020. Registration will open soon. Course descriptions are provided on the SCALE website at https://www.ornl.gov/scale/scale-training.

The 2020 schedule of the training courses is as follows:

- **October 5–9:**
  SCALE Criticality Safety Calculations
- **October 12–16:**
  TRITON Lattice Physics and Depletion
- **October 19–23:**
  ORIGEN Standalone Fuel Depletion, Activation and Source Term Analysis
- **October 26–30:**
  Nuclear Data Fundamentals and AMPX Libraries Generation

Furthermore, in response to previous user requests, the training course "SCALE Computational Methods for Burnup Credit" will be offered in February 2021.

SCALE Users' Group Workshop

The second and third meetings of the annual SCALE Users' Group Workshop were held at ORNL in August 2018 and August 2019, respectively. The full agendas with links to the presentations and photos from the meetings are available at https://scalemeetings.ornl.gov/previous-workshops.

Figure 13. Participants in the SCALE Users' Group, August 2019.

Save the Date for the 2020 SCALE Users' Group Workshop!

This year, the meeting will be held virtually from ORNL on July 27–29, 2020. All SCALE users are invited to contribute with presentations and participate in discussions on impactful, innovative applications of SCALE. Registration is open on the meeting website at https://scalemeetings.ornl.gov. The meeting will be offered free of charge to all participants. Participation will be limited to 200 attendees.

A morning plenary session is planned for day 1 of the meeting. For afternoon of day 1 and all of day 2, there will be two concurrent tracks at any time: (1) technical presentations and/or discussions, and (2) hands-on tutorials. The morning of day 3 will be devoted exclusively to hands-on tutorials, followed by a closing discussion session that will be held that afternoon.

A total of eight 2-hour tutorials will be presented by developers and expert users of the SCALE Team. To facilitate an effective instructor-attendee interaction, registration will be limited to 20 attendees per tutorial.

The working titles of the tutorials are shown below, and the schedule for when each will be offered is included in the meeting agenda.

- Frequent Fulcrum Functions: The Basics of SCALE's Graphical User Interface
- Generation of SCALE Multigroup Libraries for Advanced Reactors using AMPX
- LWR Depletion Analysis with Polaris
- SCALE Utilities for Nuclear Data Interrogation, Comparison, and Visualization
- Crossing the Streams—Sampler and the Template Engine
- Advanced User Interface for Advanced Reactors
- Activation Analysis with ORIGEN/MAVRIC for Advanced Reactors
- Advanced Reactor Safeguards Example

User Support and Training

The SCALE Team is dedicated to supporting all SCALE users. The team provides limited complimentary technical support for inquiries submitted to scalehelp@ornl.gov. For basic help getting started with SCALE, new users are encouraged to attend the public training courses in which SCALE capabilities are presented in detail and the annual SCALE Users' Group Workshop (https://scalemeetings.ornl.gov). SCALE training blocks are offered twice annually at ORNL, usually in February–March and October–November. Additionally, two SCALE training courses per year are hosted by OECD/NEA in France, usually in March. Updates on training courses are available on the SCALE website (https://www.ornl.gov/scale/scale-training).

Direct links to the SCALE manual and other user documentations are available on the SCALE website. To facilitate interaction among SCALE users and developers, the SCALE Users Group forum hosted by Google is available at https://groups.google.com/forum/?hl=en&fromgroups#!forum/scale-users-group.

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

SCALE use worldwide

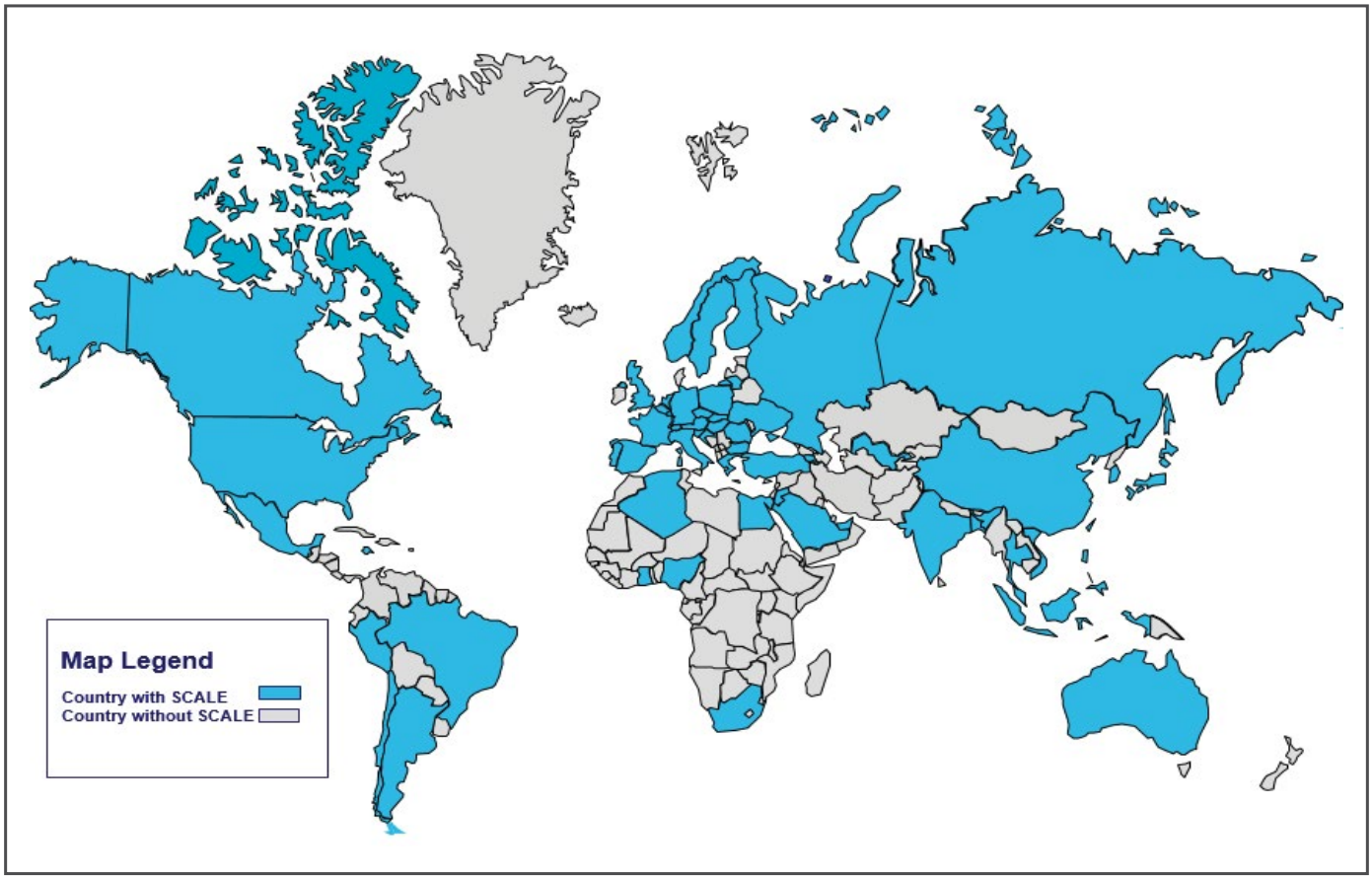

Figure 14. Nations where SCALE is licensed.

Recent SCALE Training Events

Figure 15. "SCALE Criticality Safety and Radiation Shielding" course, OECD/NEA, September 2018.

Figure 16. "SCALE/TRITON Lattice Physics and Depletion" course, ORNL, October 2018.

Figure 17. "SCALE/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis" course, ORNL, October 2018.

Figure 18. "SCALE Criticality Safety and Radiation Shielding" course, ORNL, November 2018.

Figure 19. "SCALE Criticality Safety Calculations" course, ORNL, February 2019.

Figure 20. "Nuclear Data Fundamentals and AMPX Libraries Generation" course, ORNL, February 2019.

Figure 21. "Source Terms and Radiation Shielding for Spent Fuel Transportation and Storage Applications" course, ORNL, February 2019.

Figure 22. "SCALE Criticality Safety and Radiation Shielding" course, OECD/NEA, March 2019.

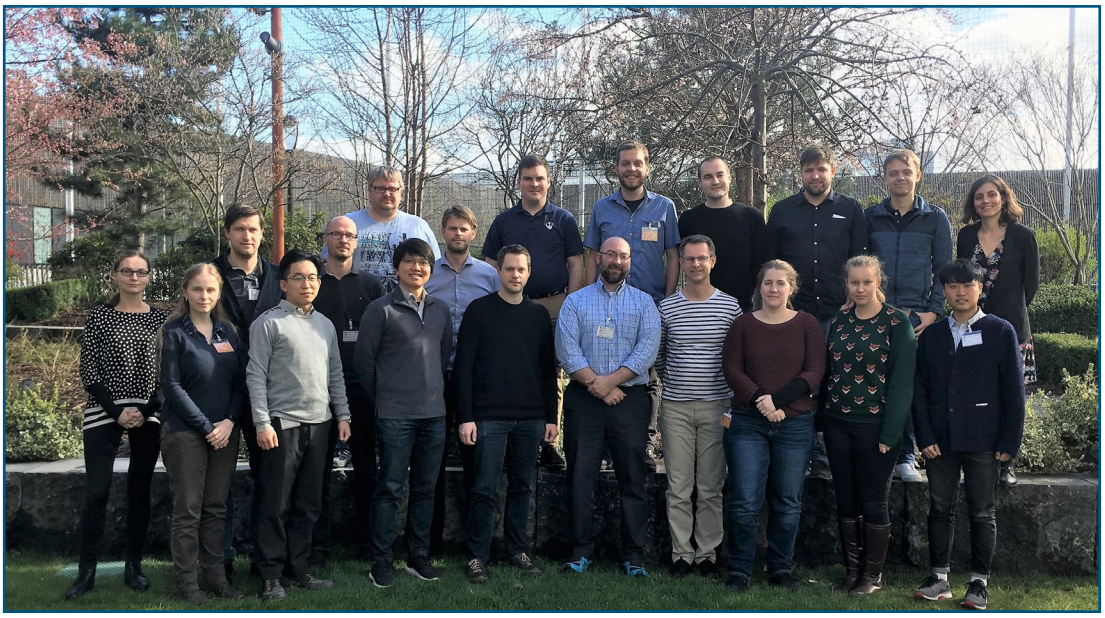

Figure 23. "SCALE/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis" course, OECD/NEA, March 2019.

Figure 24. "SCALE/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis" course, ORNL, Fall 2019.

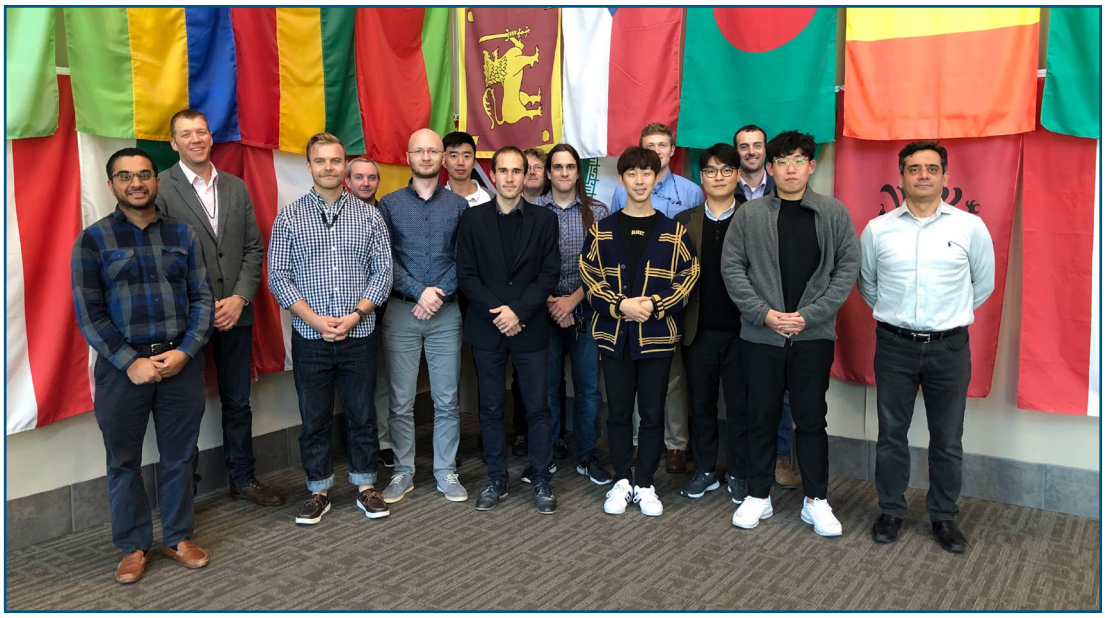

Figure 25. "SCALE/TRITON Lattice Physics and Depletion" course, ORNL, Fall 2019.

Figure 26. "SCALE/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis" course, ORNL, February 2020.

Figure 27. "SCALE Criticality Safety and Radiation Shielding" course, ORNL, February 2020.

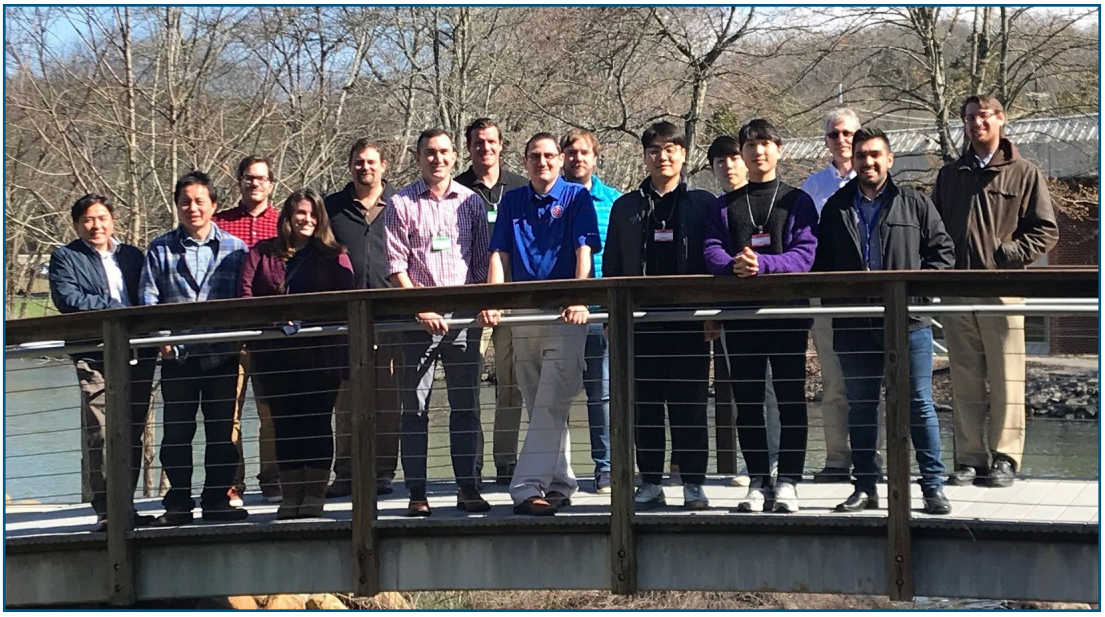

Figure 28. "SCALE Sensitivity and Uncertainty Analysis for Criticality Safety Assessment and Validation" course, ORNL, February 2020.

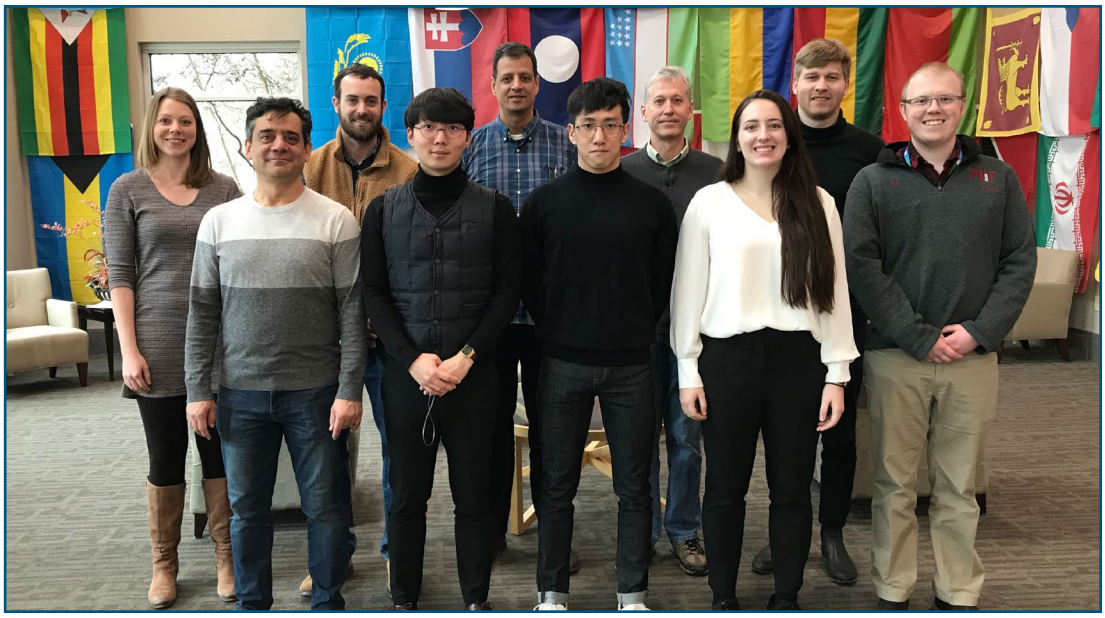

Figure 29. "SCALE/Polaris Lattice Physics, Depletion, and Uncertainty Analysis" course, ORNL, February 2020.

Nuclear Systems Modeling & Simulation

SCALE Newsletter

Oak Ridge National Laboratory
Post Office Box 2008, Bldg. 5700
Oak Ridge, TN 37831-6003

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