Oak Ridge National Laboratory

SCALE Newsletter

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IN THIS ISSUE

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Welcome to the 50th edition of the updated SCALE newsletter! Here we present the latest relevant content on the SCALE Code System in a newly designed format. Our website has also been updated with current information on our capabilities, quality assurance, training schedule, public training material, user primers, journal publications, technical reports, and additional resources. Please visit http://scale.ornl.gov to see more.

We are excited to introduce the inaugural SCALE Users' Group Workshop hosted at Oak Ridge National Laboratory (ORNL) on September 26–28, 2017. The workshop is open to anyone, with opportunities for user presentations and panel discussions on SCALE applications for neutronics analysis across our growing 8,000-member worldwide user base. The workshop schedule and registration information are provided at https://scale2017.ornl.gov.

In May of 2017, SCALE 6.2.2 was made available as a download for current users and through the Radiation Safety Information Computational Center (RSICC) for new users. The update features improvements to computational performance and the Fulcrum user interface, and several new capabilities have been introduced into the Polaris lattice physics code for boiling water reactor (BWR) modeling. Details on the SCALE 6.2.2 update and Polaris capabilities are provided on page 2.

We continue to emphasize training to help users gain practical experience using SCALE to perform design and licensing calculations. The training schedule for October 2017 is provided on pages 15 and 16, while several past training courses are highlighted on page 19.

This newsletter presents the ORNL SCALE team's continued research and development on multiple fronts, including continuous-energy Monte Carlo depletion, molten salt reactor modeling, sodium fast reactor modeling, sensitivity and uncertainty analysis for isotope production, and many others. We thank you and appreciate your continued use of SCALE, and we look forward to seeing you at the workshop this September.

scale
Nuclear Systems Modeling & Simulation

SCALE 6.2.2 Update

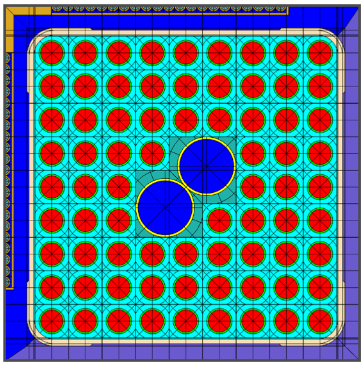
The SCALE 6.2.2 update is available for SCALE 6.2 and SCALE 6.2.1 users as of June 2017, providing enhanced features and performance in the areas detailed below. This update is provided as a download and is recommended for all SCALE 6.2 and 6.2.1 users. New licenses for SCALE 6.2.1 will include the SCALE 6.2.2 update. SCALE 6.2.2 incorporates all updates made since the SCALE 6.2 release so users can proceed directly to the SCALE 6.2.2 update even if SCALE 6.2.1 has not been applied.

General Enhancements Available in Many SCALE Sequences

Oxygen-18 (^{18}O) cross section treatment: SCALE 6.2.2 includes an update to address a deficiency in ENDF/B-VII.0 and VII.1 where no cross section data are available for ^{18}O, even though the natural abundance of oxygen includes 0.2% ^{18}O. When using the SCALE Standard Composition Library with natural abundances, materials with missing cross sections are omitted from the material data before the calculation proceeds by setting the number density to zero. As such, a small amount of mass is removed when natural abundance oxygen is used in a model. To resolve this issue, a new feature was implemented for all sequences in SCALE 6.2.2 in that a zero-valued cross section is added for ^{18}O so that material masses are maintained. Criticality and shielding calculations will generate the same results when using either a zero number density or a zero cross section. Depletion calculations may demonstrate an insignificant variation due to the use of specific powers that use the system mass, which will vary slightly with this update. However, all material tables will demonstrate that mass is preserved, while warning messages merely note that a zero cross section was used because the material is not available on the specified library.

Doppler broadening of ZrH thermal moderators: Thermal moderator Doppler broadening in continuous-energy Monte Carlo calculations was improved to address an issue that caused a large bias in results for systems containing ZrH. Any temperature-corrected continuous-energy calculations for systems with ZrH should be rerun with the new SCALE version.

Polaris



Polaris model for GE 9 × 9 assembly.

With SCALE 6.2.2, several new features were implemented for Polaris to model boiling water reactor (BWR) geometries. Moreover, the abilities to specify time-dependent state properties and to specify one or more depletion histories were added. Improvements to existing input cards were also implemented.

To maximize backwards compatibility for input files developed with SCALE 6.2 and SCALE 6.2.1, the new and modified input cards are not available by default with SCALE 6.2.2. The new and modified input cards are activated if the input file begins with =polaris_6.3 rather than =polaris. The suffix "_6.3" is an indicator to the Polaris input processor to use the SCALE 6.3 input format. For the future release SCALE 6.3, the original input cards supported in the SCALE 6.2 input format will be available if the input file begins with =polaris_6.2.

The new input cards to model BWR geometries include:

- **cross** – defines the interior water cross geometry of SVEA assembly designs
- **dxmap** (or **dymap**) – defines displacement maps that indicate translation of the pin center in the x- (or y-) direction
- **control <BLADE>** – defines the control blade geometry

- **mesh** – defines advanced spatial meshing options for different materials
- **option <GEOM>** – defines geometry tolerances, advance meshing options, and plotting options

The modified input cards to model BWR geometries include:

- **pin** – defines circular- and square-based geometry zones, as well as arbitrarily sized pins (e.g., size=1.5 water rod in some 9 × 9 BWR lattice designs
- **box** – defines channel box geometry with an arbitrary number of zones and cutout regions

The new input cards for time-dependent modeling include:

- **history** – defines one or more operating histories in the input file
- **bui** (or **ti**) – defines restart cumulative burnup (or time) values

The modified input cards for time-dependent modeling include:

- **state** – defines one or more time-independent or time-dependent state properties
- **bu** (or **t**) – defines cumulative burnup (or time) values
- **dbu** (or **dt**) – defines incremental burnup (or time) values

Example input files are included in SCALE 6.2.2 in the ${SCALE}/regression/input directory:

- polaris.6.3.atrium9x9.inp and polaris.6.3.atrium10x10.inp – prototypic ATRIUM models
- polaris.6.3.blade1.inp and polaris.6.3.blade2.inp – control <BLADE> examples
- polaris.6.3.ge7x7.inp through polaris.6.3.ge10x10.inp – prototypic GE models
- polaris.6.3.svea100.inp and polaris.6.3.svea64.inp – prototypic SVEA models
- polarisHistory.inp: history example

TRITON

T-DEPL ASSIGN capability: The TRITON T-DEPL ASSIGN feature is enabled for problems with BRANCH, TIMETABLE, and SWAP definitions.

TRITON depletion with CE-KENO: A discrepancy was introduced in SCALE 6.2.1 for continuous-energy TRITON/KENO calculations that included both a TIMETABLE input block and carbon in a depleted mixture, which can lead to erroneous isotopic predictions. This issue was not present in SCALE 6.2. Any SCALE 6.2.1 continuous-energy TRITON/KENO calculations that include a TIMETABLE and carbon in a depleted mixture should be rerun with SCALE 6.2.2.

TRITON depletion with MG-KENO: TRITON/KENO multigroup depletion with DOUBLEHET multigroup processing was enhanced to complete all requested burnup steps where previous calculations would sometimes terminate prematurely.

"nubar" component in TRITON-generated libraries for ORIGEN: ORIGEN has a special, rarely used, "k-infinity" output option. This k-infinity is calculated as "nubar*sigma_f/sigma_a," where "nubar" is the average number of neutrons per fission, "sigma_f" is the fission cross section, and "sigma_a" is the absorption cross section. The data used for this calculation are taken from the ORIGEN library file produced by TRITON (f33 file). TRITON in SCALE 6.2 and 6.2.1 is not correctly setting the "nubar" component in this file, and all ORIGEN reactor libraries distributed with SCALE (in ${DATA}/arplibs directory) are affected by this. This issue has been addressed in the SCALE 6.2.2 update. **Note, this does not affect the accuracy of depletion calculations with TRITON or ORIGEN in SCALE 6.2, only the special k-infinity output, if requested in ORIGEN.**

TRITON edits: Printed information for TRITON branch case calculations has been enhanced to provide more complete state information.

TSUNAMI

CE TSUNAMI-3D calculations using the Iterated Fission Probability (IFP) and Generalized Perturbation Theory (GPT) methods now use the variance reduction technique of Monte Carlo particle splitting which was disabled for these specific sensitivity methods in SCALE 6.2 and 6.2.1. The results for IFP and GPT calculations with SCALE 6.2.2 will vary from previous results within the stochastic uncertainty of the calculation, but the runtimes will be improved by 10–40%.

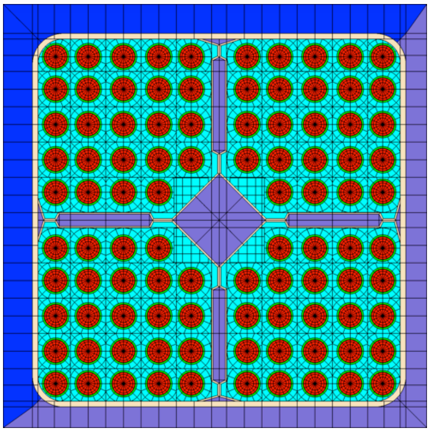
CE TSUNAMI-3D, using the CLUTCH method (i.e., CET=1), was updated to correct a rare issue. In only one case, it was found that the importance function portion of the CLUTCH calculation becomes corrupted, creating unreasonable sensitivity coefficients with very large uncertainties. CLUTCH calculations that may be corrupted by this identified bug would run to completion, but they would not match direct perturbation confirmations. Any previous CLUTCH calculations that display these aspects should be rerun with SCALE 6.2.2.

SAMS was updated to correctly process a user-specified covariance data file. Previous calculations that used the COVERX= input to specify a non-default covariance file should be checked to confirm that the desired covariance file was used.

Minor Miscellaneous Issues Resolved:

- An issue was corrected in which .plt files were sometimes not returned to the output directory when running many simultaneous calculations.
- USLSTATS was updated to improve stability for cases in which it would fail to run to completion.
- ORIGAMI was updated to correct an issue in which MCNP-formatted material cards sometimes contained incorrect number densities. Previous calculations with ORIGAMI to generate MCNP material cards should be checked to confirm the number densities.
- Sampler was enhanced for improved stability on Windows.
- Minor issues with legacy ORIGEN FIDO formatted input were corrected.
- Several minor enhancements in output information were incorporated.
- Several minor enhancements in the Fulcrum user interface were incorporated.
- Minor discrepancies in the user documentation were also corrected.

Introducing Polaris

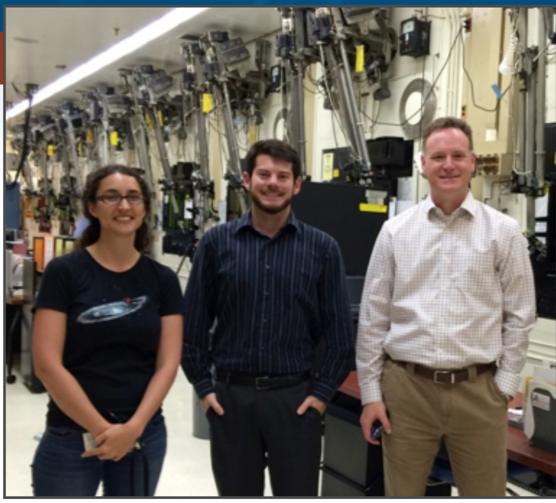


Polaris model for SVEA-96 assembly.

Polaris, an easy-to-use lattice physics capability for light water reactor assemblies, was introduced in SCALE 6.2 (April 2016). Polaris uses advanced calculation methods for performing lattice physics analysis, including (1) the embedded self-shielding method for cross section processing, (2) a new transport solver based on the method of characteristics, (3) the ORIGEN depletion solver, and (4) automated assembly geometry processing based on simplified user input format.

Several enhancements were introduced into Polaris as part of the SCALE 6.2.1 and 6.2.2 updates. In SCALE 6.2.1, Polaris' accuracy was significantly enhanced by adding anisotropic scattering (only transport-corrected isotropic scattering in SCALE 6.2) and improved hydrogen transport cross sections for diffusion coefficient calculations. In SCALE 6.2.2, several new input cards were added to Polaris to model boiling water reactor (BWR) geometries. The BWR input cards include (1) the ability to model complicated water cross geometries for SVEA assemblies, (2) a square-shaped water box for ATRIUM assembly designs, (3) the displacement of fuel pins from their nominal location, and (4) several options to model control blade insertions. An example of the geometry model for a SVEA-96 assembly is shown here.

Additional input cards have been implemented to model time-dependent changes in system properties such as void fraction, boron concentration, fuel temperature, and insertion/removal of control or insert maps. Polaris also includes the ability to specify one or more history calculations in a single input file. The new input cards are described in detail in the Polaris section of the SCALE 6.2.2 Manual. Look for new features of Polaris in featured 6.2 updates and also in SCALE 6.3.



Team members Susan Hogle, Chris Perfetti, and Brad Rearden tour ORNL's Radiochemical Engineering Development Center, where ^{252}Cf isotopes are extracted from HFIR isotope production targets.

Using Sensitivity Coefficients to Optimize the Design of ^{252}Cf Isotope Production Targets

For SCALE 6.2, the KENO-based TSUNAMI-3D sequence was enhanced with a unique capability to calculate sensitivity coefficients for ratios of reaction rates via Generalized Perturbation Theory. This was accomplished using high-fidelity continuous-energy physics. This capability was employed to optimize the design of ^{252}Cf radioisotope production targets in the High Flux Isotope Reactor at Oak Ridge National Laboratory. Only about 1% of the initial and very valuable heavy actinide feedstock is converted into ^{252}Cf – the remaining 99% of the heavy actinides are destroyed through fission reactions. This study used the TSUNAMI-3D sensitivity coefficient capabilities to predict the sensitivity of capture-to-fission ratios in ^{252}Cf isotope production targets. The goal was to identify a target design that would maximize these capture-to-fission ratios.

In addition to the parallel KENO version of TSUNAMI-3D deployed with SCALE 6.2, these new TSUNAMI-3D sensitivity analysis capabilities were also implemented in the Shift high performance computing Monte Carlo code, which is planned for initial release with SCALE 6.3. The results of this implementation were promising, resulting in sensitivity calculations that scaled in parallel simulations with reasonable efficiency on more than 1,000 processors. The TSUNAMI-3D sensitivity analyses indicated that using production targets with a lower density of heavy actinides would improve the yield of ^{252}Cf by approximately 13%. This behavior suggests that

- self-shielding effects were depressing the neutron flux inside the isotope production targets at energies likely to cause helpful neutron capture/transmutation events, and
- lowering the density of the targets helps to mitigate these self-shielding effects.

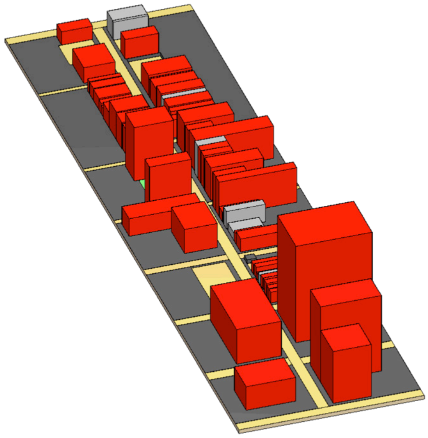
Additional analyses were performed to further optimize the ^{252}Cf isotope production target design by using neutron filter materials to block neutrons at energies likely to induce fission in heavy actinide isotopes. The net effect of the considered neutron filters was a ^{252}Cf transmutation process that may have been hundreds of percent more efficient in terms of heavy actinide feedstock consumption. However, it produced ^{252}Cf at a slower overall rate.

The results of the investigations demonstrated the potential of the TSUNAMI-3D tools for estimating the impact of design changes on the time-dependent transmutation of ^{252}Cf. The sensitivity coefficients were calculated for a single mid-cycle reactor state point and did not account for the change in sensitivity coefficients during the reactor cycle. Future studies may consider full time-dependence and could improve the predictive capability of the TSUNAMI sensitivity coefficients for time-dependent ^{252}Cf targets optimization.

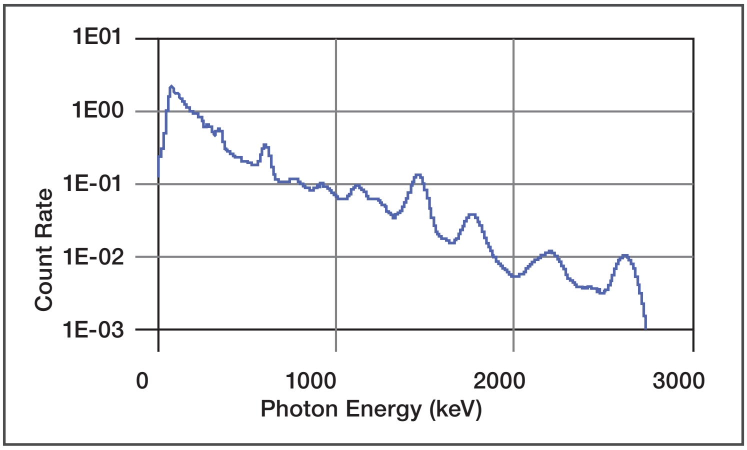
More information on this work is available in C. M. Perfetti, S. L. Hogle, S. R. Johnson, B. T. Rearden, T. M. Evans, "Optimizing HFIR Isotope Production through the Development of a Sensitivity-Informed Target Design Process," *Proc. of the 2017 International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C2017)*, Jeju, Korea, April 16–20, 2017.

Predicting Measured Count Rate Spectra with MAVRIC

An ongoing project at ORNL for the National Nuclear Security Administration is to use MAVRIC to generate synthetic detector data. These data can be used for testing source detection algorithms. Teams that search for radioactive/nuclear sources need to be able to differentiate threat sources from the background of naturally occurring radioactive materials (NORMs). With limited measurement times, it can be challenging to trigger an alarm for a threat source for the detection algorithms. This is especially true in urban environments with high NORMs. Using MAVRIC, the count rates from the K, U, and Th present in building materials, sidewalks, and roadways can be simulated. Count rates from injected threat sources can also be simulated. Using models such as the generic street model shown below, count rate spectra for vehicles driving down the street can be simulated and passed to different detection algorithms to evaluate their performance. MAVRIC uses CE-Monaco to find photon fluxes in 1 keV bins. These fluxes are then processed outside of SCALE to determine detector count rate spectra. The spectra are sampled for a number of detection events based on vehicle speed. A pilot competition open to the public will be held later this year to find the best detection algorithm.



MAVRIC model of generic urban street.



Background count rate spectra based on MAVRIC photon fluxes from all NORM sources.

References:

Douglas E. Peplow, Mathew W. Swinney, Gregory G. Davidson, Andrew D. Nicholson and Bruce W. Patton, "Initial Modeling of Urban Search Measurements," *Transactions of the American Nuclear Society* **116**, accepted for publication (2017).

Mathew W. Swinney, Douglas E. Peplow, and Andrew D. Nicholson, "Characterization of NORM in an Urban Environment using HPGe Measurements and MCNP6 Simulations," *Transactions of the American Nuclear Society* **116**, accepted for publication (2017).

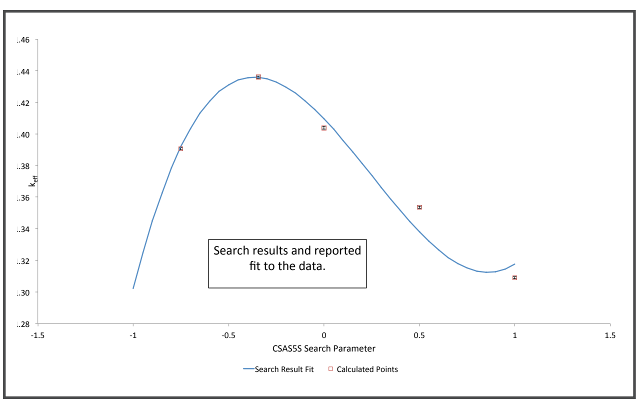
Andrew D. Nicholson, Irakli Garishvili, Douglas E. Peplow, Daniel E. Archer, William R. Ray, Mathew W. Swinney, Michael J. Willis, Gregory G. Davidson, Steven L. Cleveland, Bruce W. Patton, Donald E. Hornback, James J. Peltz, M. S. Lance K. McLean, Alexander A. Plionis, Brian J. Quiter, and Mark S. Bandstra, "Multi-Agency Urban Search Experiment Detector and Algorithm Test Bed," accepted for publication in *IEEE Transactions on Nuclear Science* **99** (2017).

A Better Option for Criticality Searches with Sampler

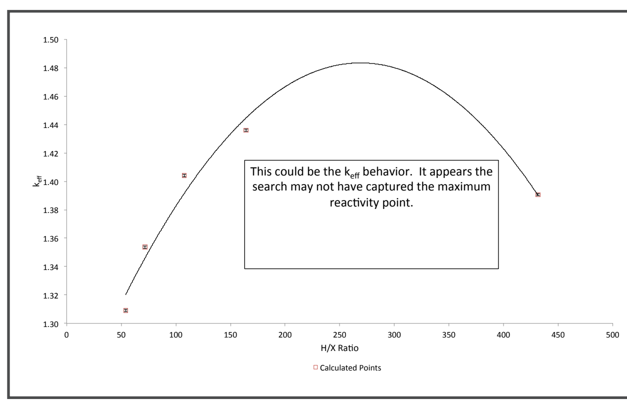
Criticality safety analysts often need to identify optimum configurations that maximize criticality, or they need to determine the combination of conditions that will lead to a desired condition (e.g., $k_{eff} = 1.0$).

Several decades ago, a search capability was included in the CSAS5S sequence. However, the capability can be difficult to use and may give the user a false sense of complete coverage of the search space. Therefore, the user is encouraged to try a more modern approach by performing CSAS calculations using the parametric mode introduced in Sampler with SCALE 6.2.1. Brief summaries of the main pitfalls of the current CSAS5S implementation, as well as an introduction to the Sampler parametric capability, are provided below.

The CSAS5S sequence provides powerful, very flexible search capabilities for the CSAS5 sequence. The first difficulty most users encounter is the input for the sequence. The input can be complicated due to the range of searches supported. Users can search on composition descriptions, array pitch, or geometric dimensions and then use a maximum, minimum, or fixed (critical) k_{eff} value as the target of the search. Other difficulties with the search capability arise from the fact that it has never been extended to CSAS6 and is no longer under active development. The results can be misleading, especially regarding the coverage of the search space with the explicit cases run. The search is performed on a search parameter which is calculated from the desired input parameters for the search. As shown in these figures, good coverage of the search parameter space does not necessarily translate into good coverage for the parameter of interest. In the example shown here, the parameter of interest was the H/X ratio.



Uniform coverage in "search parameter" space.



Nonuniform coverage in real parameter space.

Some users have recently reported having difficulty with CSAS5S in the SCALE 6.2 releases, specifically with the MAINTAIN command as part of generic geometry searches. Combined with the difficulties discussed above, this has led to the recommendation that users perform their own parametric searches of the parameters of interest within the desired range. This approach may require more calculations than the root finding approach in CSAS5S, but it is less likely to yield poor coverage. It is also easier to extract information about the general system behavior from a parametric search. The example Sampler input provided below illustrates an analysis considering the effect of variations in the outer radius of a bare sphere of uranium metal. The KENO input is embedded in a case block in the Sampler input. More details of the Sampler input are provided in Section 6.7 of the SCALE Manual. A plot of the resulting KENO k_{eff} estimates is included with the input.

Sample Setup

```
=sampler
'
read parameters
  run_cases = yes
end parameters
read parametric
  variables = radius end
  n_samples = 9 end
end parametric
'
```

CSAS input

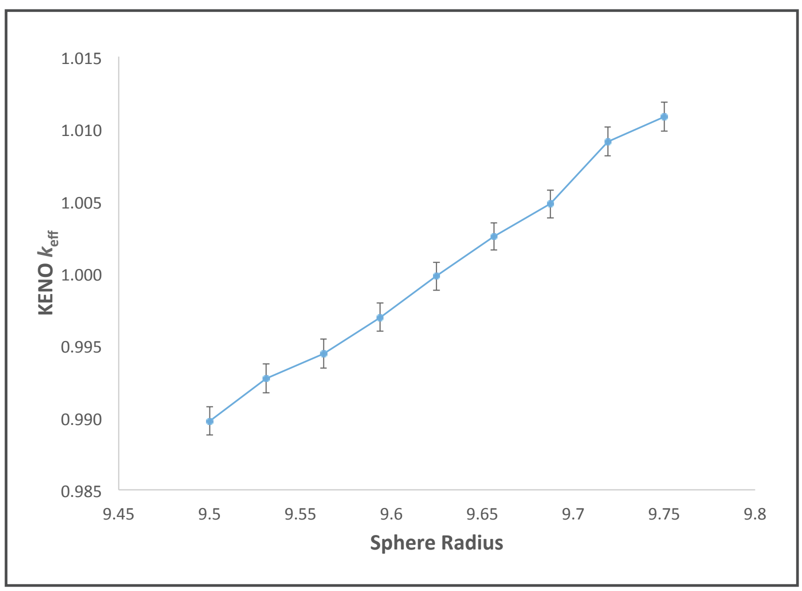
```
read case[bare_sphere]
 sequence=csas5 parm=()
bare_sphere
ce_v7.1_endf
read composition
 uranium     1 den=18.742 1 300
                         92235 80.0
                         92238 20.0 end
end composition
read parameter
 nsk=10 npg=5000 gen=10100 sig=0.001
 htm=no
end parameter
read geometry
global unit 1
 sphere 1 1   #{radius}
end geometry
end data
end sequence
end case
'
```

Establishment of Ranges

```
' sphere radius range
'
read variable[radius]
   distribution=uniform
   value=9.25
   minimum=9.5 maximum=9.75
   cases= bare_sphere end
end variable
'
```

Data collection

```
'  response block
'
read response[keff]
  type = grep
  regexp = ":kenova.keff:"
  eregexp = ":kenova.keff:"
end response
end
```



Dependency of eigenvalue on sphere radius.

Potential for Collision in Writing to Output Files

During execution, SCALE 6.2 generates the output file in the directory requested by the user. The default location of the output directory is the directory from which the input was submitted. This behavior is in most ways an improvement over the previous method of output generation. In prior versions of SCALE, each module created its portion of the output file in the temporary working directory during execution. At the completion of the execution, a script collected each of these small output files, concatenated them into the complete SCALE output file, and copied this file back to the requested location. Checking on the progress of a calculation therefore required the user to locate the temporary working directory and the appropriate file within that directory. Both complications are eliminated with the new output file generation approach in SCALE 6.2.

There is, however, a problem that can occur with the new scheme. If the same job is submitted multiple times and the calculations are running simultaneously, each instance of the job will write output to the same output file. This collision in the target output file results in a single file containing multiple complete outputs. These outputs are frequently intermingled with each other line by line. The most effective mitigation strategy available is to include the "-z" option to *scalerte* at execution. The use of this option results in the inclusion of the date and time that execution began within the output and message file names. The output file name then has the following format: BASENAME.YYYY.MM.DDTHH.MM.SS.out.

BASENAME is the name of the input file prior to the extension; for example, the BASENAME of my_final_file.inp is "my_final_file." YYYY is the four-digit year, MM is the two-digit month, and DD is the two-digit day. A capital "T" is included in the file name to separate the date from the time of execution. HH.MM.SS is the time execution of SCALE began, where HH is the two-digit hour (00–23), MM is the minute, and SS is the second. Further development is underway to design a complete solution to this issue for inclusion in a future release of SCALE.

Employee Spotlights

Sheila Walker

Appreciation for a Job Well Done

As the SCALE software coordinator, Sheila Walker has been instrumental in the development and support activities for SCALE since 2005. As of February 2017, Sheila started focusing only on her commitments and responsibilities for the Radiation Information Computational Center (RSICC). In her role as SCALE software coordinator, Sheila was responsible for supporting a wide range of tasks, including SCALE training registration and administration, SCALE manual documentation, SCALE quality assurance coordination, scalehelp@ornl.gov support, and SCALE newsletter editing. Sheila's positive attitude, energy, contagious smile, and deep well of patience dealing with SCALE managers, trainers, code developers, and occasionally users has been much appreciated by everyone. She will truly be missed. We wish Sheila all the best with her professional and personal endeavors.

Dr. Benjamin R. Betzler

Dr. Benjamin R. Betzler

Position: Research and Development Staff, Reactor Physics Group
Focus areas: Reactor physics, advanced reactor modeling and simulation, fuel cycle analysis

Most memorable projects:

Dr. Betzler joined ORNL in 2014 as a postdoctoral researcher and initially worked on updating the SCALE reactor libraries for the 6.2 release. He also supported verification and validation of the SCALE lattice physics modules Polaris and TRITON. In 2016, Dr. Betzler became an R&D staff member in the Reactor Physics Group.

His current project to implement molten salt reactor (MSR) tools into SCALE is a significant effort. For Dr. Betzler and collaborators Nicholas Brown (Penn State University), Jeff Powers, and Brad Rearden, the research is centered on improving and coupling separate simulation tools--one that looks at neutron transport and another that analyzes fuel makeup--for complete analysis of the system. Neutron transport is challenging to predict in liquid fuel MSR designs, as neutrons can be generated in the coolant loops away from the main reactor vessel. With MSR fuel, composition can change dramatically due to the ability to remove fuel and fission products during operation to keep the systems efficient and void of isotopes that could damage equipment.

Because the current fleet of light water reactors has neither of these characteristics, very few tools are able to simulate these operations. And with numerous companies working on MSR concepts, these tools are vital in determining viability of a design by identifying key issues that could arise during the life of the reactor.

“Our goal is to make the tool set as generic as possible, so it is accessible to a variety of users, easy to use, and accurate,” Betzler said. “The ultimate driver is to release the code, and whoever wants to do analysis on MSRs can take it and study the impact of different design parameters on a reactor core.”

Life outside of work:

During the summer, Dr. Betzler spends much of his time gardening. He also enjoys coaching and playing hockey, cooking, and volunteering in the local community. Dr. Betzler is also a passionate supporter of the University of Michigan—where he earned his BSE, MSE, and PhD in nuclear engineering—with a particular interest in Wolverine football. As a member of the local ANS chapter, he currently serves as the chair.

Recent Publications

Journal

B. Betzler, D. Chandler, E. Davidson, G. Ilas, "High-Fidelity Modeling and Simulation for a High Flux Isotope Reactor Low-Enriched Uranium Core Design," *Nuclear Science and Engineering* (2017). http://dx.doi.org/10.1080/00295639.2017.1292090

B. R. Betzler, J. J. Powers, and A. Worrall, "Molten salt reactor neutronics and fuel cycle modeling and simulation with SCALE," *Annals of Nuclear Energy* 101, 489–503 (2017). http://dx.doi.org/10.1016/j.anucene.2016.11.040

J. Hu, J. M. Giaquinto, I. C. Gauld, G. Ilas, and T. J. Keever, "Analysis of new measurements of Calvert Cliffs spent fuel samples using SCALE 6.2," *Annals of Nuclear Energy* 106, 221–234 (2017). http://dx.doi.org/10.1016/j.anucene.2017.04.005

G. Ilas and H. Liljenfeldt, "Decay heat uncertainty for BWR used fuel due to modeling and nuclear data uncertainties," *Nuclear Engineering and Design* 319, 176–184 (2017). https://doi.org/10.1016/j.nucengdes.2017.05.009

J. A. Favorite, Z. Perkó, B. C. Kiedrowski, and C. M. Perfetti, "Adjoint-Based Sensitivity and Uncertainty Analysis for Density and Composition: A User's Guide," Nucl. Sci. Eng. 185, 3, 384–405 (2017).

C. M. Perfetti and B. T. Rearden, "Diagnosing Undersampling in Monte Carlo Eigenvalue and Flux Tally Estimates," *Nuclear Science and Engineering 2017*185, 1 (2017).

http://dx.doi.org/10.13182/NSE16-54

Other

***Proceedings of the 2017 International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering* (M&C 2017), Jeju, Korea, April 16–20, 2017**

C. M. Perfetti, S. L. Hogle, S. R. Johnson, B. T. Rearden, and T. M. Evans, "Optimizing HFIR Isotope Production through the Development of a Sensitivity-Informed Target Design Process."

C. M. Perfetti and B. T. Rearden, "Continued Investigation of Metrics for Predicting Undersampling Biases in Monte Carlo Simulations"

A. Alhajri, V. Sobes, C. M. Perfetti, and B. Forget, "Calculating Resonance Parameter Sensitivity Coefficients in SCALE."

B. R. Betzler, J. J. Powers, N. R. Brown, and B. T. Rearden, "Molten Salt Reactor Neutronics Tools in SCALE."

B. T. Rearden, B. R. Betzler, M. A. Jessee, W. J. Marshall, U. Mertyurek, and M. L. Williams, "Accuracy and Runtime Improvements with SCALE 6.2."

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SCALE Team Structure

Leadership Team

Brad Rearden *(Manager)*
SCALE Code System

Matt Jessee *(Deputy Manager)*
SCALE Code System

Steve Bowman *(Group Leader)*
Reactor Physics

Will Wieselquist *(R&D Staff)*
Reactor Physics

Doug Bowen *(Group Leader)*
Nuclear Data and Criticality Safety

Bob Grove *(Group Leader)*
Radiation Transport

Rob Lefebvre *(R&D Staff)*
Software Development Coordinator

Infrastructure Development and and Software Support

Tony Walsh
Seth Johnson
Brandon Langley
Jordan Lefebvre
Rob Lefebvre
Adam Thompson
Marsha Henley

Quality Assurance System; Build and Test Framework; Deployment

Monte Carlo Methods

Brad Rearden
Brian Ade
Kaushik Banerjee
Kursat Bekar
Cihangir Celik
Greg Davidson
Tom Evans
Cole Gentry
Shane Hart
Germina Ilas
Seth Johnson
Tara Pandya
Chris Perfetti
Katherine Royston
Doro Wiarda
Steve Wilson

KENO/CSAS; MAVRIC/Monaco; Shift; Sourcerer

Depletion, Decay, and Activation Methods

Will Wieselquist
Ian Gauld
Shane Hart
Germina Ilas
Thomas Miller
Steve Skutnik (UT)
Doro Wiarda
Mark Williams

ORIGEN; ORIGAMI; Depletion, Decay, and Activation Data

Sensitivity and Uncertainty Analysis

Mark Williams
Goran Arbanas
Aaron Beville
Keith Bledsoe
Matt Jessee
Elizabeth Jones
Jordan Lefebvre
B.J. Marshall
Ugur Mertyurek
Thomas Miller
Chris Perfetti
Vladimir Sobes
Will Wieselquist

TSUNAMI; TSURFER; SAMPLER; Optimization and Inverse Analysis

Nuclear Data and Methods

Cihangir Celik
Charles Daily
Shane Hart
Andrew Holcomb
Matt Jessee
Seth Johnson
Kang Seog Kim
Rob Lefebvre
B.J. Marshall
Marco Pigni
Doro Wiarda
Mark Williams

XSProc; Neutron and Gamma Cross Section Data (MG&CE); Covariance D

Reactor Physics Methods

Matt Jessee
Brian Ade
Kursat Bekar
Ben Betzler
Greg Davidson
Tom Evans
Cole Gentry
Steven Hamilton
Rob Lefebvre
Ugur Mertyurek
Doro Wiarda
Will Wieselquist
Mark Williams

TRITON; Polaris; Advanced Reactor R&D

User Interface Development

Rob Lefebvre
Matt Jessee
Brandon Langley
BJ Marshall
Josh Peterson
Adam Thompson
Will Wieselquist

Fulcrum, SNAP, Geometry and Data Visualization

User Interaction and Training

Germina Ilas
Brian Ade
Ben Betzler
Cihangir Celik
Justin Clarity
Ian Gauld
Shane Hart
Marsha Henley
Matt Jessee
Henrik Liljenfeldt
B.J. Marshall
Thomas Miller
Douglas Peplow
Chris Perfetti
Will Wieselquist

Courses at ORNL, NEA Data Bank, NRC, and User Facilities; Conference Workshops; Helpline, documentation, beta distributions

SCALE Team

The SCALE team consists of over 40 talented and diverse staff members from ORNL's Reactor and Nuclear Systems Division. Most of our team members hold advanced degrees in nuclear engineering, physics, and/or computer science. SCALE development, testing, deployment, and training are organized into task-oriented teams as shown on the previous page. Many other internal and external collaborators and students also contribute to SCALE on an ongoing basis.

SCALE 6.2 Team Photo - April 2016

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

SCALE Quality Assurance Program

The SCALE quality assurance (QA) program was updated in 2013 to provide improved high-quality software and data to the user community. The new QA program is compliant with international standards in ISO 9001-2008, US Department of Energy Order 414.1D, and the ORNL Standards-Based Management System, and it is consistent with US Nuclear Regulatory Commission (NRC) guidelines in NUREG/BR-0167, as well as ASME NQA-1. The SCALE QA program implements a streamlined Kanban process with continuous integration of new features and an automated test system that performs approximately 100,000 tests per day on Linux, Macintosh, and Windows operating systems. This QA program provides for rapid introduction of new features for deployment to end users. However, the SCALE team makes no guarantees regarding the performance of SCALE for any specific purpose, and users should independently submit the software to their own site- or program-specific testing and validation prior to use. See https://www.ornl.gov/scale/qa-plan to download a copy of the SCALE QA plan.

Technical Support and Training

The SCALE team is dedicated to supporting all SCALE users, but the team can only provide limited complimentary technical support for inquiries submitted to scalehelp@ornl.gov. For basic help in getting started with SCALE, new users are encouraged to attend the public training courses where the capabilities of SCALE are presented in detail.

To facilitate interaction among SCALE users and developers, the SCALE Users Group forum hosted by Google is available at the following link: https://groups.google.com/forum/?hl=en&fromgroups#!forum/scale-users-group

SCALE primers provide detailed, step-by-step instructions to assist new users in learning how to use these modules for criticality safety, sensitivity/uncertainty, lattice physics, and source term calculations. SCALE 6.2 primers are available for Fulcrum and ORIGAMI Automator, and earlier SCALE 6.1 primers are available for KENO V.a, KENO-VI, TSUNAMI, and TRITON. Direct links to the SCALE primers are available at https://www.ornl.gov/scale/scale-manual.

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

Upcoming SCALE Training Courses

Training courses are presented by developers and expert users from the SCALE team. These courses include a review of theory, descriptions of capabilities and limitations of the software, and hands-on expertise running problems of varying levels of complexity. Please see https://www.ornl.gov/scale/scale-training for more information.

All attendees must be licensed users of SCALE 6.2.1, which is available from ORNL/RSICC in the USA, the OECD/NEA Data Bank in France, and the RIST/NUCIS in Japan.

Class size is limited, and a course may be canceled if minimum enrollment is not obtained one month prior to the start of the course. Course fees are refundable up to one month before each class.

NON US CITIZENS VISITORS TO ORNL - Payment MUST be received at least one week prior to attending the training course. All non US citizens must register 40 days before the start date of the training course that they plan to attend.

Workshop Schedule

Dates	Course	Registration Fee
October 2–6, 2017	**SCALE/TRITON Lattice Physics and Depletion** *Oak Ridge National Laboratory, Oak Ridge, TN, USA*	**$2000**
October 9–13, 2017	**SCALE/ORIGEN Fuel Depletion, Activation, and Source Term Analysis** *Oak Ridge National Laboratory, Oak Ridge, TN, USA*	**$2000**
October 16–20, 2017	**SCALE Criticality Safety and Radiation Shielding** *Oak Ridge National Laboratory, Oak Ridge, TN, USA*	**$2000**
October 23–27, 2017	**SCALE Sensitivity and Uncertainty Analysis for Criticality Safety Assessment and Validation** *Oak Ridge National Laboratory, Oak Ridge, TN, USA*	**$2000**

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

Course Description

SCALE/TRITON Lattice Physics and Depletion Course ($2,000*)

October 2–6, 2017 – Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

SCALE supports a wide range of reactor physics analysis capabilities. SCALE reactor physics calculations couple neutron transport calculations with ORIGEN to simulate the time-dependent transmutation of various materials of interest. TRITON is SCALE's modular reactor physics sequence for a wide variety of system types. Attendees of this course will learn how to use TRITON for depletion analysis. The TRITON training material is centered around using the NEWT 2-D transport module for 2-D depletion analysis and briefly touches on 3-D depletion analysis. The course will instruct users on the use of KENO in place of NEWT for 3-D Monte Carlo-based depletion; however, KENO is not covered in depth in this course. Additional applications of TRITON are incorporated into the training, including the creation of ORIGEN libraries for rapid spent fuel characterization calculations, defining appropriate unit cell calculations of various reactor types for cross section processing, performing restart calculations, and performing uncertainty analysis of reactor physics calculations using Sampler.

SCALE/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis Course ($2,000*)

October 9–13, 2017 – Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

This is a hands-on class that covers the use of ORIGEN for isotopic depletion, decay, decay heat, and radiation source-terms calculations. The course features the use of the Fulcrum consolidated SCALE graphical interface and Fulcrum plotting capabilities for displaying nuclear data and results. The class includes solving activation, spent fuel, and nuclear safeguards and security analyses. This class provides an introduction to the ORIGAMI tool for convenient characterization of spent nuclear fuel with radially and axially varying burnup. Advanced applications including simulation of chemical processing, continuous feed and removal are also covered.

SCALE Criticality Safety and Radiation Shielding Course ($2,000*)

October 16–20, 2017 – Oak Ridge National Laboratory, Oak Ridge, Tennessee

This course provides instruction on the use of the KENO-VI Monte Carlo code for criticality safety calculations and the MAVRIC (Monaco with Automated Variance Reduction using Importance Calculations) shielding sequence with 3-D automated variance reduction for deep-penetration problems. KENO-VI is a 3D eigenvalue Monte Carlo code for criticality safety and Monaco is a 3D fixed-source Monte Carlo code for shielding analysis. Both codes use the SCALE Standard Composition Library and the SCALE Generalized Geometry Package (SGGP), which allows for versatile modeling of complex geometries and provides convenient, efficient methods for modeling repeated and nested geometry configurations such as lattices. The MAVRIC sequence is based on the CADIS (Consistent Adjoint Driven Importance Sampling) methodology. For a given tally in a Monte Carlo calculation that the users wants to optimize, the CADIS method uses the result of an adjoint calculation from the Denovo 3D deterministic code to create both an importance map for weight windows and a biased source distribution. MAVRIC is completely automated in that from a single user input, it creates the cross sections (forward and adjoint), computes the adjoint fluxes, creates the importance map and biased source, and then executes Monaco. An extension to the CADIS method using both forward and adjoint discrete ordinates calculations (FW-CADIS) is included in MAVRIC so that multiple point tallies or mesh tallies over large areas can be optimized (calculated with roughly the same relative uncertainty). Both KENO and Monaco use ENDF/B-VII.0 or ENDF/B-VII.1 cross-section data distributed with SCALE to perform continuous energy (CE) or multigroup (MG) calculations. Both codes can also be used with the Fulcrum consolidated SCALE user interface and KENO3D for interactive model setup, computation, output review, and 3-D visualization. Instruction is also provided on the SCALE material input and resonance self-shielding capabilities and the data visualization capabilities within Fulcrum for visualizing fluxes, reaction rates, and cross-section data as well as mesh tallies. KENO-VI and MAVRIC can be applied together to perform an integrated criticality accident alarm system (CAAS) analysis.

SCALE Sensitivity and Uncertainty Analysis for Criticality Safety Assessment and Validation ($2000*)

October 23–27, 2017 – Oak Ridge National Laboratory, Oak Ridge, Tennessee

Sensitivity and uncertainty analysis methods provide advanced techniques for code and data validation including the identification of appropriate experiments, detailed quantification of bias and bias uncertainty, identification of gaps in available experiments, and the design of new experiments. The Sampler sequence within SCALE provides a flexible tool for quantifying uncertainties due to manufacturing tolerances as well as composition and dimensional uncertainties in criticality safety assessments. This 5-day training class provides a foundation on sensitivity and uncertainty analysis and applies these methods to criticality safety validation applications, as well as instruction on the use of Sampler for uncertainty quantification.

Topics covered include:

- The TSUNAMI sensitivity and uncertainty analysis techniques for determining the sensitivity of the k_{eff} eigenvalue to cross section uncertainties using both multigroup and continuous-energy physics.
- SCALE's comprehensive cross section covariance data library, which is applied to these sensitivity coefficients to estimate the data-induced uncertainty in k_{eff}.
- The TSUNAMI-IP code, which determines the correlation between benchmark and application systems in terms of their shared sources of data-induced uncertainty.

- The USLSTATS trending analysis tool, which uses similarity coefficients from TSUNAMI-IP (among other parameters) to estimate the computational bias and bias uncertainty for design and licensing applications.

- The TSURFER data adjustment tool, which uses generalized linear least squares to adjust nuclear data parameters to minimize discrepancies between computed predictions and the results of integral experiments; these adjustments can then be used to estimate bias and bias uncertainty in design and licensing applications.

- The SAMPLER code for uncertainty assessment, which randomly samples nuclear data and/or system compositions and dimensions to quantify the uncertainty in system k_{eff}.

This course will cover the theoretical basis for these analysis techniques and will also conduct exercises for attendees to familiarize themselves with these tools. It is recommended that attendees are familiar with the KENO Monte Carlo code or are experienced SCALE users, although these are not necessary prerequisites.

Recent SCALE Training Events

SCALE Criticality Safety and Radiation Shielding Course
ORNL, Oak Ridge, TN, February 2017

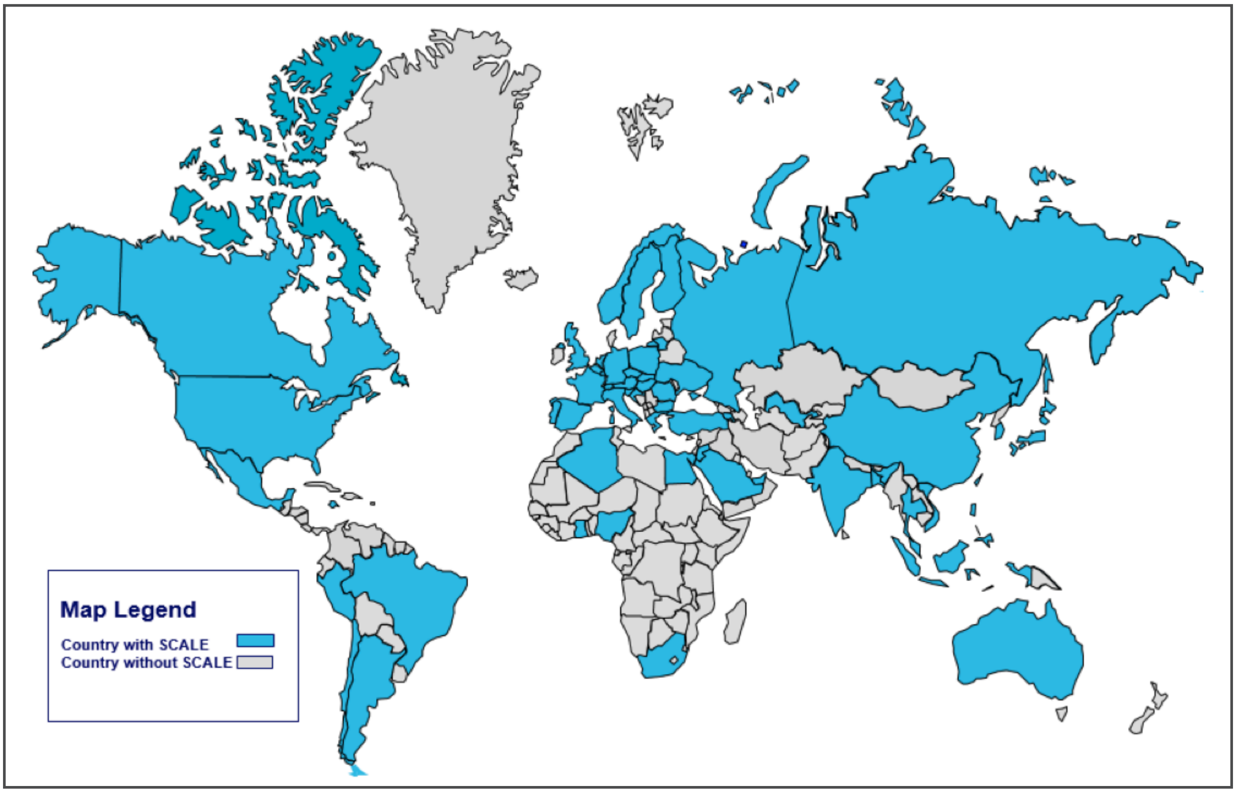
SCALE Criticality Safety Calculations Course
Areva, Lynchburg, VA, May 2017

SCALE and UNF-ST&DARDS Training:
Spent Fuel Characterization and Decay Heat
SKB HQ, Sweden, June 2017

Welcome New SCALE Users

SCALE 6.2 was released through the Radiation Safety Informational Computational Center (RSICC) in April 2016 and subsequently distributed through the Nuclear Energy Agency (NEA) Data Bank in France and the Research Organization for Information Science and Technology (RIST) in Japan. A recent update, SCALE 6.2.2, was made available in June 2017. There are currently 8,000 SCALE users in 58 different nations. If you are one of the new users of SCALE, we welcome you to our community and hope you find SCALE useful in your work.

Nations where SCALE is licensed



There are many resources for new and current users, including:

- How-to primers on many topics – https://www.ornl.gov/scale/scale-manual
- Validation reports – https://www.ornl.gov/scale/validation
- Training courses – https://www.ornl.gov/scale/scale-training

User discussion forum on Google Groups:

- https://groups.google.com/forum/?hl=en&fromgroups#!forum/scale-usersgroup
- E-mail helpline: scalehelp@ornl.gov

SCALE Newsletter

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