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SCALE Newsletter

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I am pleased to present this latest edition of the SCALE Newsletter and to report that SCALE 6.2 continues to be well received, with over 3,700 licenses issued since 2016, including distribution to over 1,200 new SCALE users. Our total user base now exceeds 8,500 individuals in 58 nations. This newsletter highlights our latest update to SCALE 6.2.3, which includes many new features requested by our community. Here we also briefly highlight several ongoing SCALE activities. We are always seeking additional partnerships, so if we can better meet your needs with specialized training, analysis support, or enhanced SCALE features, please contact me for teaming information.

The SCALE User Interaction and Training Team has updated the training course material to emphasize the new capabilities of SCALE 6.2, focusing on Polaris, Sampler, and the Fulcrum user interface. These courses continue to be in high demand through public offerings and several onsite courses tailored to the needs of individual teams.

We held the first-ever SCALE Users' Group Workshop in September 2017, attracting 130 attendees, including users from the US Nuclear Regulatory Commission (NRC), the US Department of Energy (DOE), several national laboratories, industry, and academia, as well as international participants. After receiving positive feedback from the attendees, we plan to make the Users' Group Workshop an annual event, so mark your calendars to join us at ORNL on August 27–29, 2018.

Based on the growing interest in advanced reactors and advanced technology fuels, several NRC-sponsored initiatives are underway to provide resources for the design and licensing of these new systems. Some of the features in development for SCALE 6.3 are highlighted in this newsletter.

SCALE leadership personnel were honored to receive a Technical Excellence Award from the American Nuclear Society (ANS) Nuclear Criticality Safety Division at the ANS Winter Meeting (Figure 1).

Figure 1. 2017 ANS Nuclear Criticality Safety Division Technical Excellence Award

"For Technical Excellence in the Program Management of the SCALE System of Nuclear Safety Software Spanning Four Decades." ***(Left to right)*** Cecil V. Parks (1980–1995), Stephen M. Bowman (1995–2009), and Bradley T. Rearden (2009–present).

William A. Wieselquist, PhD
Deputy Manager, SCALE Code System
Reactor Physics Group

Organizationally, we are pleased to announce that Dr. William A. (Will) Wieselquist has joined our Leadership Team as deputy manager of the SCALE Code System. Will earned a PhD in nuclear engineering from North Carolina State University in 2009. From 2009 to 2012, he was a staff member at the Paul Scherrer Institut, where he established an uncertainty quantification platform for reactor core analysis. Will joined ORNL in 2012 and quickly became the lead developer for the ORIGEN depletion/decay tools and the Sampler uncertainty quantification capabilities. Will is also a key developer of the Polaris lattice physics code. I am also grateful to Dr. Matthew (Matt) A. Jessee for his commitment to excellence and tireless service over the past 2 years as deputy manager. Matt will continue to serve as a member of the SCALE Leadership Team, leading the development of Polaris, which has quickly gained the attention of the community and continues to expand with numerous new features.

We take great pride in the many capabilities provided by SCALE, and I hope you enjoy this newsletter.

Bradley T. Rearden, PhD
Leader, Modeling and Simulation Integration
Reactor and Nuclear Systems Division

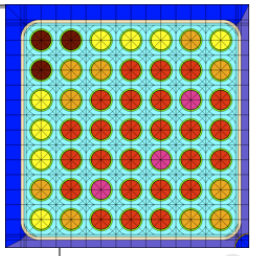
Polaris Enhancements

SCALE 6.2.3 introduces several enhancements to the Polaris lattice physics code.

- Users will notice the ~2× speedup in run time for depletion calculations.
- A new restart feature reuses the geometry data structures and flux solution from previous calculations.
- Polaris has a new detector edit capability in SCALE 6.2.3. Input examples of the detector card for a PWR 17 × 17 lattice model and for a BWR 7 × 7 lattice model are shown in Figure 2, and an example of detector response output is shown in Figure 3. The key inputs and their descriptions are given here.
  - **Detector material** (Lines 24, 25). In this input, a trace amount of ^{235}U is used to define material DET.1.
  - **Detector geometry** (Line 26). The detector geometry is provided through the Polaris pin card. In this input, the detector geometry is a simple zone of coolant with pin ID "D."
  - **Detector definition** (Line 27). In this input, the detector "d_235" is defined as pin D inserted into pin IT. The detector response is the neutron fission rate "E(n,FIS)." The detector cross section is from DET.1 (i.e., ^{235}U), and the detector flux is the COOL.2 flux inside the detector geometry.
  - **Opt FG input** (Line 48). The detector option on the opt FG card designates the detector edit to be included on the t16 file.

```
1 =polaris_6.3
2 title "Westinghouse Electric Company 17x17"
3 system PWR
4 lib "broad_n"
5 % ------------------------------------------------------- %
6 % geometry
7 % ------------------------------------------------------- %
8 geom wec17x17 : ASSM 17 1.26 SE
9 hgap 0.04
10 % ------------------------------------------------------- %
11 % comps/mats
12 % ------------------------------------------------------- %
13 comp c_uo2 : UOX 2.1
14 mat FUEL.1 : c_uo2 10.257
15 % ------------------------------------------------------- %
16 % pins
17 % ------------------------------------------------------- %
18 pin  F : 0.4096 0.4180 0.4750 : FUEL.1 GAP CLAD
19 pin IT : 0.5590 0.6050 : COOL.1 TUBE
20 pin GT : 0.5610 0.6020 : COOL.1 TUBE
21 % ------------------------------------------------------- %
22 % detector
23 % ------------------------------------------------------- %
24 comp c_u235 : CONC 92235=1.0e-15
25 mat DET.1 : c_u235
26 pin D : 0.4 : COOL.2
27 det d_235 : pin.D at=pin.IT : R(n,FIS) COOL.2 DET.1
28 % ------------------------------------------------------- %
29 % maps
30 % ------------------------------------------------------- %
31 pinmap
32   IT
33     F  F
34     F  F  F
35   GT  F  F GT
36     F  F  F  F  F
37     F  F  F  F  F GT
38   GT  F  F GT  F  F  F
39     F  F  F  F  F  F  F  F
40     F  F  F  F  F  F  F  F  F
41 % ------------------------------------------------------- %
42 % initial state HFP, avg boron
43 % ------------------------------------------------------- %
44 state temp=600 boron=900 FUEL : temp=900 COOL : dens=0.7
45 % ------------------------------------------------------- %
46 % miscellaneous
47 % ------------------------------------------------------- %
48 opt FG DetectorEdit=d_235
49 opt PRINT XFile16=yes
50 mesh FUEL    : nr=3
51 end
```

```
1 =polaris_6.3
2 title "bwr example"
3 lib "broad_n"
4 sys BWR
5 geom bwr7x7 ASSM 7 1.875
6 hgap 0.475 0.9525
7 box  0.2032 0.9652 6.7
8 comp uox_279 UOX 2.79
9 comp uox_194 UOX 1.94
10 comp uox_169 UOX 1.69
11 comp uox_127 UOX 1.27
12 comp gd_fuel WT GD2O3=4 uox_279=-100
13 mat FUEL.1 uox_279 10.32
14 mat FUEL.2 uox_194 10.32
15 mat FUEL.3 uox_169 10.32
16 mat FUEL.4 uox_127 10.32
17 mat FUEL.5 gd_fuel 10.16
18 pin 1 : 0.607 0.622 0.716 : FUEL.1 GAP CLAD
19 pin 2 : 0.607 0.622 0.716 : FUEL.2 GAP CLAD
20 pin 3 : 0.607 0.622 0.716 : FUEL.3 GAP CLAD
21 pin 4 : 0.607 0.622 0.716 : FUEL.4 GAP CLAD
22 pin 5 : 0.607 0.622 0.716 : FUEL.5 GAP CLAD
23 pinmap
24    4
25    4 2
26    3 2 1
27    3 1 1 1
28    3 1 1 1 5
29    2 1 5 1 1 1
30    3 2 1 1 1 2 2
31 % ------------------------
32 % Detector insertion
33 % ------------------------
34 comp c_u235 : CONC 92235=1.0e-10
35 mat DET.1 : c_u235
36 pin GD : 0.81280 0.88900 : MOD.1 STRUCT
37 det D1 : pin.GD : E(n,FIS) MOD.1 DET.1
38 opt FG DetectorEdit=D1
39 opt PRINT xfile16=yes
40 end
```



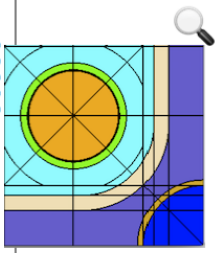


Figure 2. Example detector card for a Westinghouse 17 × 17 model (left) and a BWR 7 × 7 model (right).

```
Detector Response
-----------------

Name               = d_235
Flux particle      = NEUTRON
Flux material      = COOL.2
Reaction material  = DET.1
Reaction type      = FIS
Reaction units     = RATE
Reaction volume    = 1.257E-01

|Fine |    Det     |  Neutron   | Reaction  |
|Group|    XS      | Vol*Flux   |   Rate    |
|-----|------------|------------|-----------|
|   1 | 1.614E+00 | 2.809E-04 | 4.532E-04 |
|   2 | 1.092E+00 | 1.007E-03 | 1.099E-03 |
|   3 | 1.171E+00 | 1.630E-03 | 1.910E-03 |
|   4 | 1.263E+00 | 3.502E-03 | 4.424E-03 |
|   5 | 1.259E+00 | 1.393E-03 | 1.753E-03 |
|   6 | 1.220E+00 | 1.543E-03 | 1.883E-03 |
|   7 | 1.179E+00 | 2.052E-03 | 2.419E-03 |
|   8 | 1.115E+00 | 1.074E-03 | 1.198E-03 |
|   9 | 1.117E+00 | 1.555E-03 | 1.737E-03 |
|  10 | 1.129E+00 | 1.508E-03 | 1.703E-03 |
|  11 | 1.209E+00 | 1.467E-03 | 1.773E-03 |
|  12 | 1.235E+00 | 1.012E-03 | 1.250E-03 |
|  13 | 1.300E+00 | 1.252E-03 | 1.627E-03 |
|  14 | 1.553E+00 | 4.327E-03 | 6.721E-03 |
|  15 | 2.034E+00 | 1.976E-03 | 4.019E-03 |
|  16 | 2.428E+00 | 3.186E-04 | 7.736E-04 |
|  17 | 3.274E+00 | 2.823E-03 | 9.243E-03 |
|  18 | 5.099E+00 | 8.893E-04 | 4.534E-03 |
|  19 | 1.191E+01 | 4.134E-03 | 4.922E-02 |
|  20 | 1.138E+01 | 2.863E-05 | 3.258E-04 |
|  21 | 2.196E+01 | 7.488E-04 | 1.644E-02 |
|  22 | 1.863E+01 | 1.685E-05 | 3.140E-04 |
|  23 | 1.557E+01 | 1.577E-04 | 2.455E-03 |
|  24 | 2.044E+01 | 5.219E-05 | 1.067E-03 |
|  25 | 2.574E+01 | 6.287E-04 | 1.619E-02 |
|  26 | 6.233E+00 | 5.164E-05 | 3.219E-04 |
|  27 | 4.081E+01 | 8.473E-04 | 3.458E-02 |
|  28 | 1.296E+01 | 3.792E-05 | 4.913E-04 |
|  29 | 4.845E+01 | 7.316E-04 | 3.544E-02 |
|  30 | 1.711E+01 | 3.362E-05 | 5.753E-04 |
|  31 | 7.646E+01 | 3.863E-05 | 2.954E-03 |
|  32 | 5.646E+01 | 1.479E-03 | 8.350E-02 |
|  33 | 1.948E+01 | 2.089E-05 | 4.069E-04 |
|  34 | 7.915E+00 | 5.924E-05 | 4.689E-04 |
|  35 | 8.030E+01 | 4.371E-05 | 3.510E-03 |
|  36 | 1.803E+01 | 2.764E-04 | 4.983E-03 |
|  37 | 2.085E+01 | 1.962E-03 | 4.092E-02 |
|  38 | 1.021E+02 | 6.131E-05 | 6.256E-03 |
|  39 | 8.128E+01 | 9.149E-05 | 7.437E-03 |
|  40 | 5.868E+01 | 6.812E-04 | 3.997E-02 |
|  41 | 7.780E+01 | 5.131E-04 | 3.992E-02 |
|  42 | 1.126E+02 | 3.276E-04 | 3.688E-02 |
|  43 | 1.420E+02 | 1.387E-04 | 1.969E-02 |
|  44 | 1.623E+02 | 1.617E-04 | 2.624E-02 |
|  45 | 1.885E+02 | 7.116E-04 | 1.342E-01 |
|  46 | 1.781E+02 | 8.217E-04 | 1.464E-01 |
|  47 | 1.848E+02 | 1.348E-03 | 2.490E-01 |
|  48 | 2.266E+02 | 2.153E-03 | 4.879E-01 |
|  49 | 2.730E+02 | 1.125E-03 | 3.072E-01 |
|  50 | 3.236E+02 | 1.242E-03 | 4.018E-01 |
|  51 | 3.739E+02 | 6.391E-04 | 2.390E-01 |
|  52 | 4.231E+02 | 6.264E-04 | 2.651E-01 |
|  53 | 5.150E+02 | 8.351E-04 | 4.301E-01 |
|  54 | 7.309E+02 | 6.232E-04 | 4.555E-01 |
|  55 | 1.159E+03 | 1.218E-04 | 1.411E-01 |
|  56 | 1.997E+03 | 2.672E-05 | 5.337E-02 |
| Sum |            |            | 3.830E+00 |
|-----|------------|------------|-----------|

Nodal Detector Data
-------------------

|Broad|    Det     |    Det     |
|Group|    XS      |    FF      |
|-----|------------|------------|
|   1 | 9.484E+00| 9.734E-01|
|   2 | 3.008E+02| 1.142E+00|
|-----|------------|------------|
```

Figure 3. Example of detector response output.

User Notice for Polaris Boron Property Update in SCALE 6.2.2. A Polaris feature introduced in SCALE 6.2.1 allows the user to define the initial coolant density (DC) and the boron poison concentration (PC) and then modify them throughout a depletion cycle with input on both state and branch cards. However, in SCALE 6.2.1 and SCALE 6.2.2, incorrect behavior is observed when applying user input to modify both DC and PC. This issue is resolved in SCALE 6.2.3. The issue is best described through an example in which DC is initially defined as 0.6 g/cm^3 and PC is defined as 1,000 ppm boron. The results shown in the table below are obtained with SCALE versions 6.2.1, 6.2.2, and 6.2.3.

Table 1. Polaris Calculation Status for Different Coolant State Properties

Case	Initial		Final		SCALE version		
					6.2.1	6.2.2	6.2.3
DC only	boron = 1000	dens = 0.6	boron = 1000	dens = 0.7	OK	OK	OK
PC only	boron = 1000	dens = 0.6	boron = 100	dens = 0.6	OK	OK	OK
PC+DC	boron = 1000	dens = 0.6	boron = 100	dens = 0.7	OK	Wrong	OK
DC+PC	boron = 1000	dens = 0.6	boron = 100	dens = 0.7	Wrong	Wrong	OK

Keep in mind the following results for each case:

- **DC only** changes work on all versions.
- **PC only** changes work on all versions.
- **DC+PC** changes always fail in version 6.2.2 and sometimes fail in version 6.2.1.

Polaris applies a DC change to coolant concentrations using a fractional multiplier: new_conc = old_conc* (new_dc/old_dc). The bug in Polaris results in the internal coolant density variable not being updated to the new density value. For a follow-on change to PC, Polaris will compute the fractional multiplier for H, O, and B isotopes using the old coolant density value instead of the updated density.

The coolant property update works in SCALE 6.2.1 because the state variables are updated in alphabetical order, so the PC update comes before the DC update ("boron" before "dens"). In the DC+PC case, the PC update comes after the DC update, which leads to a bad calculational result.

In SCALE 6.2.2, ORNL staff added the history card option, which required an overhaul to the manner in which state changes are stored internally. In version 6.2.2, temperatures and densities were updated before boron properties; therefore, the code bug always led to bad results using SCALE 6.2.2. This issue has been corrected in version 6.2.3.

SCALE 6.2.3 Update

The SCALE 6.2.3 update is available for SCALE 6.2 users as of April 2018, providing enhanced features and performance in the areas detailed below. This update is provided as a download and is recommended for all SCALE 6.2.0, 6.2.1, and 6.2.2 users. The 6.2.3 update includes all previous updates and can be applied directly on any SCALE 6.2 release.

XSPROC

Self-shielding method selection logic: SCALE 6.2.3 includes improved consistency for self-shielding logic across all sequences and now enables the user to use the BONAMI-only methodology for faster calculations or in cases where the CENTRM methodology is not suitable. In SCALE 6.2.3, the logic has been streamlined as follows:

1. CENTRM for double-heterogeneous cells,
2. BONAMI for infinite homogeneous (inf. hom.) cells without fissionable nuclides,
3. For inf. hom. cells with fissionable nuclides, choose
    a. method specified by user in parm data (CENTRM, BONAMI, XSLEVEL, 2REGION) or
    b. sequence defaults
        i. CENTRM for t-newt, t-xsdrn, t-depl-1d, t-depl, csas1x, csas5, csas6, t keno, t-depl-3d, tsunami-1d, tsunami-3d
        ii. BONAMI for Mavric, XSProc sequence

Numerical stability in CENTRM MoC solver: An issue was identified with the default option for lattice cell self-shielding in cases with very small macroscopic cross section < 10^{-7} cm^{-1}. During the calculations, CENTRM produced nonphysical fluxes, shown as *not a number*, or NaN. Analyses of typical LWR configurations are not expected to be affected. The issue was resolved in SCALE 6.2.3 by introducing a more robust way to handle very small macroscopic cross sections, with negligible impact on memory and runtime.

Coupled neutron/gamma: An issue was discovered in CENTRM in which enabling upscattering in a coupled neutron/gamma problem produced erroneous results. This was recognized due to no gammas leaving the problem domain. As a temporary stop-gap for SCALE 6.2.3, upscattering will not be allowed in coupled neutron/gamma calculations.

Minor miscellaneous issues resolved in XSPROC

In the output of XSProc with lattice cell self-shielding, the printout was corrected where a radius quantity was incorrectly labeled as a diameter.

The XSDRN Balance table file (ft76.btf) was missing its lambda value. The lambda value is now included in the balance table file.

The XSPROC section of the manual has been updated to include a description of the double-heterogeneous self-shielding treatment (e.g., for TRISO particle models) for SLAB geometry. Previously, only a description of the capability for SPHERE geometry was present.

There has been some confusion over the filenames used by the various SCALE sequences/modules that write a cross section library to disk. In SCALE 6.2.3, the various filenames used by each sequence/module have been clearly documented in the SCALE manual. For SCALE 6.3, a more consistent naming scheme will be implemented, perhaps with the additional capability for the user to choose the name.

KENO

KENO-V.a boundary condition: An issue was identified in SCALE 6.1–6.2.2. An unexpected behavior can occur when a user generates an input that is inconsistent with the documentation and training materials and the code does not detect the input error before executing. SCALE behaves as intended if users generate models consistent with the documentation and training materials. Details and corrective actions are presented in the section below entitled "SCALE 6.1–6.2.2 KENO-V.a boundary condition issue."

Reaction cross sections: In continuous energy (CE) KENO, the method for calculating average reaction cross sections, which are of particular importance in CE TRITON depletion calculations, has been modified to increase robustness. Previously, multigroup reaction cross sections were calculated at each active generation and were averaged over all active generations to arrive at the best estimate. For SCALE 6.2.3, the methodology has changed so that the multigroup reaction rates and fluxes (instead of reaction cross sections) are accumulated over active generations and after all active generations are complete, the reaction cross sections are calculated as the reaction rate divided by flux. An additional positive effect of the change is that the options for tallying reaction cross sections, cxm=2 (multigroup xs) and cxm=4 (1-group xs), generally show better agreement.

Reaction rate output: An output processing issue was discovered in the KENO reaction rate output: absorption (MT=27) and capture (MT=101) cross sections were not being updated when constituent cross sections for scattering (MT=2), fission (MT=18), inelastic scattering to the first excited state (MT=51), and n,gamma (MT=102) cross sections are sampled from probability tables in the unresolved resonance region (URR). This does not impact the transport calculation or depletion calculations under t5-depl or t6-depl that use the constituent cross sections directly. This issue was discovered by a user attempting to calculate k_{eff} from reaction rate output and match the result to the output eigenvalue. **Analysis using the reaction rate output where the URR range is important should be repeated with SCALE 6.2.3.**

Minor miscellaneous issues resolved in KENO

The output for the Shannon entropy convergence test has been updated in SCALE 6.2.3 to emphasize where active generations are used.

The nuclide identifiers for metastables and bound nuclides were not correctly displayed in the KENO output. These isotope edits are now correct.

Filenames for reaction rates have been tallied. Instead of ${BASENAME}.keno_micro_rr.* in SCALE 6.2.2, KENO in SCALE 6.2.3 writes reaction rate tallies in ${BASENAME}.keno_rr.*.

The Doppler broadening of CE cross sections to user-specified temperatures in KENO now allows for four options for the DBX parameter:

- 0 = No problem-dependent or on-the-fly Doppler broadening
- 1 = Perform problem-dependent Doppler Broadening for 1D cross sections only
- 2 = Perform problem-dependent Doppler Broadening for both 1D and 2D (thermal scattering data) cross sections
- 3 = Broaden 2D cross sections normally, and broaden 1D cross sections using a less robust but faster interpolation method.

DBX=3 was previously only supported as an option in Monaco.

Occasionally, the Doppler broadening of very small cross sections can result in very small negative values for a few data points. The effect of these values on criticality and reaction rates is undetectable, but these very small negative values could cause CE TSUNAMI sensitivity calculations to fail. In SCALE 6.2.3 these values are set to zero.

NEWT

Undefined mixtures: For cases that have undefined mixtures referenced in the geometry, NEWT calculations assumed that any mixture that did not include any data in the cross section library was a void material with a cross section of zero. This issue has been fixed in SCALE 6.2.3, and additional checks and error messages have been added to verify that every mixture referenced in the geometry is defined in the composition block. This issue affects all uses of NEWT, including the t-newt and t-depl sequences.

ORIGEN

Neutron emission calculations: An issue was found in ORIGEN in which a tolerance for including a nuclide in the emission calculation did not include the initial isotopics. Thus, any nuclide that fell below the threshold over the first timestep would not be included in the neutron emission calculation for the entire case. For common timestep sizes on the order of days, the main effect was that the delayed neutron emitters, which have effective time ranges of much less than a day, are bypassed, and no delayed neutron information is shown. The issue was fixed in SCALE 6.2.3 by including the initial isotopics in the time-averaging to determine the active nuclides for an emission calculation. A workaround for SCALE 6.2.0, 6.2.1, and 6.2.2 is to add a very small, initial timestep (on the order of milliseconds).

Volume input: ORIGEN volume input is only used when the user specifies the isotopic input by number density, and the volume is needed to convert the number density to ORIGEN's internal mole units. However, unlike other SCALE sequences, number density input is not commonly used in ORIGEN. Volume input was not being correctly handled in SCALE 6.2.2. Any calculations using the number density input option should be rerun using SCALE 6.2.3.

Elemental input: A minor change was made regarding how ORIGEN handles elemental input. It is now flagged as an error which specifies any element for which the natural abundances sum to zero (e.g., Tc) according to the data on the specified ORIGEN library. Note that the current ORIGEN library format only allows abundances for light nuclides (hydrogen to lead), so it does not include natural uranium.

ARPLIB utility module: This module, which is used to manipulate the number of burnup-dependent data sets on an ORIGEN library, was not properly processing libraries in the SCALE 6.2 format. In SCALE 6.2.3, ARPLIB properly reads the SCALE 6.2 library format (and SCALE 6.1 format) and has been redesigned to allow the user to easily create an arbitrary library from cross sections using data from a number of other available libraries. Note that this utility module is rarely used for thinning or combining existing libraries. The module does not intervene in any ORIGEN calculation or SCALE sequences involving ORIGEN.

Polaris

Significant Polaris enhancements are discussed in this newsletter under "Polaris Enhancements." A new preview capability is available for basic detector modeling and gamma transport. This is fully described in the appendix of the Polaris manual in SCALE 6.2.3. As with earlier previews, =polaris_6.3 must be used as the sequence name. Users may experience a runtime reduction of 10–50% due to optimization of some internal initialization routines.

Minor issues resolved in Polaris

Mismatches between user-specified symmetry and actual problem symmetry are now better recognized. Defining compositions with names that are also element symbols (e.g., Zr or F) is no longer allowed. Rare convergence issues occurring with CMFD and buckling calculations are now fixed. In the Polaris nodal data file (T16 or X16 file): energy release per fission parameters now properly include energy released from capture, and few-group flux is normalized as per source neutron instead of per source neutron per unit volume.

Sampler

Perturbed decay data: The uncertainty in the decay energy release (aka Q-value) for primary alpha emitters was found to be at least 50% larger than the actual value due to an issue in the sampling code that is used to generate the 1,000 perturbed decay data files. The code error has been fixed. The updated perturbed decay data files are not available as part of the SCALE 6.2.3 release, but they will be made available as an additional download. This only affects Sampler uncertainty calculations with perturb_decay="yes" (the default is "no"). Moreover, it only affects the decay heat uncertainty prediction; it does not affect the decay heat prediction itself. Validation of calculated decay heat against measured spent fuel decay heat has shown good agreement, typically within 2%, between predicted and measured values. SCALE developers are

committed to making uncertainty calculations a simple, routine part of nuclear engineering analysis. Additional tests will be applied to the current data set, along with new uncertainty data from ENDF/B-VIII.

Minor issues resolved in Sampler: The output to additional auxiliary files (recommended for post-processing of the sampled results with a tool external to SCALE) only contained a single significant digit instead of the desired five significant digits. If the input only used a single sample, then Sampler would show standard deviations of 0.0 (or for some outputs, NaN) instead of the more appropriate infinity.

TRITON

Calculations using thorium: TRITON did not correctly include thorium (atomic number 90) in the definition of initial heavy metal (IHM) for the purpose of setting specific power levels (units of MW/MTIHM) and reporting burnup (MWd/MTIHM). The error has been corrected in SCALE 6.2.3, and a verification problem using ^{232}Th was added to the regression suite. The error made it impossible to deplete a thorium-only mixture, and for a mixture that included thorium, the input power was misinterpreted, and burnup was misreported. Any depletion calculations for thorium in SCALE 6.2.0–6.2.2 are incorrect and should be rerun with 6.2.3.

Keep block: In TRITON, keeping the ORIGEN output (origen keyword found in the keep block) would lead to extremely large transition coefficient tables in the TRITON output file, and cases with many burnup points could have output file sizes in gigabytes. In SCALE 6.2.3, requesting TRITON to keep origen will only enable output of detailed depletion number density tables. To recover the previous output, which may be useful in small problems to understand specific depletion pathways, the user must indicate to keep both ORIGEN and COUPLE output in the keep block.

Self-shielding and material swap: In TRITON (MG) within SCALE 6.2, the interaction between self-shielding and the material swap (and control rod branch) has changed. In previous versions, the mixture swap occurred before self-shielding. This required users to take the swap into account when creating the celldata block. In SCALE 6.2 and later versions, self-shielding in the celldata block is based only on the defined mixtures. This difference only affects calculations in which latticecell or multiregion self-shielding is used with swaps or control rod branches. It does not affect the default inf. hom. In SCALE 6.2.3, the user is warned when these conditions are present. Details are presented in the section below entitled "SCALE 6.2 TRITON backwards compatibility break."

Fulcrum

Autocomplete: SCALE 6.2.3's Fulcrum now has the ability to validate and autocomplete the MAVRIC input.

Visualization: Lines in OPUS plot files now display in different colors instead of only blue. Covariance data color bar limits and axis fonts can now be changed.

Input Editor: Input validation is now faster by a factor of two, is fully case insensitive, accounts for all possible SCALE sequences (including utility modules), and is no longer disrupted by uncommented text preceding a sequence. New error messages are emitted if a user attempts to create a new file without the proper write permissions. If a user attempts to view a geometry for an input that has no geometry, then appropriate error messages are displayed. The cursor retains its original position when a text file is reloaded instead of moving to the top of the file.

Other Minor Miscellaneous Issues Resolved in SCALE 6.2.3

The legacy addnux value of -2, which was disabled in TRITON in SCALE 6.2.2, has been included again in SCALE 6.2.3.

In SCALE 6.2.3, various updates have been implemented in the STARBUCS burnup credit analysis sequence for consistency with updates in KENO and ARP.

ORIGAMI now allows the simulation of an initial decay interval, for example, to simulate some initial decay time before the first irradiation. This is accomplished by entering a power level of zero for the first cycle, which would previously cause the calculation to fail. Additionally, the format MCNP source output (enabled with mcnp=yes) has been updated for improved compatibility with MCNP.

In TSURFER, a minor issue was corrected in which the printout of cross section adjustment information (print_adjustments) did not work.

An issue was discovered with the SCALE composition block's atom type input in which the atom fractions that were entered were being treated as weight fractions. This issue has been resolved in SCALE 6.2.3. Note that this only affects atom composition inputs (e.g., "atom 1 19.0 2 92235 0.1 92238 0.9 end"), which is a rarely used form.

SCALE 6.1–6.2.2 KENO-V.a boundary condition issue

An issue was identified in SCALE 6.1–6.2.2. An unexpected behavior can occur when a user generates an input that is inconsistent with the documentation and training materials and the code does not detect the input error before executing. SCALE behaves as intended if users generate models consistent with the documentation and training materials.

In all versions of SCALE, the Monte Carlo code KENO V.a implements the use of non-vacuum albedo boundary conditions (e.g., mirror, periodic, white) only when the outermost geometry region of the model is a cuboidal region. This limitation is noted in the user documentation in the section on Albedo data, where it is stated that **"Albedo boundary conditions are applied only to the outermost region of a problem. In KENO V.a this geometry region must be a rectangular parallelepiped."**

It was recently discovered—beginning with the release of SCALE 6.1 in 2011— that KENO V.a will accept noncompliant input that specifies albedo boundary conditions for non-cuboidal outer shapes and then attempt to complete the calculation. For example, a user can specify a cylinder as the outermost region and add a mirror boundary condition on the top or bottom to effectively double the volume of the system considered. A user can also add a mirror boundary condition to both the top and the bottom of the cylinder to simulate a bounding case of an infinite system. While these scenarios are accepted and perform as expected in KENO-VI, ***KENO V.a requires the addition of a cuboidal region (typically an empty void region) to enable the use of these albedo boundary conditions.***

For calculations using KENO V.a in SCALE 6.1–6.2.2 with noncompliant input, in which albedo boundary conditions are applied but without the required cuboidal outermost region, the calculation will proceed without warning, and an underestimation of k_{eff} often results. The magnitude of underestimation in k_{eff} can vary widely, depending on the system modeled and the desired boundary conditions, but it **can exceed several percent in k_{eff}.**

It is strongly recommended that users who rely on albedo boundary conditions in KENO V.a review their input models to ensure that the outermost region is a cube or cuboid, per the documentation requirement. Note that input models that were generated and applied with SCALE 6 and earlier versions, which included the check for the cuboidal outer boundary, will continue to produce the expected results with SCALE 6.1–6.2.2.

In testing the extent of this issue by placing mirror boundary conditions on non-cuboidal outer shapes, it was found that cylinders oriented along the x-, y-, or z-axis most often produce nonconservative results without warning. The calculation will terminate prior to completion for cases in which a sphere is the outermost shape. The calculation will terminate with an error message for cases in which a hemicylinder or hemisphere is the outermost shape. The calculation performs as expected for cases in which a cube or cuboid is the outermost shape.

This issue applies to all SCALE 6.1–6.2.2 sequences that implement KENO V.a, including csas5, tsunami-3d-k5, t5-depl, and starbucs. No other SCALE sequences are impacted by this issue. The error condition for the attempted use of albedo boundary conditions on non-cuboidal outer shapes in KENO V.a was restored in SCALE 6.2.3, thus preventing users from inadvertently entering noncompliant input.

SCALE 6.2 TRITON backwards compatibility break: affects TRITON control rod branch calculations and TRITON timetable swap function

Although SCALE 6.2 can run most SCALE 6.1 TRITON inputs without modification, in SCALE 6.2, the method for handling the mixtures involved in a control rod branch calculation has changed. Therefore, users may need to modify inputs to properly self-shield control rod materials. In addition, the new timetable swap feature performs in a manner similar to the control rod branch calculations.

Description

Four blocks of the TRITON input are involved:

1. The ***celldata block***, where self-shielding models are defined.
2. The ***branch block***, where crin and crout material lists are defined and where the nominal condition (crin or crout) is specified. Depletion is performed under the nominal conditions.
3. The ***timetable block***, where swap mixtures are defined and used. Note that the timetable swap function is only available in SCALE 6.2, but its behavior is similar to the branch crin and crout functionality.
4. The ***geometry block***, where the geometry is defined, including associating mixtures to the various volumes via media inputs.

In SCALE 6.1, the material swapping performed with crin and crout mixtures for control rod branch calculations literally replaces mixtures in the celldata and geometry blocks as needed. This leads to non-intuitive celldata inputs in which it appears that the crout moderator mixtures are receiving control rod self-shielding, but because the swap is defined, the crin mixtures will replace those in the celldata input before self-shielding.

In SCALE 6.2, the celldata block is independent from the branch and timetable blocks, and material swaps only affect the geometry—materials are NOT swapped within the celldata block. Below are some important rules to remember when setting up control rod branch calculations and timetable swap calculations:

1. The celldata block defines the self-shielding of the mixtures declared in the composition block. In SCALE 6.2, material swaps are not performed on mixtures within the celldata block.
2. The branch block defines the crin and crout mixtures.
3. The geometry block defines media in terms of the nominal mixtures.

For example, if the nominal condition is control rods out, using crout mixtures, then the geometry must contain those crout mixture IDs. When a branch to crin mixtures is performed, TRITON substitutes the crin number densities and cross sections into the nominal mixtures only in the geometry block, which in this example are the crout mixtures. A message in the output file indicates the following:

Property changes for this branch:

- Swap material CROUT1 to CRIN1
- Swap material CROUT2 to CRIN2

Therefore, for this calculation, the cross sections and number densities for CROUT1 are equal to those of CRIN1, and for CROUT2 they are equal to those of CRIN2, and so on. While this implementation detail would not typically be exposed to the user, highlighting it here helps the user understand how to reference mixtures for homogenization (use nominal mixture IDs) and for other outputs in which the nominal mixture identifiers are potentially changing in every way (different number densities, cross sections, etc.) except for the mixture ID itself.

Other Information

The importance of self-shielding control rod materials containing resonance absorbers was documented in the 2014 spring edition of the SCALE Newsletter (No. 46). Although the guidance on self-shielding is still valid, note that the directions to model crin and crout branches in TRITON are correct for SCALE 6.1, but they are incorrect for SCALE 6.2.

The following examples show the correct method for performing self-shielding of control rod mixtures used in TRITON control rod branches and material swaps.

1. The first example addresses the scenario in which nominal corresponds to crout.
2. The second example addresses the scenario in which nominal corresponds to crin. The celldata block is the same in both examples. Only the branch blocks differ in what is defined as nominal, which then forces those nominal mixtures to be associated with media in the geometry block.
3. In the third example, mixture swaps in SCALE 6.2 are not performed within the celldata block; they are only performed within the geometry block.

Note that in the following examples, specifying the crout mixtures with inf (infinite homogeneous medium) treatment is redundant, which is the default for all mixtures in TRITON.

Branch example: nominal conditions with control rods out

```
=t-depl parm=(addnux=2, centrm)
...
read composition
  silver    1   den=10.16      0.85     581.34    end
  indium    1   den=10.16      0.15     581.34    end
  cadmium   1   den=10.16      0.05     581.34    end
  he-4      2   den=1.4485e-4  1.0      581.34    end
  ss304     3   den=7.8620     1.0      581.34    end

  h2o       4   den=0.65649    1.0000   581.34    end
  h2o       5   den=0.65649    1.0000   581.34    end
  h2o       6   den=0.65649    1.0000   581.34    end
...
end composition
read celldata
...
  multiregion cylindrical right_bdy=white end
      1   0.4000
      2   0.4400
      3   0.4900
    300   0.5600
    200   0.6000
    400   0.7109
    100   2.8490   end
  inf 4 5 6 end
end celldata
...
read branch
...
  define crin  1  2  3   end
  define crout 4  5  6   end
  cr=0         end
  cr=1         end
...
end branch
...
read model
...
unit 36
  com='guide tube'
  cylinder 10 0.4000
  cylinder 20 0.4400
  cylinder 30 0.4900
  cylinder 40 0.5600
  cylinder 50 0.6200
  cuboid 60 4p0.6300
  media 4   1 10
  media 5   1 20 -10
  media 6   1 30 -20
  media 311 1 40 -30
  media 211 1 50 -40
  media 311 1 60 -50
  boundary 60
...
end model
```

Define self-shielding for control materials (1,2,3)

Define self-shielding for water fill mixtures (4,5,6)

Nominal conditions are defined as those with crout mixtures (4,5,6)

Branch condition using crin where nominal mixtures (4,5,6) in geometry are given xs and numden from crin mixtures (1,2,3)

Geometry defined using nominal mixture IDs (4,5,6)

Figure 4. Branch example: nominal conditions with control rods out.

Branch example: nominal conditions with control rods in

```
=t-depl parm=(addnux=2, centrm)
...
read composition
  silver    1   den=10.16      0.85     581.34   end
  indium    1   den=10.16      0.15     581.34   end
  cadmium   1   den=10.16      0.05     581.34   end
  he-4      2   den=1.4485e-4  1.0      581.34   end
  ss304     3   den=7.8620     1.0      581.34   end

  h2o       4   den=0.65649    1.0000   581.34   end
  h2o       5   den=0.65649    1.0000   581.34   end
  h2o       6   den=0.65649    1.0000   581.34   end
...
end composition
read celldata
...
  multiregion cylindrical right_bdy=white end
       1   0.4000
       2   0.4400
       3   0.4900
     300   0.5600
     200   0.6000
     400   0.7109
     100   2.8490    end
  inf 4 5 6 end
end celldata
...
read branch
...
  define crin   1   2   3    end
  define crout  4   5   6    end
  cr=1        end
  cr=0        end
...
end branch
...
read model
...
unit 36
  com='guide tube'
  cylinder 10 0.4000
  cylinder 20 0.4400
  cylinder 30 0.4900
  cylinder 40 0.5600
  cylinder 50 0.6200
  cuboid 60 4p0.6300
  media 1    1 10
  media 2    1 20 -10
  media 3    1 30 -20
  media 311  1 40 -30
  media 211  1 50 -40
  media 311  1 60 -50
  boundary 60
...
end model
```

Define self-shielding for control materials (1,2,3)

Define self-shielding for water fill mixtures (4,5,6)

Nominal conditions are defined as those with crin mixtures (1,2,3)

Branch condition using crout where nominal mixtures (1,2,3) in geometry are given xs and numden from crout mixtures (4,5,6)

Geometry defined using nominal mixture IDs (1,2,3)

Figure 5. Branch example: nominal conditions with control rods in.

Swap example: nominal conditions with control rods out

```
=t-depl parm=(addnux=2, centrm)
...
read composition
  silver   1   den=10.16      0.85     581.34   end
  indium   1   den=10.16      0.15     581.34   end
  cadmium  1   den=10.16      0.05     581.34   end
  he-4     2   den=1.4485e-4  1.0      581.34   end
  ss304    3   den=7.8620     1.0      581.34   end

  h2o      4   den=0.65649    1.0000   581.34   end
  h2o      5   den=0.65649    1.0000   581.34   end
  h2o      6   den=0.65649    1.0000   581.34   end
...
end composition
read celldata
...
  multiregion cylindrical right_bdy=white end
      1   0.4000
      2   0.4400
      3   0.4900
    300   0.5600
    200   0.6000
    400   0.7109
    100   2.8490   end
  inf 4 5 6 end
end celldata
...
read timetable
...
  swap 1 4
          0.0  0
        100.0  1 end
  swap 2 5
          0.0  0
        100.0  1 end
  swap 3 6
          0.0  0
        100.0  1 end
...
end timetable
...
read model
...
unit 36
  com='guide tube'
  cylinder 10 0.4000
  cylinder 20 0.4400
  cylinder 30 0.4900
  cylinder 40 0.5600
  cylinder 50 0.6200
  cuboid 60 4p0.6300
  media 4   1 10
  media 5   1 20 -10
  media 6   1 30 -20
  media 311 1 40 -30
  media 211 1 50 -40
  media 311 1 60 -50
  boundary 60
...
end model
```

Define self-shielding for control materials (1,2,3)

Define self-shielding for water fill mixtures (4,5,6)

Nominal conditions are defined as those with crout mixtures (4,5,6). At 100 days, the crout mixtures are swapped out and the crin mixtures (1,2,3) are swapped in.

Geometry defined using nominal mixture IDs (4,5,6)

Figure 6. Swap example: nominal conditions with control rods out.

NEWT User Guidance

Whether used with the SCALE/TRITON sequence or run standalone, SCALE/NEWT is a flexible, discrete ordinates transport tool with the capability to model a variety of two-dimensional geometries. To ensure proper execution, here are a few reminders to maximize SCALE/NEWT performance.

1. **Geometry verification:** We recommend that all users verify their geometry by including drawit=yes in the parameters block. The resulting "*matl.ps" file may be used to generate a PDF within MacOS or Windows using a GhostScript utility. Review of the resulting graphic representation is recommended to ensure that (a) the materials are in the correct location in the geometry, (b) no cells are missing, and (c) no grid lines are missing or are irregular. The graphic illustrates the geometry as understood by SCALE/NEWT. The visualization generated in Fulcrum, the graphical interface to SCALE, may be used to aid in construction of the model, but the model should always be checked by viewing the "*matl.ps" file before execution.
2. **Unit clipping:** We advise all users not to clip units being filled into arrays. This can cause unexpected results that would be flagged when reviewing the geometry.
3. **Hexagonal arrays:** When the outer units in a hexagonal array overlap the boundaries containing the array, SCALE/NEWT may have some difficulties generating the solution grid. This commonly occurs when the hexagonal array cells overlap an enclosing surface and a subgrid is specified in the unit cell. These issues are apparent when viewing the "*matl.ps" file generated by NEWT. Eliminating the unit cell subgrids will fix the issue. When eliminating the unit cell subgrids, we recommend the use of a fine grid on the global unit.

Example 1: SCALE/NEWT has problems processing the geometry of this input (see Figure 7). The steps to rectify this problem are:

1. Review the "*matl.ps" file and determine whether there is an issue with the south boundary in the model.

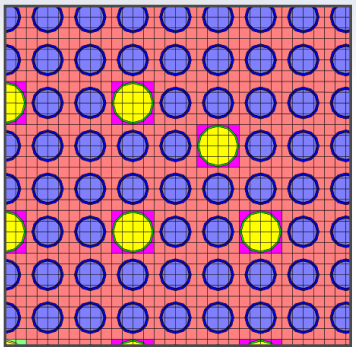


Figure 7. SCALE/NEWT representation of a PWR lattice with a geometry construction error.

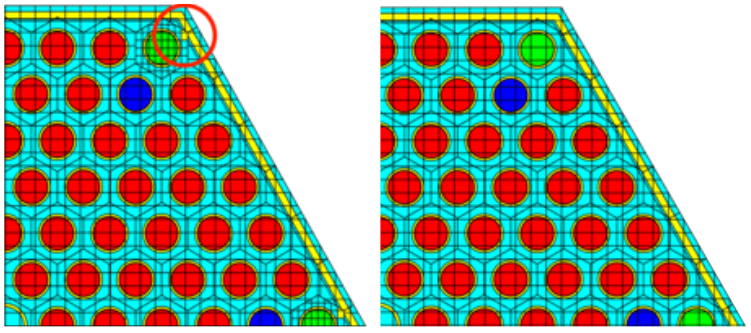
2. Investigate each unit on the south face in the model, ensuring that the height of the boundary in these units is consistent.

The issue is due to the center pin (bottom left unit) in this problem having a height that is 0.00002 cm greater than the other units along this boundary.

Example 2: SCALE/NEWT has issues generating the geometry and solution grid of this hexagonal geometry-based input (see Figure 8a, green fuel pin, circled in red). The steps to rectify this problem are:

1. Review the "*matl.ps" file and recognize that there is an issue with the diagonal boundaries of the array and the enclosing geometry.
2. Remove the subgrid from the array element in which materials have been erroneously placed into grid cells.

After the subgrid is removed from the green unit cell (see Figure 8b), the geometry construction issue will be resolved.



(a) NEWT grid construction error

(b) NEWT model using not unit cell subgrid

Figure 8. Illustration of (a) NEWT hexagonal geometry construction issue problem and (b) the solution using no unit cell subgrid.

SCALE 6.3 Development for Advanced Reactors and Advanced Technology Fuels

Several FY18 projects are underway to develop new code and data capabilities in SCALE 6.3 for modeling advanced reactors and advanced technology fuels (ATFs), which are sometimes referred to as *accident-tolerant fuels*. Historically, many of SCALE's capabilities have been developed and applied to light water reactor (LWR) fuel applications. Enhancements for non-LWR applications are being implemented in the Polaris lattice physics code and the high performance massively parallel Monte Carlo code Shift. In addition, new cross section libraries are being developed for non-LWR applications.

Polaris

Advanced Reactors

Non-LWR capabilities under development for **Polaris** include:

- hexagonal geometry support to simulate high temperature gas cooled reactors (HTGRs), sodium fast reactors (SFRs), and prismatic assembly designs,
- a double-heterogeneity modeling capability to support HTGR prismatic analysis and ATFs based on TRISO-particle fuel forms,
- integration of a time-dependent chemical processing model and a delayed neutron precursor drift model for integration of molten salt reactors (MSRs) into Polaris (to allow time-dependent modeling of the molten salt fuel (already implemented in TRITON for SCALE 6.3 for MSR analysis), and
- definition of the branch and history requirements in Polaris for advanced reactor modeling with PARCS or other nodal core simulators.

Advanced Technology Fuels (ATFs)

Several ATF and advanced cladding concepts are being considered by industry. Some of these concepts are planned for lead test rods over the next two years. We are assessing SCALE neutronics capabilities for ATF designs, including the identification of relevant benchmark experiments for validation, and code enhancements to improve SCALE modeling accuracy. The focus is on lattice level investigations for ATF concepts such as

- Cr-doped UO_2,
- greater-than-5% enriched UO_2,
- advanced cladding types, and
- uranium-silicide fuel.

Once the assessment is complete, we will implement the necessary changes into Polaris to provide accurate modeling of ATF concepts. Potential enhancements may include:

- modifications to the energy group structure in the multigroup library,
- updates to the nuclear data library such as modified self-shielding factors or scattering data, and
- updates to the Polaris input interfaces for simple definition of ATF compositions or geometries.

Shift

Lattice Physics Calculations

Another capability under development will enable lattice physics calculations with Shift through Polaris' established input and output definitions. This capability will provide reference solutions for non-LWR fuel designs, and nodal cross section data will be generated via Shift's CE Monte Carlo solution using the same inputs as those used in the Polaris MG approach. Polaris, which is designed for MG calculations, uses (1) the Embedded Self-Shielding Methodology (ESSM) to generate problem-dependent cross sections and (2) an MoC transport solver to generate flux solutions that are subsequently used to produce nodal core simulator data for PARCS. The Shift Monte Carlo interface will allow definition of Monte Carlo sampling parameters and tallies needed for nodal cross section generation. The construction of the lattice geometry will be updated to create Shift native geometry.

TRITON Depletion Sequence

Shift is also being implemented in the TRITON depletion sequence. CE depletion is now available in the SCALE TRITON depletion sequence through use of the KENO Monte Carlo code for neutron transport calculations. However, the KENO solution involves large parallel calculations that require significant computational resources which are prohibitive for full core reactor analysis. A highly parallelizable reference solution is needed to support simulation of advanced reactor concepts, which Shift will provide.

Few-Group Nodal Cross Sections

Additional features are being added to generate few-group nodal cross sections using Shift. Currently, nodal data can only be generated for 2-D geometries in SCALE using NEWT or Polaris. Advanced reactors differ significantly from LWRs in geometry and neutron spectra, so different solution methods are required. The current multigroup methods are highly optimized for LWRs. Rather than generate a new group structure and cross section processing method for each advanced reactor class, a CE Monte Carlo nodal data generation solution using Shift will be applicable for any solid-fuel reactor design, and it will be scalable to high-performance computing platforms.

Particle-Based Fuel Designs

Particle-based fuel designs such as TRISO require the user to develop significantly complex models. Shift will allow the random geometric placement of individual fuel grains and/or fuel pebbles to be automated so the user may simply specify the number of particles in a fuel volume or the number of pebbles in a core.

Criticality Safety and Sensitivity Analysis

Shift is also being implemented into SCALE to replace KENO for criticality safety analysis sequence (CSAS) and sensitivity/uncertainty (TSUNAMI) calculations.

Hybrid Deterministic / Monte Carlo Radiation Shielding

A new MAVRIC radiation shielding sequence using Shift is under development that will use Shift instead of Monaco for hybrid deterministic / Monte Carlo radiation shielding applications.

The existing KENO- and Monaco-based sequences will still be available in SCALE 6.3.

For nuclear data to support advanced reactors and ATFs, we are developing a generic very fine (VF) 1000+ group library that is applicable to a wide range of reactor spectra, including both thermal and fast systems. This VF library will be available to generate collapsed application-specific libraries. Recommended collapsed group structures may be provided for different reactor concepts, but only the generic VF library will be maintained and distributed with SCALE. An automated capability for users to collapse reactor-specific libraries from the generic VF library is also planned for development in 2019 (after SCALE 6.3).

Employee Spotlight: William J. (B.J.) Marshall

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

Focus areas: Criticality safety of LWR fuel, PWR and BWR burnup credit, SCALE testing and training, criticality safety validation, application of sensitivity/uncertainty methods to criticality safety, critical experiment correlations, nuclear data testing

Figure 9. With my son Ian, about to collect some counties in Kentucky.

Most memorable projects:

Of all the projects I've worked on since joining ORNL in June 2010, validation of KENO and the associated testing of nuclear and covariance data have been the most memorable. This work has increased my understanding and appreciation of the complexity of nuclear data and its use in transport codes. It has also put me in a position where I can have broad and hopefully positive impacts through careful analysis of discrepancies between measured and calculated benchmark experiments. Working with the nuclear data community has also been an entirely new opportunity for me.

Providing SCALE training has also been very memorable for me. I started training users in the Fall of 2010: there really is no way to increase your understanding of something more than by teaching it. I have enjoyed meeting a huge number of people in the various classes I've taught over the years. Many of these people have helped broaden my technical and personal experience base in valuable ways. Hopefully at least some of the trainees have found the classes as enjoyable and informative as I have.

Overall it has been a lot of fun carving out a niche for myself where the SCALE developers view me as a user and the SCALE users view me as a developer.

Life outside of work:

I recently completed a PhD in nuclear engineering at the University of Tennessee, so I haven't had a lot of life outside of work over the last few years. When I do have spare time, I enjoy reading (usually ~25 books/~10,000 pages per year on history; math, science and technology; and comparative religions) and watching sports, especially baseball, hockey, and college football. My most infamous hobby is "collecting" counties around the United States. I have been in 1,565 (49 states) of the 3,142 counties in the country. You can check out the up-to-date map of my progress at http://www.mob-rule.com/user-gifs/USA/caviebjm.gif.

Recent SCALE Publications

Peer-Reviewed Journal Articles

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J. B. Clarity, K. Banerjee, H. K. Liljenfeldt, and W. J. Marshall, "As-Loaded Criticality Margin Assessment of Dual-Purpose Canisters Using UNF-ST&DARDS," *Nucl. Technol.* **199**(3), 245–275 (2017).

G. G. Davidson, T. M. Pandya, S. R. Johnson, T. M. Evans, A. E. Isotalo, C. A. Gentry, and W. A. Wieselquist, "Nuclide Depletion Capabilities in the Shift Monte Carlo Code," *Ann. Nucl. Energy* 114, 259–276 (2018). DOI: https://doi.org/10.1016/j.anucene.2017.11.042

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M. Duluc, D. Heinrichs, S. Kim, T. Miller, C. Celik, C. Hopper, et al., "Introduction of Plutonium Systems to the Nuclear Criticality Slide Rule."

A. Holcomb, D. Wiarda, and W. J. Marshall, "ENDF/B-VIII.0 Testing with AMPX and SCALE."

R. A. Lefebvre and W. J. Marshall, "Template Engine Applied to Rapid Modeling."

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W. J. Marshall, B. T. Rearden, and R. E. Pevey, "Determination of Critical Experiment Correlations for Experiments Involving Highly Enriched Uranium Solutions."

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SCALE Team Structure

Leadership Team

Brad Rearden *(Manager)*
SCALE Code System

Will Wieselquist *(Deputy Manager)*
SCALE Code System

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

Kevin Clarno *(Group Leader)*
Reactor Physics

Bob Grove *(Group Leader)*
Radiation Transport

Rob Lefebvre *(Software Development Coordinator)*

Matt Jessee *(Senior R&D Staff)*

Infrastructure Development and Software Support

Rob Lefebvre
Seth Johnson
Brandon Langley
Jordan Lefebvre*
Paul Miller
Tony Walsh

**advisor*

Quality Assurance System; Build and Test Framework; Deployment

Monte Carlo Methods

Brad Rearden
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Kaushik Banerjee
Kursat Bekar
Cihangir Celik
Greg Davidson
Tom Evans
Shane Hart
Seth Johnson
Tara Pandya
Chris Perfetti
Doro Wiarda

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
Keith Bledsoe
Matt Jessee
Rob Lefebvre
B. J. Marshall
Ugur Mertyurek
Chris Perfetti
Vladimir Sobes
Will Wieselquist

TSUNAMI; TSURFER; SAMPLER; Optimization and Inverse Analysis

Nuclear Data and Methods

Cihangir Celik
Charles Daily
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 Data

Reactor Physics Methods

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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 Interfaces

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

Fulcrum, 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
B. J. Marshall
Thomas Miller
Douglas Peplow
Chris Perfetti
Will Wieselquist

Courses at ORNL, NEA Data Bank, NRC, and User Facilities, Conference Workshops Helpline, User Groups Documentation

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 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. 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.

All attendees must be licensed users of SCALE 6.2, which is available from ORNL/RSICC in the USA, the OECD/ NEA Data Bank in France, and the RIST/NUCIS in Japan.

The next SCALE training block at Oak Ridge National Laboratory will be held October 15 – November 9, 2018. The course schedule will be announced soon. Please see https://www.ornl.gov/scale/scale-training for more information.

SCALE Users' Group Workshop 2017

The first SCALE Users' Group Workshop was held at ORNL on September 26 -28, 2017, with 130 registered participants from the NRC, DOE, national laboratories, industry, and academia. The opening plenary session featured two keynote speakers. Drew Barto from the NRC described the SCALE Code System's 41-year history of use for criticality, shielding, and source-term analysis of spent fuel, and Larry Wetzel from BWXT described 30 years of applying SCALE for criticality safety assessment and criticality accident alarm analysis.

Technical sessions covered the following topics:

- Criticality safety
- Depletion and source terms
- Nuclear data
- Radiation shielding
- Reactor physics
- Sensitivity and uncertainty analysis

Five ORNL staff members held a discussion on the 41-year heritage of SCALE:

- Mike Westfall (retired), originator of SCALE, 1976
- Lester Petrie (retired), principal developer and architect of SCALE, 1976–2016
- Cecil Parks, SCALE project leader, 1979–1994
- Steve Bowman, SCALE project leader, 1995–2009
- Brad Rearden (moderator), manager, SCALE Code System, 2009–present

Tutorial sessions were provided on the following topics:

- ORIGAMI spent fuel characterization
- TSUNAMI sensitivity/uncertainty analysis
- Polaris lattice physics calculations
- Sampler uncertainty quantification

Technical tours of the following ORNL facilities were offered:

- High Flux Isotope Reactor
- Spent Fuel Experimental Facility
- Historic ORNL Graphite Reactor
- National Center for Computational Sciences

The full agenda with links to the presentations is available at:
https://www.ornl.gov/scale/scale/2017-scale-users-group-workshop

Figure 10. Participants in the 2017 SCALE Users' Group Workshop.

Figure 11. Brad Rearden introduces SCALE.

Figure 12. Drew Barto of the NRC delivers a keynote address.

Figure 13. Larry Wetzel of BWXT delivers a keynote address.

Figure 14. Participants in the SCALE Heritage Panel
(Left to right) Brad Rearden, Steve Bowman, Cecil Parks, Lester Petrie, and Mike Westfall.

See more photos from the workshop at:
https://www.ornl.gov/scale/cale/2017-scale-users-group-workshop-photos

Save the Date for SCALE Users' Group Workshop 2018

The second SCALE Users' Group Workshop will be hosted at ORNL on August 27–29, 2018. All users are invited to contribute presentations on impactful, innovative applications of SCALE. More details will be available on the SCALE website (https://scale.ornl.gov).

Recent SCALE Training Events

Figure 15. SCALE Training at Air Force Institute of Technology,
November 2017.

Figure 16. SCALE Training on TRITON/Sampler,
North Carolina State University, March 2017.

Figure 17. SCALE/ORIGEN Fuel Depletion, Activation, and Source Term Analysis Course, ORNL, Oak Ridge, TN, October 2017.

Figure 18. SCALE Sensitivity and Uncertainty Analysis for Criticality Safety Assessment and Validation Course, ORNL, Oak Ridge, TN October 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 new update, SCALE 6.2.3, will be made available in April 2018. There are currently more than 8,500 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.

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

- User documentation and 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-users-group
- E-mail helpline: scalehelp@ornl.gov

Nations where SCALE is licensed

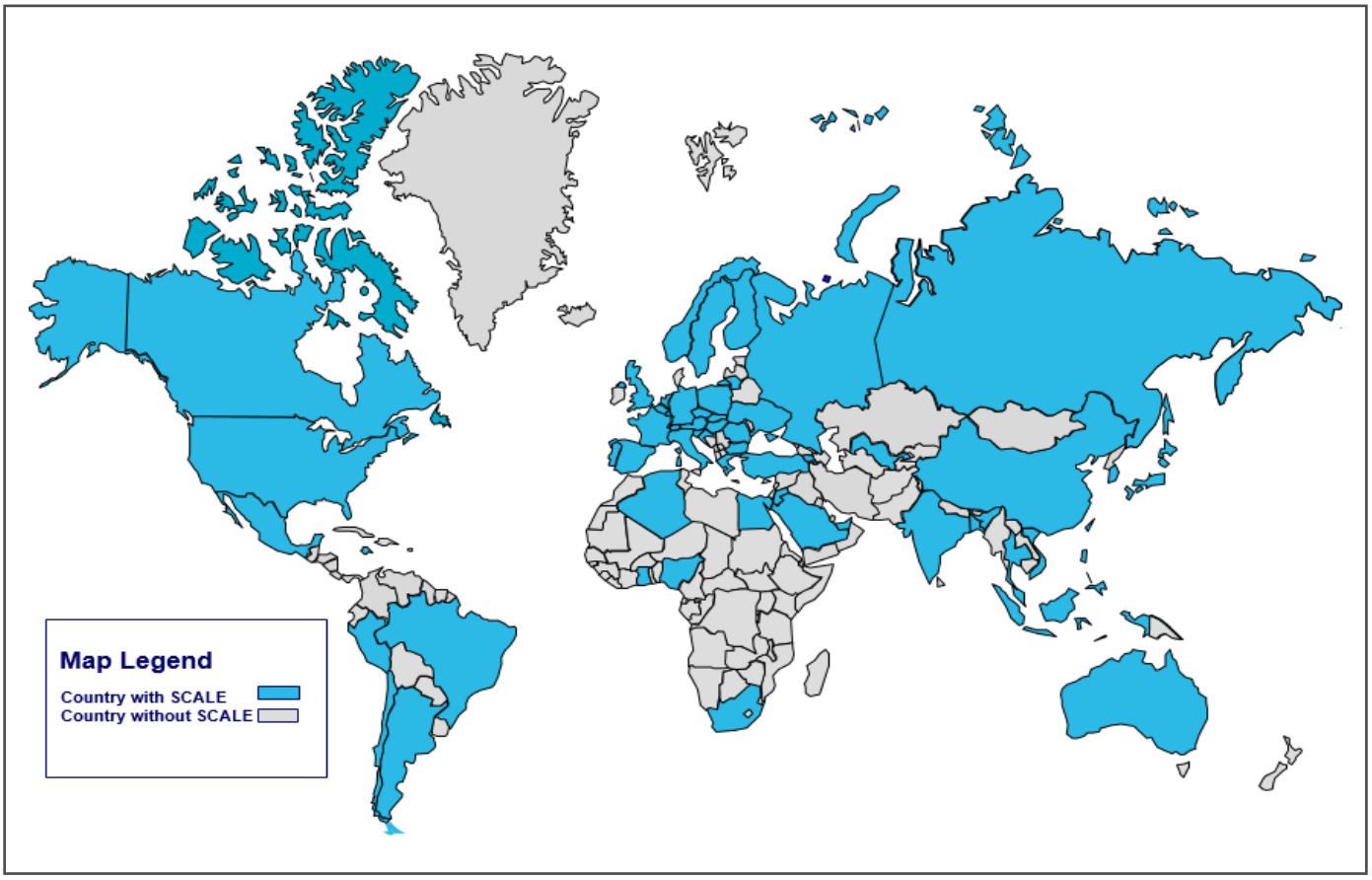
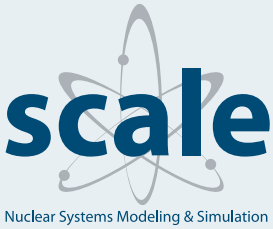


Figure 19. Nations where SCALE is licensed.



SCALE Newsletter

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