Recent Developments in SCALE

Presented to:

Nuclear Criticality Safety Program Technical Program Review

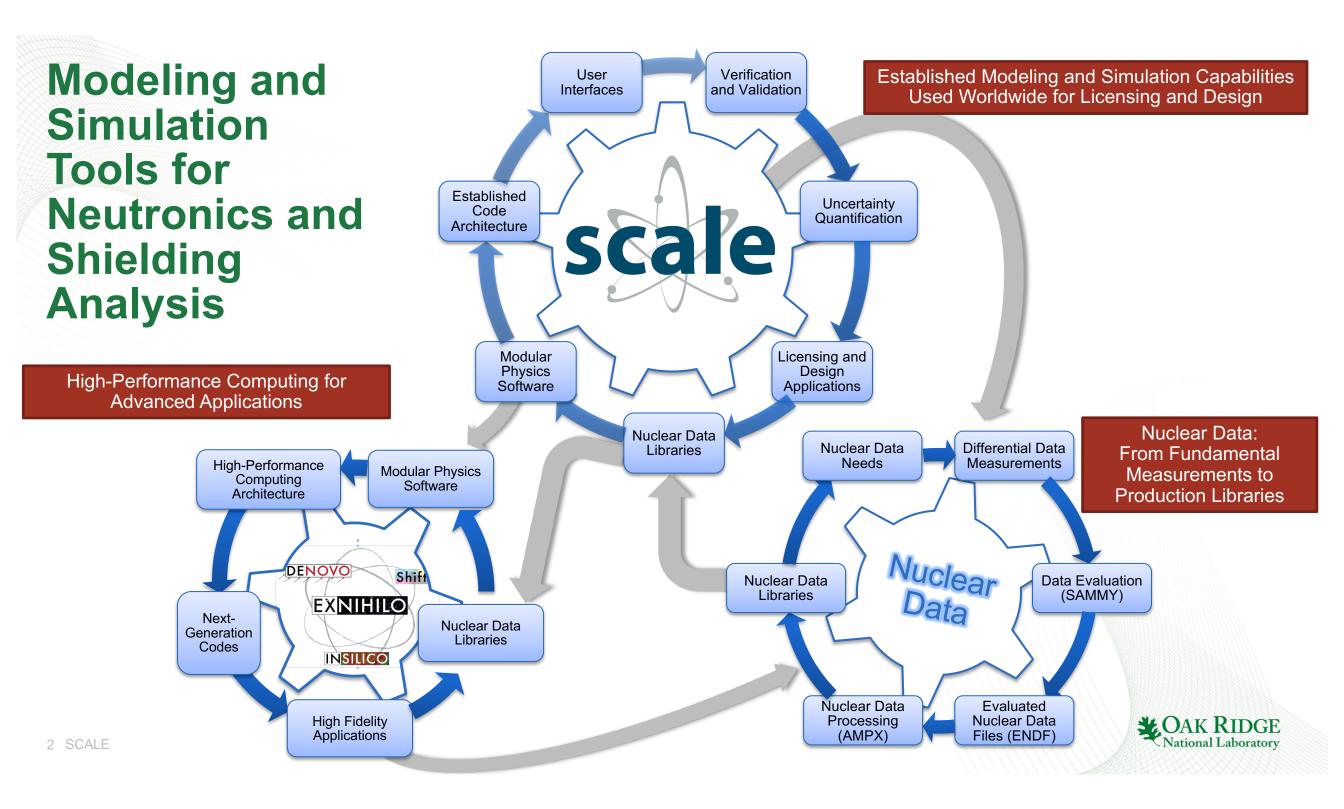
Bradley T. Rearden, PhD

Leader, Modeling and Simulation Integration Manager, SCALE Code System Reactor and Nuclear Systems Division

March 27, 2018

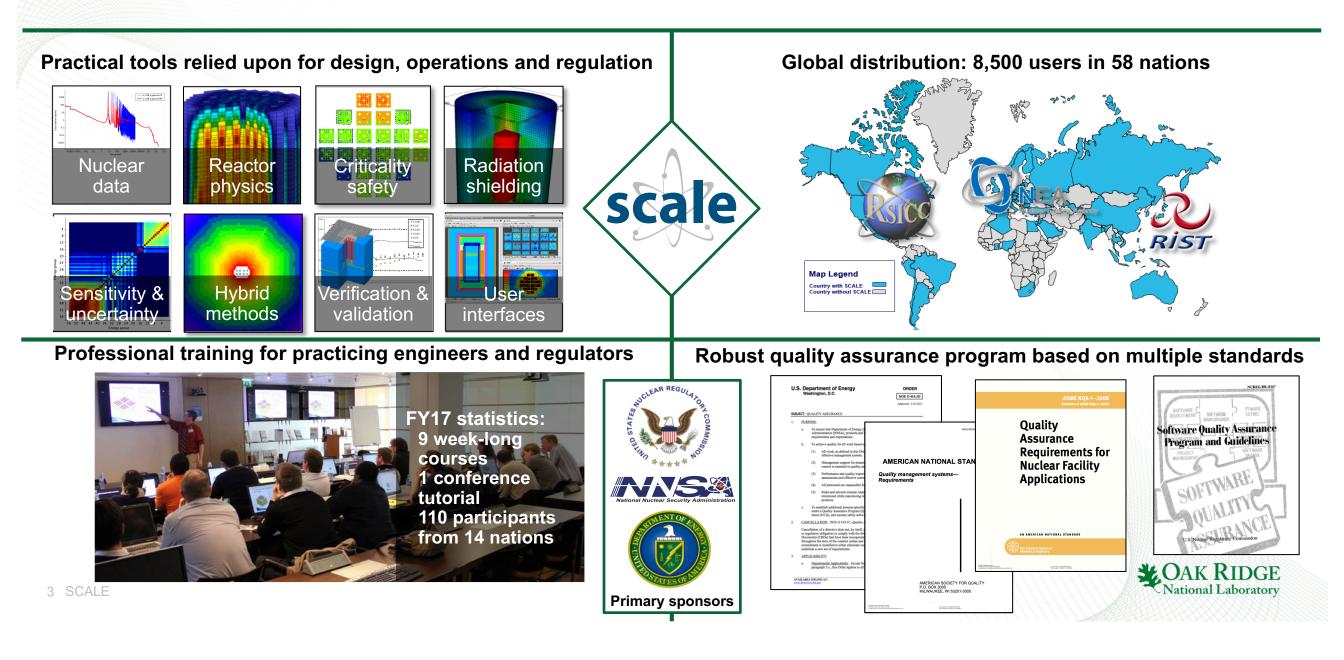
ORNL is managed by UT-Battelle for the US Department of Energy

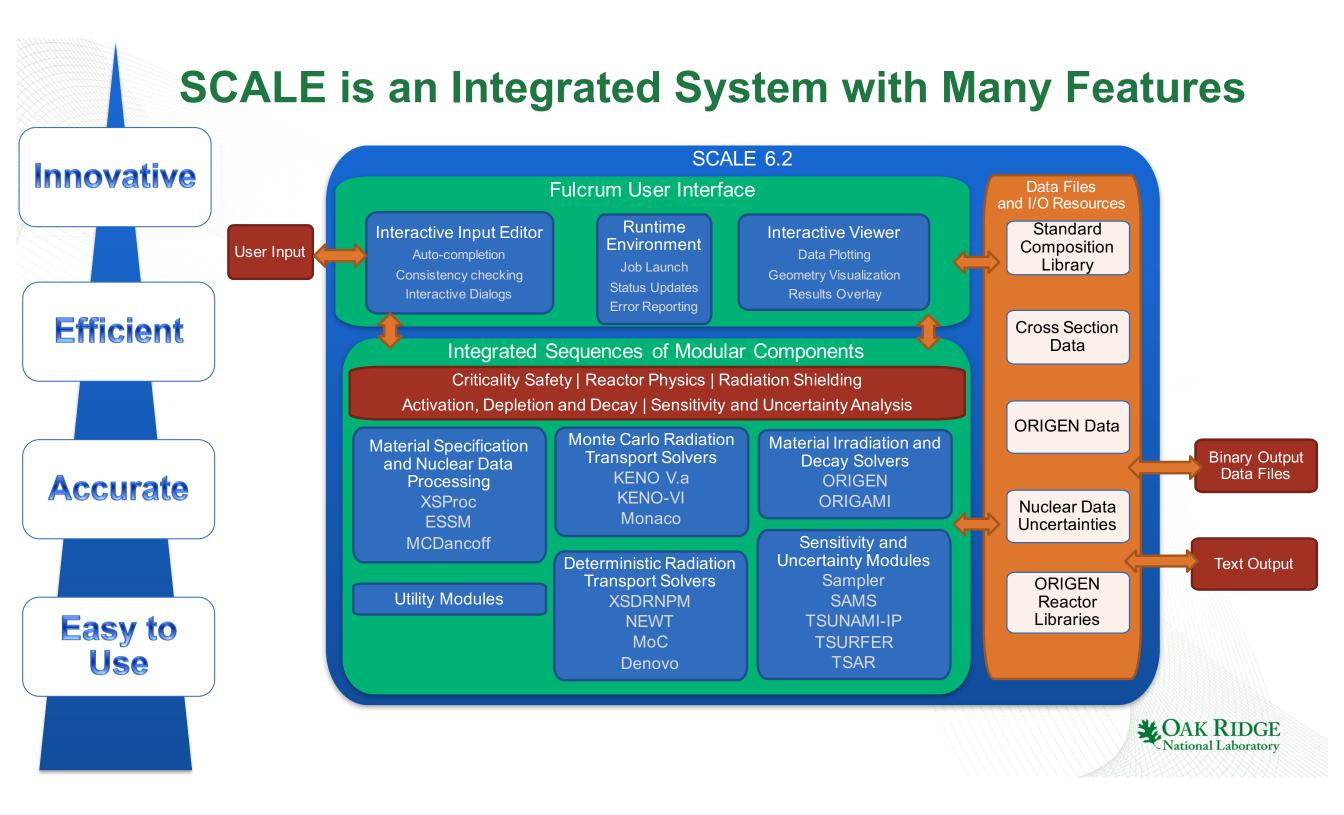




SCALE Code System:

Neutronics and Shielding Analysis Enabling Nuclear Technology Advancements – http://scale.ornl.gov





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SCALE 0.0 – SCALE 4.4a

SCALE Evolution

1980 - 2000

Established for Nuclear Regulatory Commission

Provides an independent rigorous nuclear safety analysis capability for out-ofreactor license reviews

Key Capabilities

Criticality safety

Radiation source term characterization

Radiation shielding

Heat transfer

SCALE 5.0 – SCALE 6.1

2004 – 2011

Expanded Capabilities to Address a Broader Class of Problems & Sponsors

Reactor physics

Shielding analysis with automated variance reduction

Sensitivity and uncertainty analysis

High-fidelity criticality safety in continuous energy

Graphical user interfaces and visualization tools

Expanded visibility

Used in 56 nations by regulators, industry, utilities, and researchers

SCALE 6.2

2016 – 2018

Increased Fidelity, Infrastructure Modernization, Parallelization, Enhanced Quality Assurance

Solutions for extremely complex systems

High-fidelity shielding, depletion and sensitivity analysis in continuous energy

Simplified and efficient lattice physics

Unified user interface

Initiated modern, modular software design

Expanded Use

Over 8,500 users in 58 nations Tools leveraged by many projects

SCALE 6.3 – SCALE 7.0

2018 –

High-performance Monte Carlo, Capabilities for Advanced Reactors and Advanced Fuels, Integration with Many other Tools

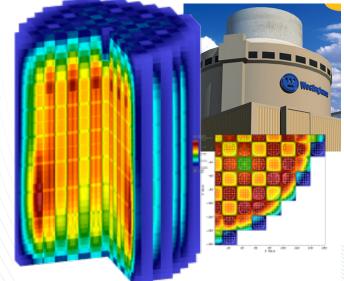
Solutions for extremely complex systems

High-fidelity, highly parallelized criticality shielding, depletion and sensitivity analysis in continuous energy

Extended modern, modular software design

Expanded Integration

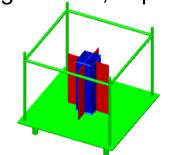
Tools directly integrated with many projects



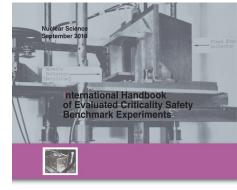
SCALE criticality validation: Verified, Archived Library of Inputs and Data (VALID)

- 611 configurations from International Criticality Safety Benchmark Evaluation Project (ICSBEP)
- 200 additional configurations, especially for ²³³U systems







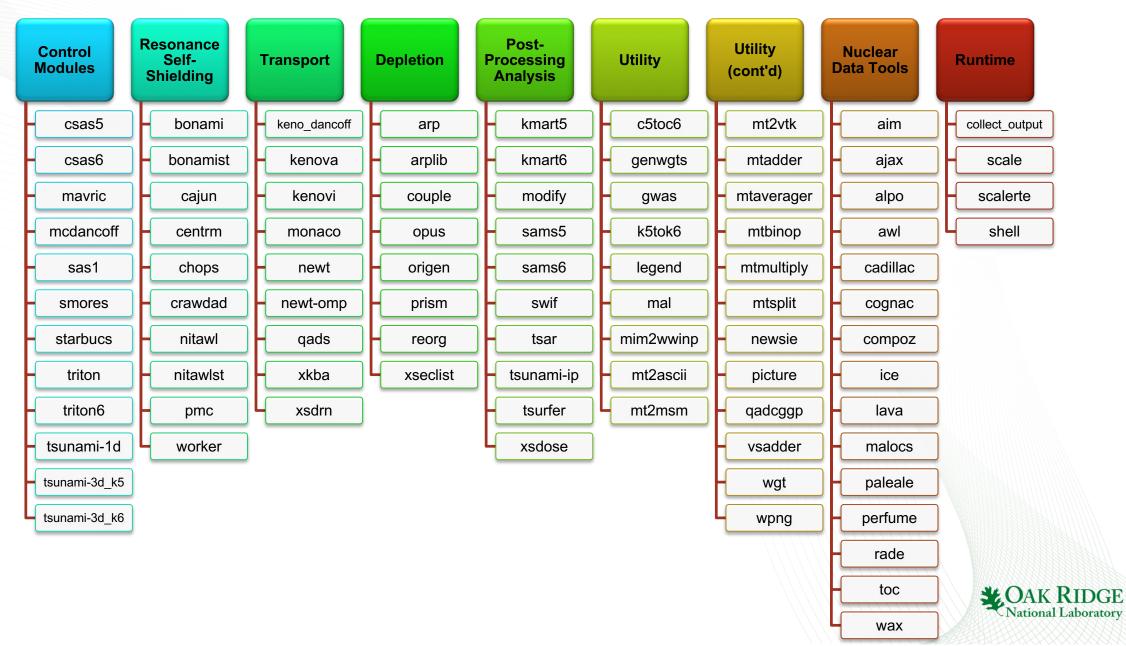


PONE /

Sequence / Geometry	Experiment class	ICSBEP case numbers	Number of configurations	
CSAS5 / KENO V.a	HEU-MET-FAST HEU-SOL-THERM IEU-MET-FAST LEU-COMP-THERM LEU-SOL-THERM MIX-MET-FAST MIX-COMP-THERM MIX-SOL-THERM PU-MET-FAST PU-SOL-THERM U233-COMP-THERM U233-SOL-THERM U233-SOL-MIXED U233-SOL-THERM	15, 16, 17, 18, 19, 20, 21, 25, 30, 38, 40, 52, 65 1, 13, 14, 16, 28, 29, 30 2, 3, 4, 5, 6, 7, 8, 9 1, 2, 8, 10, 17, 42, 50, 78, 80 2, 3, 4 5, 6 1, 2, 4 2, 7 1, 2, 5, 6, 8, 10, 18, 22, 23, 24, 25, 26 1, 2, 3, 4, 5, 6, 7, 11, 20 1 1, 2, 3, 4, 5, 6 1 1, 2 1, 2, 3, 4, 5, 8, 9, 11, 12, 13, 15, 16, 17	19 52 8 140 19 2 21 10 12 81 3 10 29 8 140	 Fissile materials High-enriched uranium (HEU), Intermediate-enriched uranium (IEU) Low-enriched uranium (LEU) Plutonium (Pu) Mixed uranium/plutonium oxides (MOX) Uranium-233 (U233) Fuel form Metal (MET), Fissile solution (SOL) Multi-material composition (e.g. fuel pins – COMP) Neutron spectra
CSAS6 / KENO-VI SCALE	HEU-MET-FAST IEU-MET-FAST MIX-COMP-THERM	5, 8, 9, 10, 11, 13, 24, 80, 86, 92, 93, 94 19 8	27 2 28	Fast Intermediate (INTER) Thermal Mixed

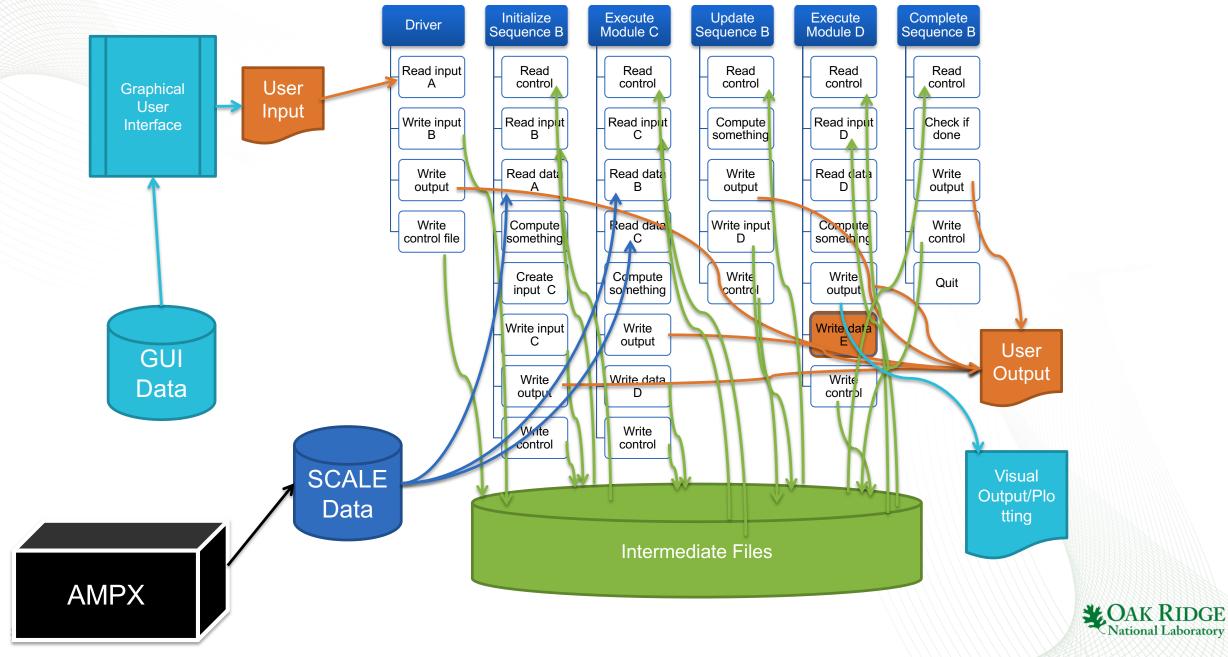
SCALE Modernization Plan:

89 Independent Executable Modules in SCALE 6.1

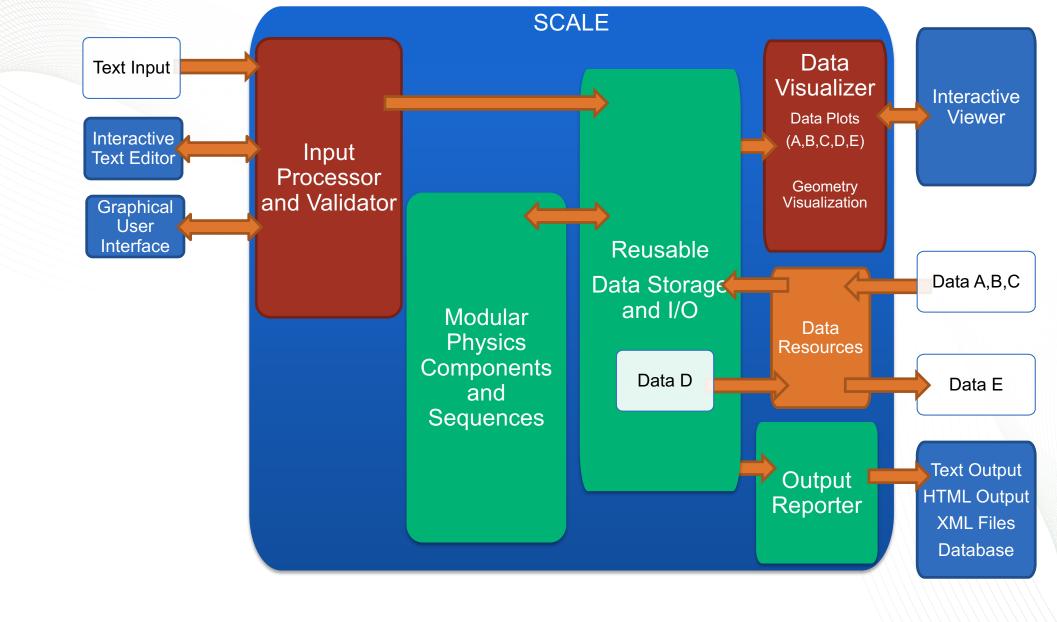


7 SCALE

Hypothetical SCALE 6.1 Calculation

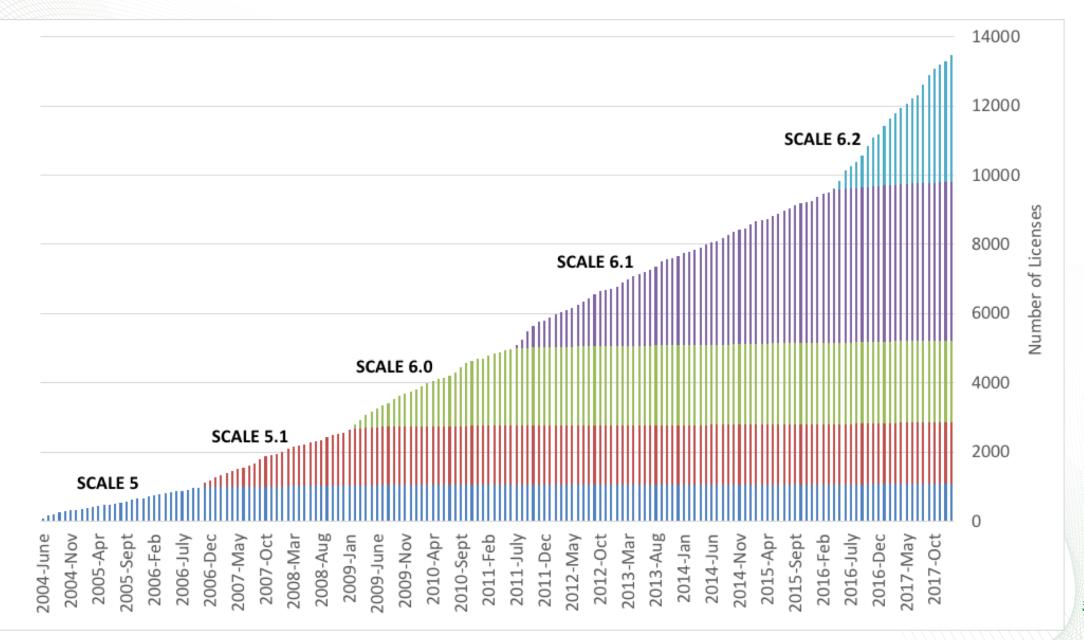


SCALE 7 Modernized Concept



CAK RIDGE

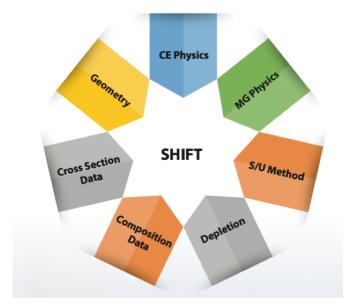
SCALE licenses by version



CAK RIDGE

Shift Monte Carlo code system

- Flexible, high-performance Monte Carlo radiation transport *framework*
- Shift is physics agnostic
 - SCALE CE physics
 - SCALE MG physics
- Shift is geometry agnostic
 - SCALE geometry
 - Exnihilo RTK geometry
 - MCNP geometry
 - DagMC-CUBIT CAD geometry



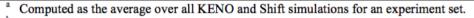
- Fixed-source and eigenvalue solvers
- Integrated with Denovo for hybrid methods
- Multiple parallel decompositions and concurrency models
- Shift is designed to scale from supercomputers to laptops



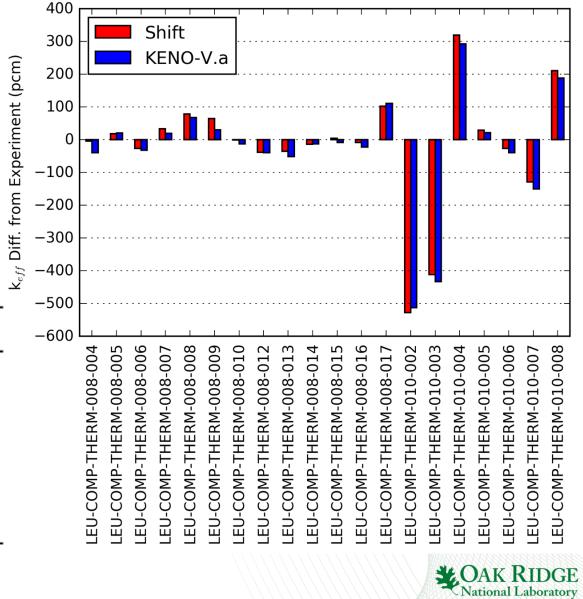
Validation of CSAS5-Shift

- VALID results for Shift correspond well with KENO V.a and KENO-VI results
- VALID calculations were run on a single processor, to compare computational time between KENO and Shift

Experiment type	Number of cases	Difference from KENO ^a (pcm)	Standard deviation ^b (pcm)
LEU-COMP-THERM	128	21	31
IEU-MET-FAST	11	16	160
PU-MET-FAST	10	-23	27
MIX-SOL-THERM	3	23	21
MIX-COMP-FAST	2	506	19
MIX-COMP-THERM	20	18	17
HEU-MET-FAST	22	-14	18
PU-SOL-THERM	81	6	20

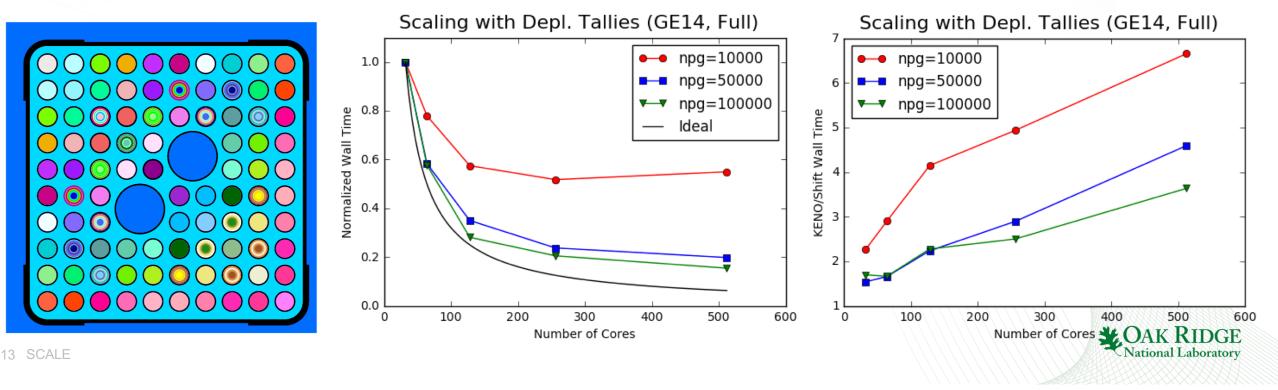


^b Computed as the standard deviation of the difference in k_{eff} between Shift and KENO.

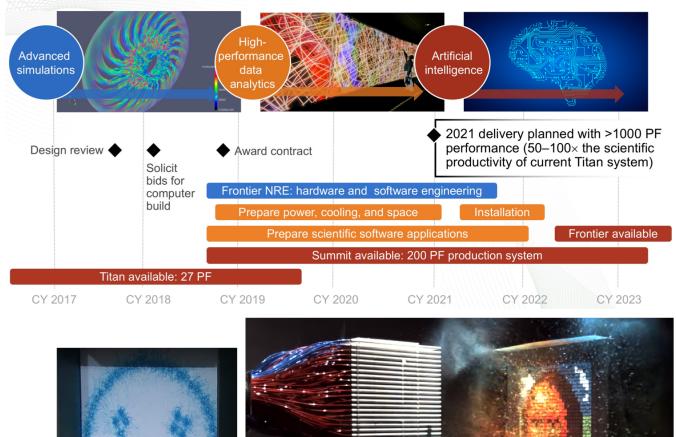


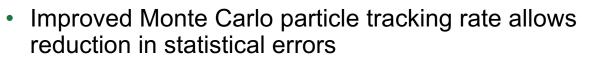
Shift parallel scaling compared to KENO

- Test Case: GE14 fuel assembly with depletion tallies
 - A number of identical simulations were run and the average time over the set simulations was used to
 estimate CPU time
- Shift is only slightly faster than KENO on a single node (1.5x 2x), but much faster on many nodes (3x - 7x)
- Shift scales close to ideally up to hundreds of processors when using O(50k) particles per generation

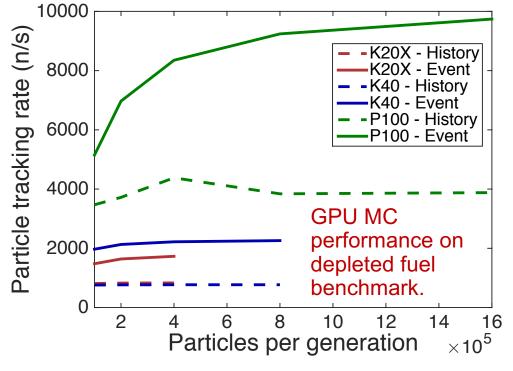


Shift is being extended for operation on GPUs as part of the Exascale Computing Project





- Cost of tallies and data access is implicit in this measure
- Improved device performance yields better results Algorithms are tracking hardware improvements



⁴ http://www.nvidia.com/object/what-is-gpu-computing.html

GE

EXASCALE COMPUTING PROJECT

Shift/SCALE integration

Integrated in CSAS criticality sequence

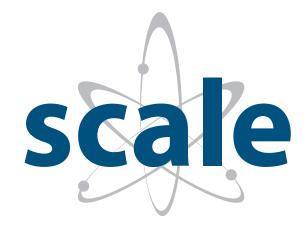
- Eigenvalue mode for criticality safety
- KENO V.a and KENO-VI geometry
- Uses standard SCALE geometry, material, and control specifications
- Validated with over 400 benchmark experiments

Integration in TRITON depletion sequence

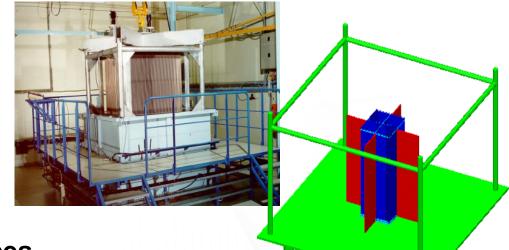
- Currently in development
- Flux-solver
- Depletion
- Multigroup cross section generation for nodal codes
- Randomized geometry for TRISO and pebble bed

Integration in TSUNAMI sensitivity/uncertainty sequences

- Capability demonstrated
- Eigenvalue and generalized perturbation theory sensitivity coefficients with CE physics
- Integration in MAVRIC shielding sequence
 - Fixed-source shielding problems using hybrid methods, especially for large facility and site modeling
 - Currently in development



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SCALE User Notice – March 2018

- A check that users enter a required cuboidal outer boundary if using non-vacuum boundary conditions was disabled for SCALE 6.1–6.2.2
- Check enabled again for SCALE 6.2.3

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SCALE User Notice

March 8, 2018

The KENO <u>V</u>, a Monte Carlo code in SCALE 6.1–6.2.2 does not include an input check to ensure compliance with the requirement that albedo boundary conditions other than vacuum (e.g., mirror, periodic, white) are only applied to cuboidal outer shapes. Users who do not follow this requirement per the user documentation may generate non-conservative <u>keff</u> results without warning.

Per the requirements of the *Quality Assurance Plan for the SCALE Code System* [1] and specifically the *SCALE Procedure for Discrepancy Reports* [2], this issue is being categorized as a *Significant Software Error* and is reported in this User Notice.

Summary

In all versions of SCALE, the Monte Carlo code KENO <u>Y</u>, a only implements the use of nonvacuum albedo boundary conditions (e.g., mirror, periodic, white) 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 <u>Y</u>, this geometry region must be a rectangular parallelepiped"[3][4].

Correct Cuboid boundary k_{eff} = 1.03599 +/- 0.00063

I have to say I am very impressed by the SCALE team's response here. This is a code system that is clearly professionally run and most importantly communicative with its users. – Don Algama – U.S. Nuclear Regulator Commission

Modernization of USLSTATS

Statistical package for determining upper subcritical limits using traditional or S/U-based parameters



scale

Nuclear Systems Modeling & Simulation

Sequence

Module

- Java code not routinely tested with rest of SCALE
- USL 1 and USL 2 Methods only

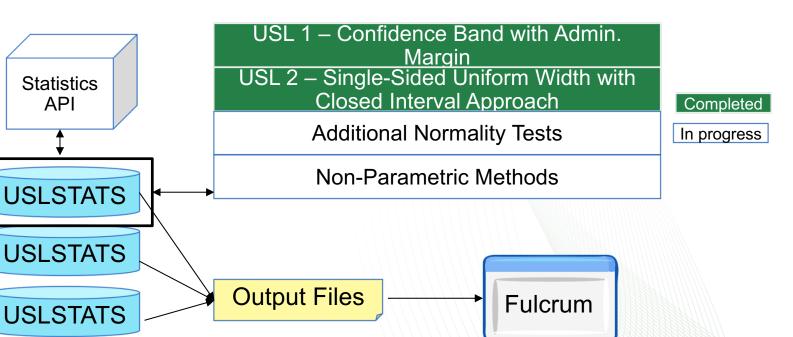
SCALE 6.3:

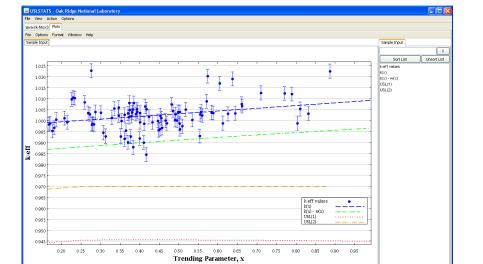
- Uses modern SCALE Sequence flow
- Fulcrum GUI for Input/Output
- Easier to add new methods

Input File(s)

Fulcrum

Uses new Statistics API

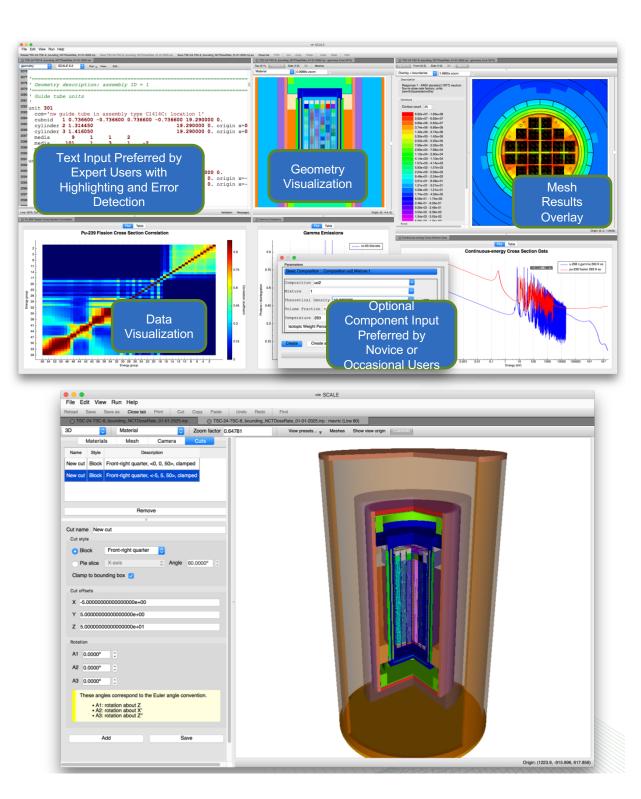




CAK RIDGE National Laboratory

Fulcrum: SCALE's integrated user interface

- Input generation and checking
- Geometry and nuclear data visualization
- Output review and visualization
- New 3D visualization for KENO V.a and KENO-VI
 - Multiple cuts with "undo"
 - Transparency
 - Rotation
 - Hide/Show materials
- Pending development:
 - AMPX integration (currently uses ExSITE)
 - Coloring for computed values instead of just materials
 - Mesh results overlay in 3D
 - Expanded use of input generation from dialog boxes, especially for new users



Uncertainty Analysis for Criticality Safety Assessment (UACSA)

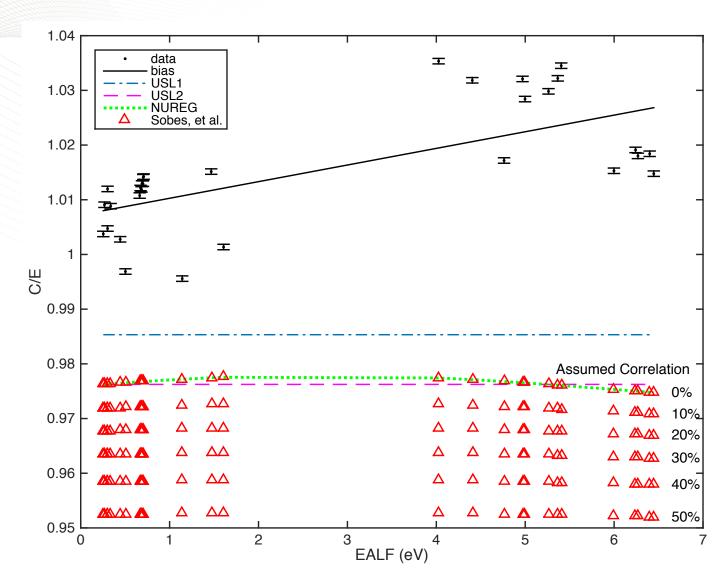
- OECD/NEA expert group under Working Party on Nuclear Criticality Safety
- Nearly 40 participants
- Phase IV Benchmark on Role of Integral Experiment Covariance Data for Criticality Safety Validation
- Phase V Benchmark
 Blind Benchmark on MOX Wet
 Powders





Phase IV Benchmark

Role of Integral Experiment Covariance Data for Criticality Safety Validation



Using data from a previous transportation package criticality safety assessment, the inclusion of experimental correlations impacts the USL by as much as 3% Δk/k

V. Sobes, B. T. Rearden, D. E. Mueller,
W. J. Marshall, J. M. Scaglione, and M.
E. Dunn, "Upper Subcritical Calculations Based on Correlated Data," ICNC 2015
– International Conference on Nuclear Criticality Safety, Charlotte, NC, September 13–17, 2015.

WPNCS/UACSA results

Fully correlated

	7-1	7-2	7-3	39-1	39-2	39-3	39-4	39-5	39-6	39-7	39-8	39-9	39-10	39-11	39-12	39-13	39-14	39-15	39-16	39-17
7-1	1.000	0.933	0.391	0.978	0.975	0.974	0.974	0.956	0.957	0.974	0.971	0.978	0.969	0.977	0.972	0.980	0.979	0.973	0.977	0.978
7-2	0.933	1.000	0.557	0.923	0.920	0.925	0.930	0.925	0.929	0.933	0.920	0.936	0.940	0.925	0.924	0.928	0.933	0.928	0.937	0.931
7-3	0.391	0.557	1.000	0.405	0.390	0.409	0.417	0.459	0.463	0.415	0.389	0.434	0.451	0.384	0.406	0.405	0.382	0.399	0.418	0.420
39-1	0.978	0.923	0.405	1.000	0.978	0.970	0.973	0.957	0.958	0.976	0.972	0.970	0.973	0.979	0.976	0.976	0.981	0.977	0.972	0.977
39-2	0.975	0.920	0.390	0.978	1.000	0.972	0.970	0.953	0.954	0.975	0.967	0.968	0.963	0.974	0.974	0.976	0.977	0.970	0.972	0.977
39-3	0.974	0.925	0.409	0.970	0.972	1.000	0.967	0.945	0.954	0.971	0.963	0.971	0.966	0.974	0.969	0.974	0.971	0.967	0.972	0.970
39-4	0.974	0.930	0.417	0.973	0.970	0.967	1.000	0.956	0.954	0.971	0.965	0.968	0.965	0.972	0.971	0.973	0.974	0.968	0.973	0.978
39-5	0.956	0.925	0.459	0.957	0.953	0.945	0.956	1.000	0.946	0.958	0.944	0.955	0.955	0.953	0.949	0.952	0.952	0.954	0.951	0.958
39-6	0.957	0.929	0.463	0.958	0.954	0.954	0.954	0.946	1.000	0.956	0.953	0.960	0.961	0.955	0.954	0.963	0.955	0.957	0.958	0.960
39-7	0.974	0.933	0.415	0.976	0.975	0.971	0.971	0.958	0.956	1.000	0.973	0.974	0.970	0.979	0.978	0.974	0.979	0.974	0.979	0.978
39-8	0.971	0.920	0.389	0.972	0.967	0.963	0.965	0.944	0.953	0.973	1.000	0.964	0.970	0.973	0.966	0.970	0.973	0.964	0.964	0.966
39-9	0.978	0.936	0.434	0.970	0.968	0.971	0.968	0.955	0.960	0.974	0.964	1.000	0.967	0.976	0.968	0.976	0.976	0.969	0.975	0.974
39-10	0.969	0.940	0.451	0.973	0.963	0.966	0.965	0.955	0.961	0.970	0.970	0.967	1.000	0.964	0.968	0.969	0.966	0.964	0.968	0.970
39-11	0.977	0.925	0.384	0.979	0.974	0.974	0.972	0.953	0.955	0.979	0.973	0.976	0.964	1.000	0.973	0.980	0.979	0.977	0.977	0.977
39-12	0.972	0.924	0.406	0.976	0.974	0.969	0.971	0.949	0.954	0.978	0.966	0.968	0.968	0.973	1.000	0.978	0.976	0.968	0.972	0.976
39-13	0.980	0.928	0.405	0.976	0.976	0.974	0.973	0.952	0.963	0.974	0.970	0.976	0.969	0.980	0.978	1.000	0.977	0.979	0.976	0.976
39-14	0.979	0.933	0.382	0.981	0.977	0.971	0.974	0.952	0.955	0.979	0.973	0.976	0.966	0.979	0.976	0.977	1.000	0.976	0.977	0.979
39-15	0.973	0.928	0.399	0.977	0.970	0.967	0.968	0.954	0.957	0.974	0.964	0.969	0.964	0.977	0.968	0.979	0.976	1.000	0.970	0.973
39-16	0.977	0.937	0.418	0.972	0.972	0.972	0.973	0.951	0.958	0.979	0.964	0.975	0.968	0.977	0.972	0.976	0.977	0.970	1.000	0.976
39-17	0.978	0.931	0.420	0.977	0.977	0.970	0.978	0.958	0.960	0.978	0.966	0.974	0.970	0.977	0.976	0.976	0.979	0.973	0.976	1.000

Pitch sampled: all pitches are the same and are the same for all cases

Coefficients range from 0.96 to 0.98 (For cases with the same pitch)

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Independent

	7-1	7-2	7-3	39-1	39-2	39-3	39-4	39-5	39-6	39-7	39-8	39-9	39-10	39-11	39-12	39-13	39-14	39-15	39-16	39-17
7-1	1.000	0.034	0.023	0.012	0.005	-0.040	0.069	-0.009	0.071	0.067	0.082	0.088	0.049	0.044	0.042	0.063	0.088	0.139	-0.021	0.082
7-2	0.034	1.000	0.074	-0.045	0.020	0.040	0.181	0.086	0.065	0.041	-0.028	-0.034	0.009	-0.030	0.018	0.047	-0.041	0.023	0.061	-0.028
7-3	0.023	0.074	1.000	0.118	0.063	0.094	0.061	0.086	0.201	0.079	0.100	0.134	0.047	0.091	0.012	0.125	0.050	0.117	0.172	0.055
39-1	0.012	-0.045	0.118	1.000	0.121	0.138	0.076	0.071	0.124	0.034	0.100	0.085	0.135	0.023	0.037	0.037	0.087	0.083	0.115	0.149
39-2	0.005	0.020	0.063	0.121	1.000	0.034	0.075	0.037	0.130	0.041	0.055	0.049	0.009	0.025	0.095	0.100	-0.050	0.124	-0.003	0.115
39-3	-0.040	0.040	0.094	0.138	0.034	1.000	0.079	0.077	0.044	0.007	0.048	-0.064	0.145	0.076	0.061	0.090	0.067	0.059	0.088	0.116
39-4	0.069	0.181	0.061	0.076	0.075	0.079	1.000	-0.051	0.090	-0.012	-0.017	0.036	0.026	-0.021	0.034	0.088	0.042	-0.004	0.025	-0.018
39-5	-0.009	0.086	0.086	0.071	0.037	0.077	-0.051	1.000	0.138	0.081	0.043	0.140	0.112	0.059	0.085	0.131	0.184	0.001	0.161	0.093
39-6	0.071	0.065	0.201	0.124	0.130	0.044	0.090	0.138	1.000	0.103	-0.014	0.035	0.149	0.051	0.062	0.116	0.013	0.074	0.153	0.127
39-7	0.067	0.041	0.079	0.034	0.041	0.007	-0.012	0.081	0.103	1.000	0.131	0.007	0.004	0.024	-0.003	0.111	0.053	0.081	0.173	0.035
39-8	0.082	-0.028	0.100	0.100	0.055	0.048	-0.017	0.043	-0.014	0.131	1.000	-0.067	0.047	-0.016	0.063	0.004	0.030	0.013	0.050	0.070
39-9	0.088	-0.034	0.134	0.085	0.049	-0.064	0.036	0.140	0.035	0.007	-0.067	1.000	0.082	0.041	0.070	0.000	0.046	-0.081	-0.009	0.077
39-10	0.049	0.009	0.047	0.135	0.009	0.145	0.026	0.112	0.149	0.004	0.047	0.082	1.000	0.080	0.069	-0.004	0.041	0.115	0.119	0.047
39-11	0.044	-0.030	0.091	0.023	0.025	0.076	-0.021	0.059	0.051	0.024	-0.016	0.041	0.080	1.000	0.115	0.022	-0.087	-0.048	0.112	0.046
39-12	0.042	0.018	0.012	0.037	0.095	0.061	0.034	0.085	0.062	-0.003	0.063	0.070	0.069	0.115	1.000	0.132	0.112	0.006	0.065	0.069
39-13	0.063	0.047	0.125	0.037	0.100	0.090	0.088	0.131	0.116	0.111	0.004	0.000	-0.004	0.022	0.132	1.000	0.184	0.206	0.232	0.138
39-14	0.088	-0.041	0.050	0.087	-0.050	0.067	0.042	0.184	0.013	0.053	0.030	0.046	0.041	-0.087	0.112	0.184	1.000	0.148	0.051	0.204
39-15	0.139	0.023	0.117	0.083	0.124	0.059	-0.004	0.001	0.074	0.081	0.013	-0.081	0.115	-0.048	0.006	0.206	0.148	1.000	0.090	0.037
39-16	-0.021	0.061	0.172	0.115	-0.003	0.088	0.025	0.161	0.153	0.173	0.050	-0.009	0.119	0.112	0.065	0.232	0.051	0.090	1.000	-0.023
39-17	0.082	-0.028	0.055	0.149	0.115	0.116	-0.018	0.093	0.127	0.035	0.070	0.077	0.047	0.046	0.069	0.138	0.204	0.037	-0.023	1.000

All fuel rod positions are sampled independently and differently in each case

Coefficients range from ~0 to ~0.23

Fuel rod position modeling makes a difference!

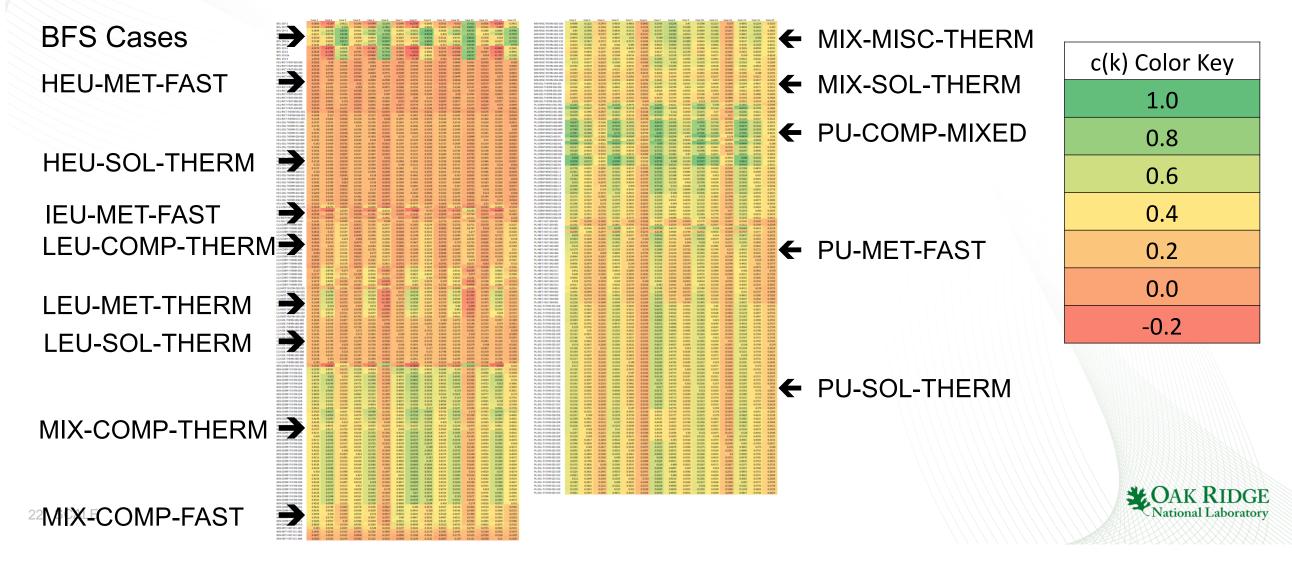
W. J. Marshall and B. T. Rearden, "Determination of Critical Experiment Correlations for Experiments Involving Arrays of Low-Enriched Fuel Rods," *Proc. of ANS NCSD 2017 - Criticality safety - pushing the boundaries by modernizing and integrating data, methods, and regulations,* Carlsbad, NM, September 10–15, 2017.



Phase V Benchmark

Blind Benchmark on MOX Wet Powders

- Challenging criticality safety validation with few applicable benchmark
- Advanced validation methods such as TSURFER and Whisper are required



Phase V Benchmark Blind Benchmark on MOX Wet Powders

 USLs vary from 0.74 to 0.99 based on selected benchmarks and validation approach

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9	Case 10	Case 11	Case 12	Case 13	Case 14	Case 15
USLSTATS Trending with PU-COMP-MIXED Experiments															
c(k) > 0.2	0.9861	0.9772	0.9845	0.9856	0.9765	0.9912	0.9886	0.9818	0.9882	0.9860	0.9819	0.9886	0.9861	0.9762	0.9818
c(k) > 0.55	0.9754	0.9262	0.9883	0.9758	0.9462	0.9856	0.9832	0.9461	0.9895	0.9748	0.9641	0.9825	0.9754	0.9039	0.9775
	USLSTATS Trending without PU-COMP-MIXED Experiments														
c(k) > 0.2	0.9861	0.9772	0.9845	0.9856	0.9765	0.9912	0.9886	0.9818	0.9882	0.9860	0.9819	0.9886	0.9861	0.9762	0.9818
c(k) > 0.55	0.9088	0.9461	0.9883	0.7751	0.9703	0.9856	0.9794	0.9681	0.9898	0.9436	0.9420	0.9825	0.7425	0.9418	0.9775
						Whi	sper Met	hodolog	y						
c(k) > 0.2	0.9657	0.9645	0.9627	0.9654	0.9646	0.9773	0.9668	0.9651	0.9663	0.9662	0.9649	0.9740	0.9652	0.9642	0.9611
c(k) > 0.55	0.9856	0.9665	0.9909	0.9881	0.9693	0.9843	0.9706	0.9659	0.9719	0.9832	0.9671	0.9843	0.9878	0.9663	0.9924
						TSURF	ER Data	Assimila	tion						
USLTSURFER	0.9924	0.9935	0.9889	0.9921	0.9928	0.9871	0.9946	0.9958	0.9950	0.9930	0.9936	0.9896	0.9916	0.9926	0.9885



New ENDF/B-VIII.0 disclaimer

 Added to ENDF repository by head of National Nuclear Data Center after issues were raised at November 2017 CSEWG meeting

Readme for ENDF/B-VIII.0

Comments about the covariance in current ENDF evaluations

- 1. The covariance data in the ENDF evaluations represents uncertainties and correlations in differential data.
- 2. The use of this covariance to calculate uncertainties for integral quantities such as K_{eff} will usually result in an overestimate of the uncertainty.
- 3. The recommended methodology to overcome this problem is to adjust the covariance to add information from set of integral data that represents the physics of the system for which the adjusted covariance will be used.
- 4. More information on this topic: <u>https://www.oecd-nea.org/science/wpec/sg33/</u>
- 5. CSEWG is currently studying the best covariance representation for future releases.



²³⁸U inelastic scattering cross section uncertainty differences between international libraries

Incident neutron data / / U238 MAT9237 / MAT9237 / MT4= (n,n') /MT=4 : (z,n') / Covariances data (BOXER) Relative standard deviation 50 U238-n.JEFF-3.3T4 U238-n.ENDF/B-VIII.0b6 Relative standard deviation (%) U238-n.ENDF/B-VII.1 30 ENDF/B-VII.1 U238-n.JENDL-4.0u1 20 Europe 10 Japan 7 Proposed 5 **ENDF/B-VIII** 3 0,005 0.5 0,001 0.01 0.05 0.1 10 5 Incident energy (MeV) CAK RIDGE



SCALE training courses are routinely provided to the user community at ORNL and NEA, regulatory training is provided twice annually to NRC, and application-specific training provided at user facilities



- FY17 statistics:
- 10 one-week courses
- 4 conference tutorials
- 150 participants from 15 nations









SCALE Users' Group Workshop 2017



- The first ever SCALE Users' Group Workshop was held at ORNL, September 26-28, 2017
 - attended by 117 participants from academia, industry, research institutions, and government agencies
 - provided an interactive forum for discussions between SCALE end users and developers

