SCALE in a nutshell

Presented by: SCALE Director and SCALE Team Members

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Oak Ridge National Laboratory

February 1, 2024

Outline

- SCALE overview
- SCALE validation:
  - shielding
  - criticality safety
  - nuclide inventory and decay heat
- SCALE/ORIGEN sensitivity
- Reactor physics calculations with SCALE/TRITON
- Sampler uncertainty quantification tool in SCALE
- Path to automated validation of ENDF/B-VIII.1
- New project: Impact of nuclear data on advanced reactor metrics

SCALE Overview

Oak Ridge National Laboratory
February 1, 2024

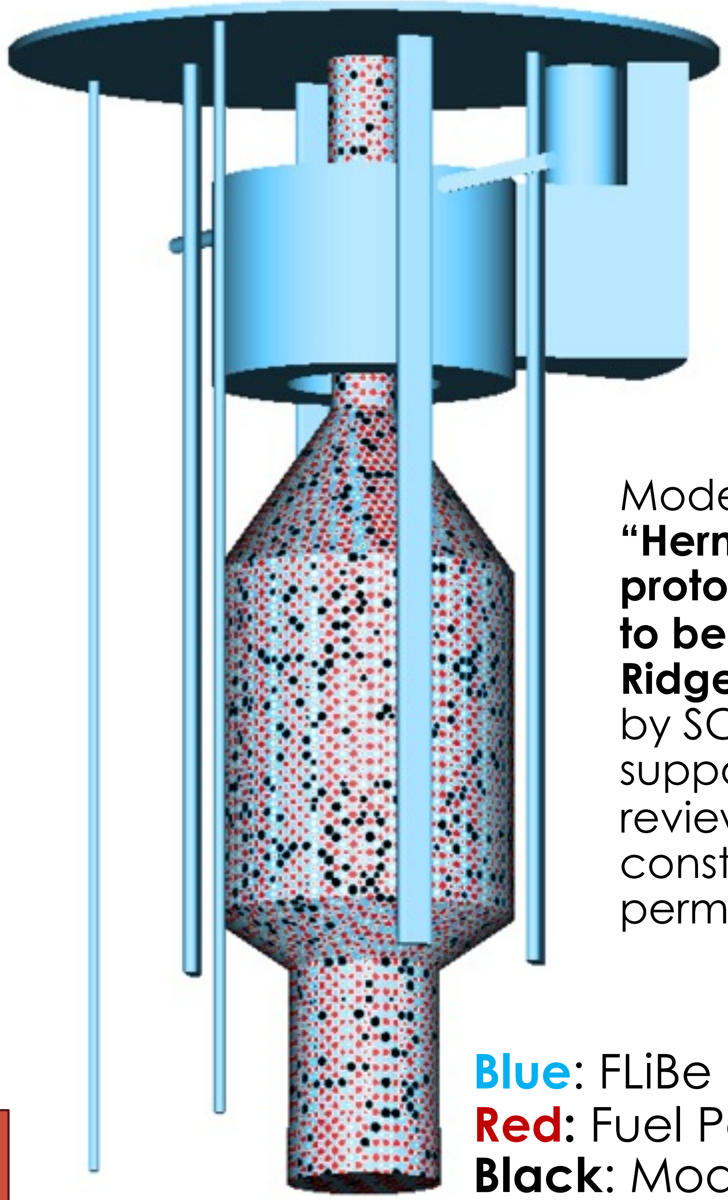
Will Wieselquist, Rob Lefebvre, Shane Hart

SCALE

Code System for Nuclear Modeling and Simulation

- Initiated by NRC in the 1980s to provide confirmatory analysis capabilities for light water reactor (LWR) criticality, transportation, and spent fuel applications
  - Sponsors include DOE Nuclear Criticality Safety Program, NNSA, and NRC
  - Over 11k users, ~100 trainees/year
- General capabilities for neutron/photon transport, energy generation, nuclide transmutation
- User-friendly capabilities for applications in
  - Criticality safety
  - Radiation shielding
  - Spent fuel inventory
  - Reactor physics/operation
  - Activation/Isotope production

Goal to be the top nuclear data assessment platform for nuclear energy and safety



Model of **Kairos "Hermes" prototype reactor to be built in Oak Ridge TN,** created by SCALE team to support NRC review of construction permit

Blue: FLiBe Coolant
Red: Fuel Pebble
Black: Moderator Pebble

Sensitivity, uncertainty propagation, and similarity capability in SCALE

- **Perturbation theory-based sensitivity methods** generate sensitivity coefficients of outputs like critical eigenvalue, k_{eff}, to all nuclear data
- **Sampling-based methods** allow sampling of any input parameter, including nuclear data, to **propagate uncertainty**
- New **similarity metrics** allow comparing two systems for **shared bias and uncertainty**—allows computational bias observed in a measurement to be associated to *similar* applications

TABLE 5 Summary of key observations.

All considered non-LWRs	FHR
• Large differences exist between ENDF/B library releases for relevant nominal and uncertainty data: neutron multiplicity, fission, capture, scattering for ^{235}U, ^{238}U, and major Pu isotopes • Reactivity uncertainty is driven by fission, capture and scattering reactions of ^{235}U, ^{238}U, and major Pu isotopes	• No graphite thermal scattering data uncertainties are available • No thermal scattering data for salts (e.g., FLiBe) are available • Significant update from ENDF/B-VII.0 to VII.1 in the carbon (n,γ) cross section • Large ^{7}Li (n,γ) cross section uncertainty • Significant update from ENDF/B-VII.0 to VII.1 in the ^{6}Li (n,t) cross section
HPR and SFR	**Graphite-moderated MSR**
• No angular scattering uncertainties are available • Large ^{235}U (n,γ) cross section uncertainty causes large uncertainties in system using ^{235}U-enriched fuel • Large ^{238}U inelastic scattering uncertainty causes large uncertainties in U/TRU-fueled systems • Large impact of scattering reactions of coolant and structural materials	• No cross section data are available for ^{135m}Xe • No thermal scattering data are available for salts (e.g., FLiBe) • No graphite thermal scattering data uncertainties are available • Large ^{7}Li (n,γ) cross section uncertainty • Significant update from ENDF/B-VII.0 to VII.1 in the ^{6}Li (n,t) cross section
HTGR	**Fast spectrum MSR**
• Significant update from ENDF/B-VII.0 to VII.1 in the carbon (n,γ) cross section • No graphite thermal scattering data uncertainties	• Significant update from ENDF/B-VII.0 to VII.1 in the ^{35}Cl (n,p) significant cross section • Large impact of ^{24}Mg elastic scattering uncertainty on uncertainties

Friederike Bostelmann, Germina Ilas, and William A. Wieselquist, "Key nuclear data for non-LWR reactivity analysis," *Frontiers in Energy Research*, **11,**1159478 (April 2023).

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Availability and open-source efforts

- SCALE is export-controlled technology under 10 CFR Part 810
  - **Free to ORNL staff**
  - As of 2023, available for free to non-commercial entities under a government-use agreement (GUA)
    - Enables a site license for NRC and other national labs
    - Handled through ORNL tech transfer
    - Email Rob Lefebvre (lefebvrera@ornl.gov) for details

- SCALE team has **open-sourced** fundamental data libraries and the AMPX nuclear data processing components

- **Public materials**
  - Manual https://scale-manual.ornl.gov
  - Reports and journal papers https://ornl.gov/scale/references
  - Open-source **code** (subset) https://code.ornl.gov/scale/code/scale-public
  - Open-source SCALE **models** https://code.ornl.gov/scale/analysis

SCALE 6.3 Shielding Validation

Oak Ridge National Laboratory
February 1, 2024

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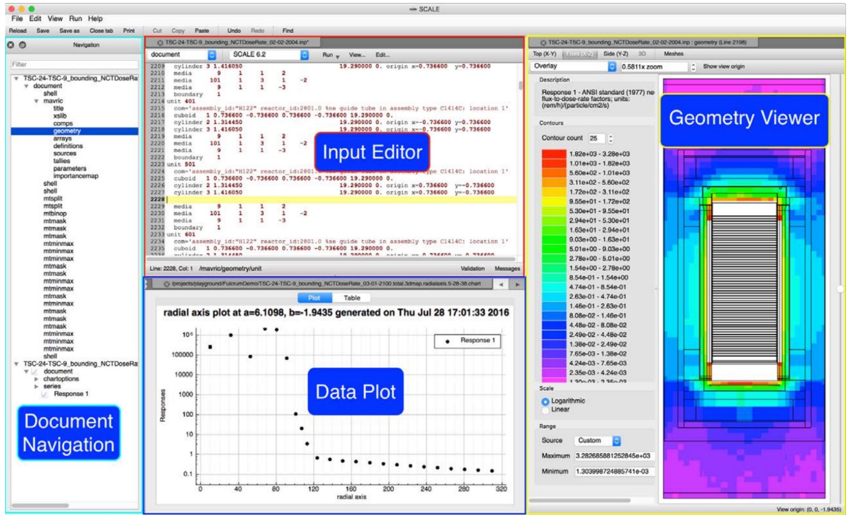
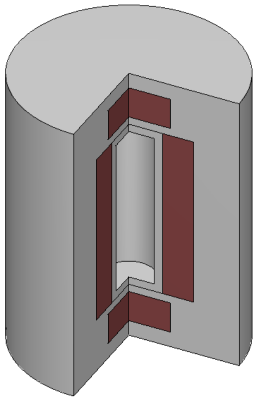
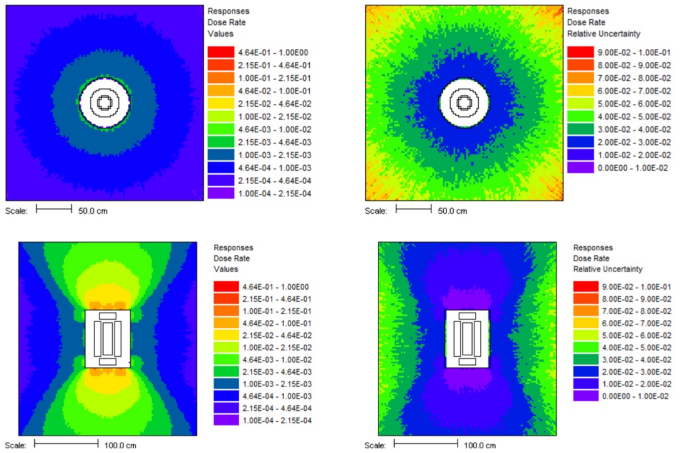
MAVRIC

- **Recognized shielding analysis tool**
  - NRC, NCSP, industry, and more
  - Validated (ICSBEP, SINBAD)
  - NQA-1 compatible
- **3D Monte Carlo particle transport**
  - Multigroup and continuous energy libraries
  - Neutron, photon, or coupled
  - Parallel processing
- **Powerful methods**
  - Doppler broadening
  - Probability tables for the URR
  - Photonuclear physics
  - Thick-target Bremsstrahlung
  - Automated variance reduction
- **Multiple tally types**
  - Point detectors, region, and mesh tallies
  - Flux, reaction and dose rates, energy deposition, and user-defined responses
  - Fulcrum GUI integration



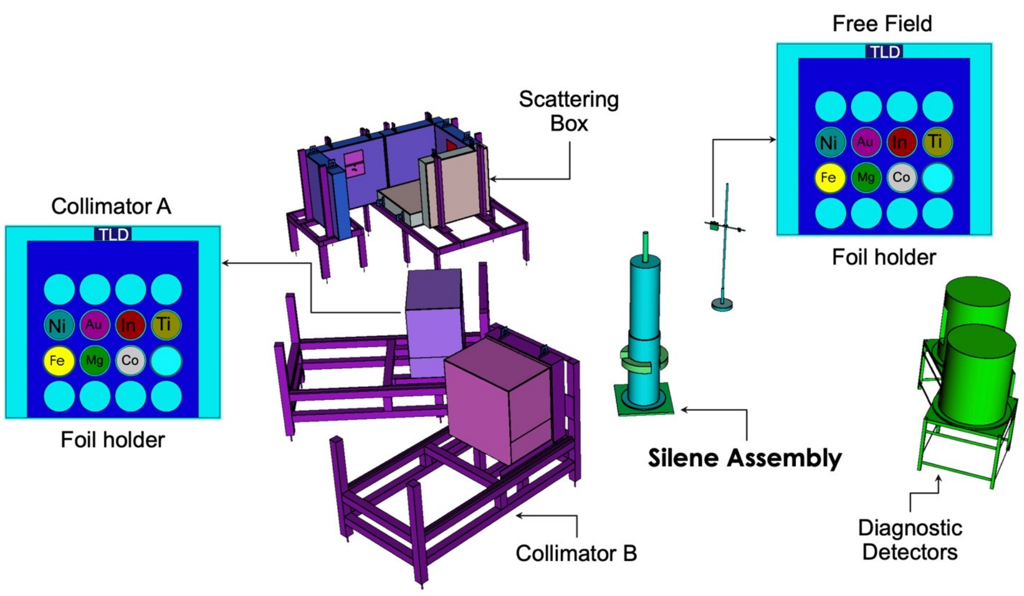




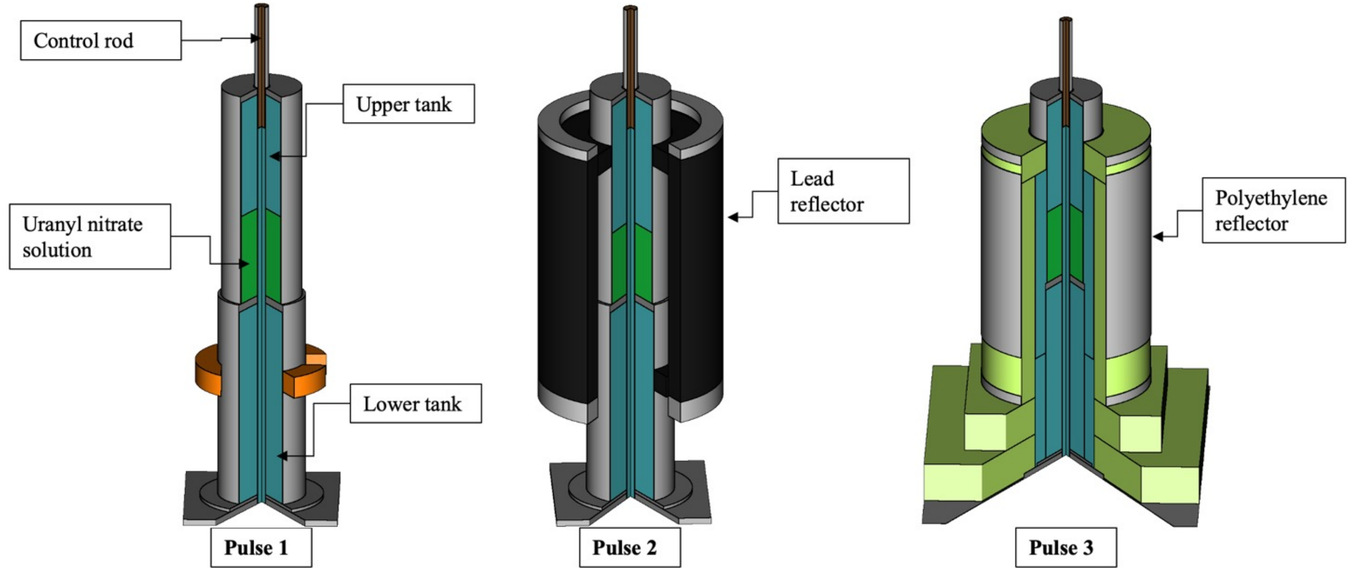
SCALE 6.3.0 Validation: Radiation Shielding Benchmarks

Benchmark No.	Benchmark	Origin	Radiation of interest	Source	Material interaction of interest	Quantity of interest
1	Neutron transmission through an iron sphere	Annals of Nuclear Energy (1993)	Neutron	^{252}Cf	Fe	Neutron flux spectrum
2	Neutrons through a heavy water sphere	Annals of Nuclear Energy (1997)	Neutron	^{252}Cf	Heavy water	Neutron flux spectrum
3	Concrete Labyrinth	ICSBEP (2007)	Neutron	^{252}Cf	Concrete (borated), PE, Cd	Count rate in Bonner sphere
4	Americium–beryllium Neutrons Leakage Through Several Materials	Nuclear Science and Engineering (1971)	Neutron	Am-Be	PE, Be, Pb, Nb, Mo, Ta, W	Neutron flux spectrum
5	Deuterium–tritium neutrons through an Iron Sphere	SINBAD (2006)	Neutron	D-T	Fe	Neutron flux spectrum
6	Ueki shielding measurements	Nuclear Science and Engineering (1996)	Neutron	^{252}Cf	Paraffin, steel, PE	Neutron dose rate
7	Skyshine benchmark	SINBAD (2012)	Gamma	^{60}Co	Air, soil	Gamma dose rate skyshine
8	SILENE critical assembly benchmark	ICSBEP (2016)	Neutron	Uranyl nitrate solution	Foils (Co, Au, In, Fe, Mn, Mg, Ni)	Neutron activation
9	NIST sphere experiments for fission rates	ICSBEP (2006)	Neutron	^{252}Cf	Stainless steel and stainless steel/water	^{235}U, ^{239}Pu, ^{238}U, ^{237}Np fission rates
10	NIST sphere experiments for cadmium covered fission chambers	ICSBEP (2007)	Neutron	^{252}Cf	Stainless steel and stainless steel/water	^{235}U, ^{239}Pu, ^{238}U, ^{237}Np fission rates
11	H. B. Robinson Unit 2 pressure vessel benchmark	SINBAD (1997)	Neutron	^{235}U and ^{239}Pu fission spectra	Pressure vessel/ reactor dosimetry	Reaction rate / specific activity

SILENE Critical Assembly Benchmark



SCALE model of SILENE Pulse 1



SILENE assembly models: bare (left), lead reflector (center), and polyethylene reflector (right) were used for Pulses 1, 2, and 3, respectively

The SILENE critical assembly is a uranyl nitrate solution with 93.5 wt % enriched ^{235}U

SILENE Critical Assembly Benchmark: Pulse 2 Results

Comparison of activities for the **lead-shielded** SILENE assembly using **ENDF/B-VII.1 CE** libraries and IRDFF responses

Position/Reaction		Measured		Calculated		C/E	
		Activity (Bq/g)	Relative experimental uncertainty[a] (%)	Activity[b] (Bq/g)	Relative simulation uncertainty[c] (%)	ENDF/B-VII.1	ENDF/B-VIII.0
CA	^{59}Co (n,g) ^{60}Co	6.09E+01	7.06	7.33E+01	0.54	1.20	1.20
	^{197}Au (n,g) ^{198}Au	6.88E+04	6.81	8.40E+04	1.26	1.22	1.22
	^{115}In (n,g) ^{116m}In	7.95E+06	7.44	9.35E+06	1.31	1.18	1.17
	^{115}In (n,n'g) ^{115m}In	6.10E+03	6.33	5.94E+03	0.52	0.97	0.92
	^{56}Fe (n,p) ^{56}Mn + ^{55}Mn (n,g) ^{56}Mn	2.02E+03	6.89	2.37E+03	0.72	1.17	1.16
	^{24}Mg (n,p) ^{24}Na	2.48E+01	6.47	2.97E+01	3.69	1.20	1.15
	^{58}Ni (n,p) ^{58}Co	6.86E+00	6.35	7.75E+00	0.77	1.13	1.09
FF	^{59}Co (n,g) ^{60}Co	6.27E+01	7.02	7.21E+01	0.96	1.15	1.09
	^{197}Au (n,g) ^{198}Au	6.43E+04	6.59	6.99E+04	2.30	1.09	1.05
	^{115}In (n,g) ^{116m}In	7.85E+06	7.11	8.27E+06	2.98	1.05	1.01
	^{115}In (n,n'g) ^{115m}In	5.21E+03	6.31	5.05E+03	0.84	0.97	0.94
	^{56}Fe (n,p) ^{56}Mn + ^{55}Mn (n,g) ^{56}Mn	2.08E+03	6.44	2.43E+03	0.97	1.16	1.11
	^{24}Mg (n,p) ^{24}Na	2.64E+01	7.08	3.10E+01	6.40	1.18	1.05
	^{58}Ni (n,p) ^{58}Co	6.34E+00	6.34	7.04E+00	1.24	1.11	1.10

[a] Largest contributor is the uncertainty in the number of fission events.
[b] Average value of 16 runs with different random seeds.
[c] Calculated relative error is the one-sigma statistical uncertainty for the Monte Carlo simulation and does not include uncertainties related to benchmark specifications.

Questions?

SCALE 6.3 Criticality Safety Validation

Oak Ridge National Laboratory
February 1, 2024

Travis Greene, B. J. Marshall, Alex Shaw

Process for criticality safety validation

1. **Generate models of critical benchmark experiments**
   – High-quality, well qualified experiments used as benchmarks
   – Currently all benchmarks drawn from the International Criticality Safety Benchmark Evaluation Project Handbook (ICSBEP)
   – Confirm model is correct and accurate via Verified, Archived Library of Input and Data (**VALID**) process

2. **Compare calculated k_{eff} results to expected k_{eff} results from benchmarks**
   – Expected result may not be a k_{eff} of 1.0 based on modeling simplifications, experimental conditions, approach parameter, etc.

3. **Analyze results for different categories and groups** of categories, potentially for multiple data libraries

Brief introduction to VALID

(Verified, Archived Library of Input and Data)

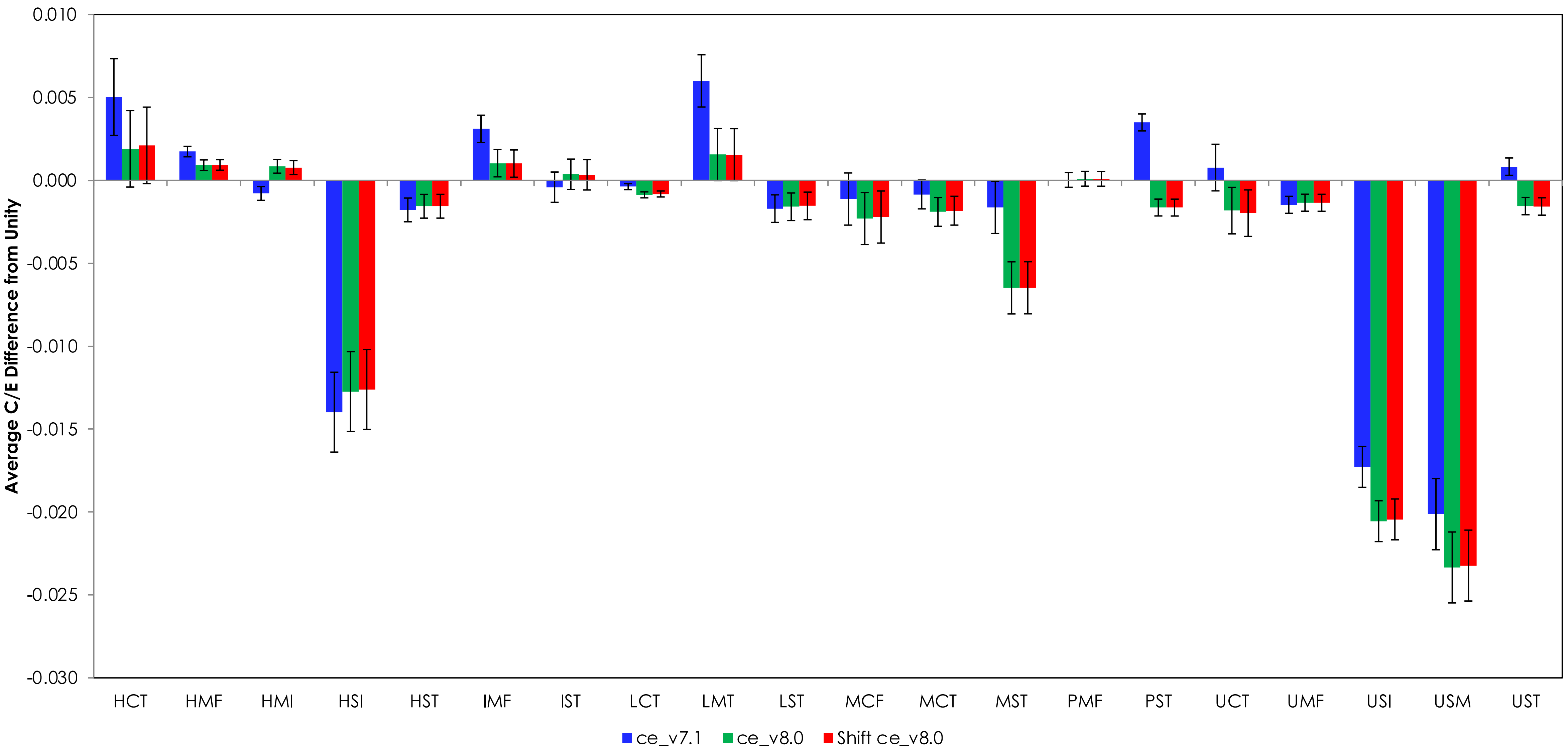
- Quality assurance-like process to generate high quality models from reliable reference descriptions
  - Separate origination and review by qualified individuals
  - Documentation of model generation, results, and checks
  - Results are controlled to prevent inadvertent modification
- Primarily includes ICSBEP Handbook evaluations
- Most models include both eigenvalue and sensitivity results
- Basis for SCALE/KENO validation reports, papers, and studies since SCALE 6 in 2010

Summary of benchmarks in SCALE 6.3.1 validation report

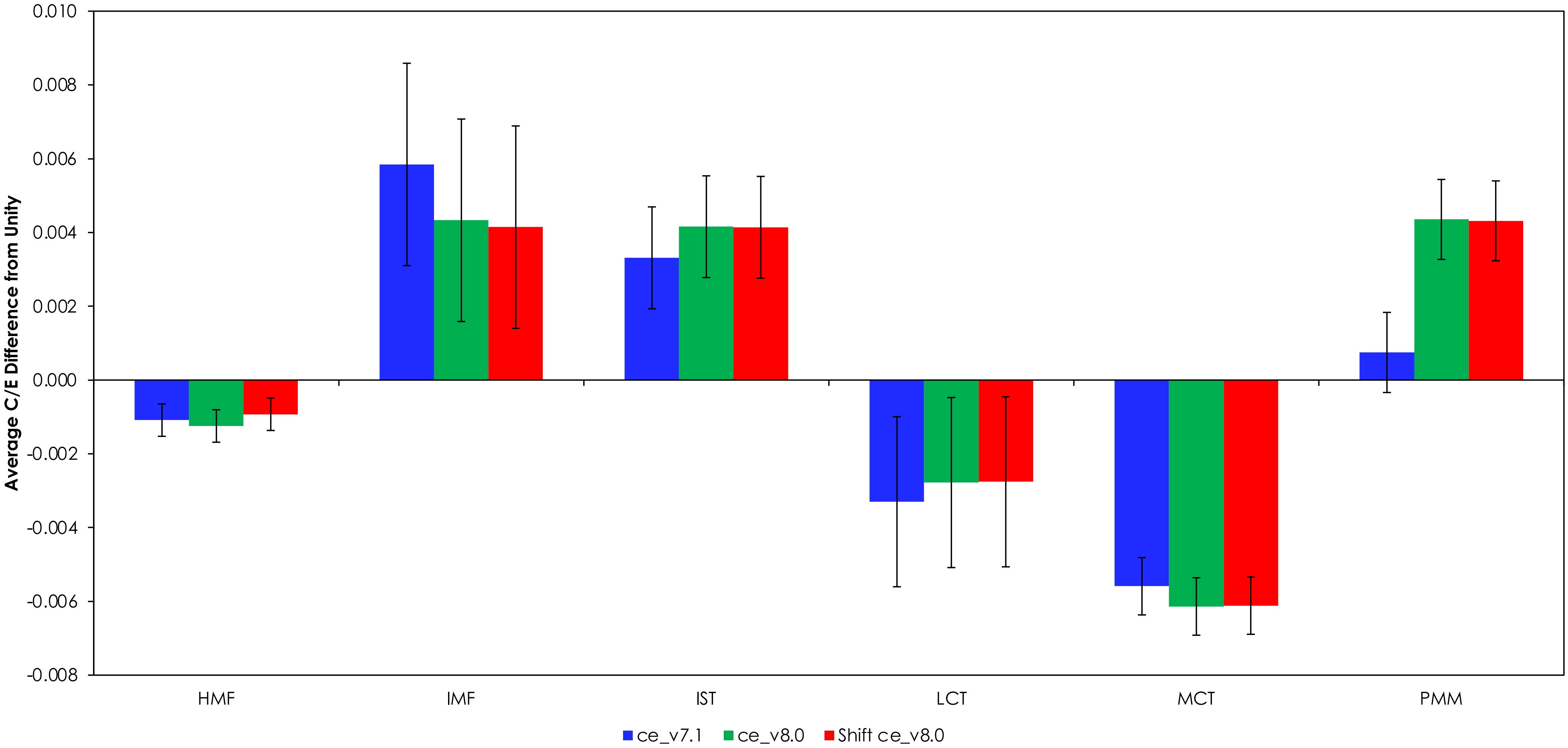
Sequence	Benchmark class	ICSBEP case numbers	Number of configurations
CSAS5/KENO V.a	HEU-COMP-THERM	17	9
	HEU-MET-FAST	1, 15, 16, 17, 18, 19, 20, 21, 25, 30, 38, 40, 52, 63, 65, 72, 73, 84, 85	60/64[a]
	HEU-MET-INTER	6	4
	HEU-SOL-INTER	1	2
	HEU-SOL-THERM	1, 4, 13, 14, 16, 20, 28, 29, 30	61
	IEU-MET-FAST	2, 3, 4, 5, 6, 7, 8, 9	8/11[a]
	IEU-SOL-THERM	3	46
	LEU-COMP-THERM	1, 2, 8, 10, 17, 42, 50, 78, 80	140
	LEU-MET-THERM	1, 2, 15	35
	LEU-SOL-THERM	2, 3, 4	19
	MIX-COMP-FAST	5, 6	2
	MIX-COMP-THERM	1, 2, 4	21
	MIX-SOL-THERM	2, 7	10
	PU-MET-FAST	1, 2, 5, 6, 8, 9, 10, 11, 18, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 35, 36, 39, 40, 41	25
	PU-SOL-THERM	1, 2, 3, 4, 5, 6, 7, 11, 16, 20	92
	U233-COMP-THERM	1	3[c]
	U233-MET-FAST	1, 2, 3, 4, 5, 6	10
	U233-SOL-INTER	1	29
	U233-SOL-MIXED	1, 2	8
	U233-SOL-THERM	1, 2, 3, 4, 5, 8, 9, 11, 12, 13, 15, 16, 17	140
CSAS6/KENO-VI	HEU-MET-FAST	5, 8, 9, 10, 11, 13, 24, 80, 86, 92, 93, 94	27
	IEU-MET-FAST	19	2
	IEU-SOL-THERM	2	13
	LEU-COMP-THERM	25	4
	MIX-COMP-THERM	8	28
	PU-MET-MIXED	2	5

[a]The larger number includes simplified cases that are duplicate cases for which detailed models are also available in the library.

KENO V.a results



KENO-VI results



Questions?

SCALE Validation for Nuclide Inventory and Decay Heat

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February 1, 2024

Germina Ilas

Experimental Radiochemical Assay (RCA) Data for SCALE 6.2.4 Validation

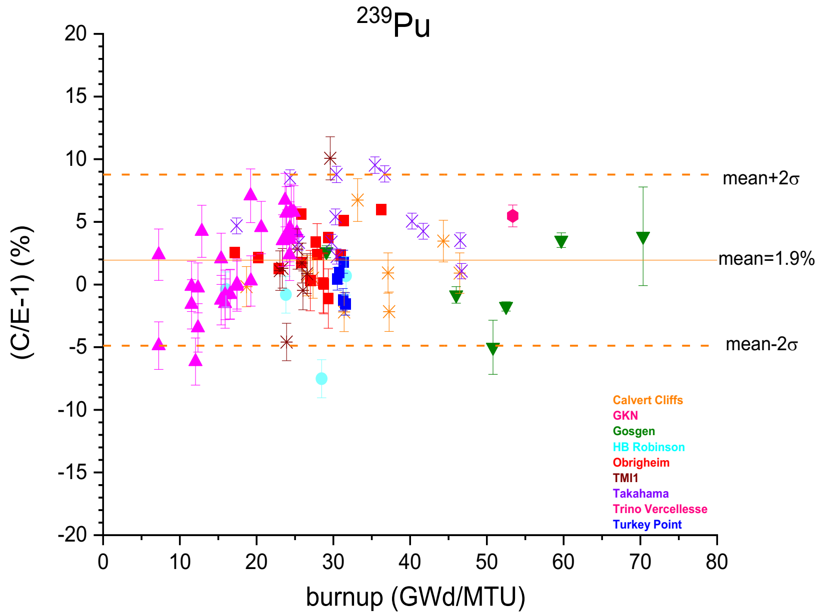
92 samples of fuel irradiated in Pressurized Water Reactors (PWRs)

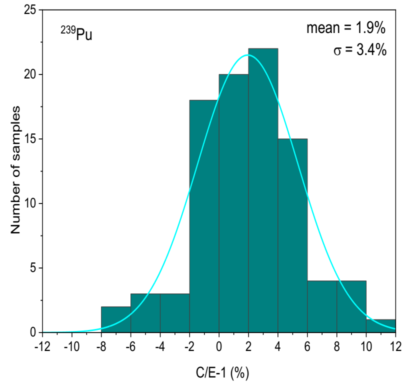
Reactor	Measurement Laboratory	Experimental Program	Assembly Design	Enrichment (wt % ^{235}U)	No. of Samples / Fuel Rods	Burnup (GWd/MTU)
Trino Vercellese	Ispra, Karlsruhe	JRC	15 × 15	2.72, 3.13, 3.897	15/5	7.2–17.5
	Ispra, Karlsruhe	JRC	15 × 15	3.13	16/5	12.8–25.2
Obrigheim	Ispra, Karlsruhe	JRC	14 × 14	2.83, 3.00	10/1	15.6–38.1
	ITU, IRCh, WAK, IAEA	ICE	14 × 14	3.13	5/5	27.0–29.2
H. B. Robinson-2	PNNL	ATM-101	15 × 15	2.561	4/1	16.0–31.7
Turkey Point-3	Battelle-Columbus	NWTS	15 × 15	2.556	5/1	30.5–31.6
Calvert Cliffs-1	PNNL, KRI	ATM-104	14 × 14	3.038	3/1	27.4–44.3
	PNNL	ATM-103	14 × 14	2.72	3/1	18.7–33.2
	PNNL, KRI	ATM-106	14 × 14	2.453	3/1	31.4–46.5
Takahama-3	JAERI	JAERI	17 × 17	2.63, 4.11	13/3	14.3–47.3
TMI-1	GE-VNC	DOE YMP	15 × 15	4.657	8/3	22.8–29.9
Gösgen	SCK•CEN, ITU	ARIANE	15 × 15	3.5, 4.1	3/2	29.1–59.7
	SCK•CEN, PSI, CEA	MALIBU	15 × 15	4.3	3/1	47.2–70.4
GKN II	SCK•CEN	REBUS	18 × 18	3.8	1/1	54.0

Source of data: Spent Fuel Composition Database SFCOMPO (OECD/NEA web database)
https://www.oecd-nea.org/sfcompo/

Results: Nuclide Inventory in PWR Fuel
comparison calculation-experiment for actinides

SCALE 6.2.4/ENDF/B-VII.1			
Nuclide	No. samples	C/E average	C/E stdev
^{234}U	55	1.127	0.173
^{235}U	**92**	**1.013**	**0.036**
^{236}U	77	0.981	0.034
^{238}U	92	0.999	0.004
^{238}Pu	77	0.959	0.074
^{239}Pu	**92**	**1.019**	**0.034**
^{240}Pu	92	1.005	0.035
^{241}Pu	92	0.978	0.047
^{242}Pu	91	0.959	0.064
^{237}Np	36	1.024	0.199
^{241}Am	39	1.043	0.192
^{243}Am	38	0.933	0.125
^{244}Cm	57	0.987	0.113
^{245}Cm	24	0.987	0.150
^{246}Cm	14	0.930	0.224





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Results: Nuclide Inventory in PWR fuel

comparison calculation-experiment for fission products

SCALE 6.2.4/ENDF/B-VII.1			
Nuclide	No. samples	C/E average	C/E stdev
^{90}Sr	15	0.991	0.066
^{99}Tc	**20**	**1.164**	**0.158**
^{101}Ru	**7**	**1.056**	**0.113**
^{106}Ru	**31**	**1.059**	**0.218**
^{103}Rh	**8**	**1.115**	**0.106**
^{109}Ag	**6**	**1.764**	**0.683**
^{125}Sb	**18**	**1.988**	**0.450**
^{133}Cs	10	1.023	0.017
^{134}Cs	**59**	**0.898**	**0.070**
^{135}Cs	16	1.021	0.036
^{137}Cs	73	0.989	0.032
^{143}Nd	36	1.008	0.021
^{145}Nd	36	1.002	0.011

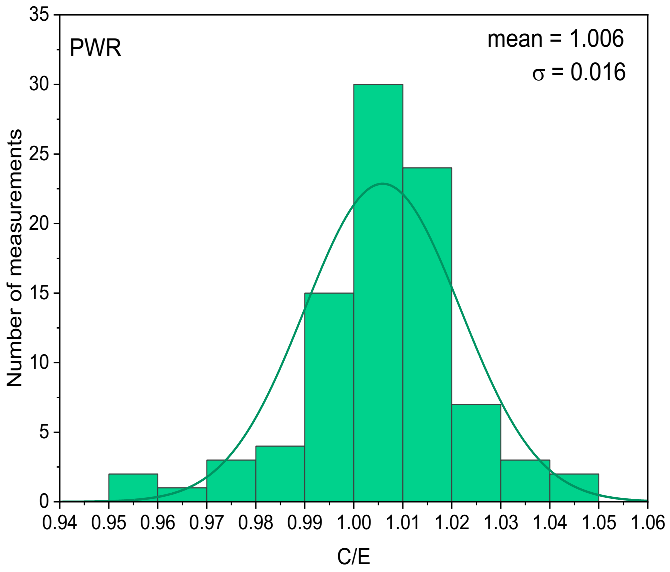
SCALE 6.2.4/ENDF/B-VII.1			
Nuclide	No. samples	C/E average	C/E stdev
^{144}Ce	**32**	**0.968**	**0.075**
^{147}Sm	24	1.016	0.034
^{149}Sm	20	1.019	**0.062**
^{150}Sm	24	1.008	0.032
^{151}Sm	24	0.979	0.044
^{152}Sm	24	1.016	0.037
^{151}Eu	**12**	**0.893**	**0.198**
^{153}Eu	19	0.991	0.031
^{154}Eu	**44**	**1.042**	**0.104**
^{155}Eu	**11**	**0.956**	**0.077**
^{155}Gd	**19**	**0.916**	**0.144**

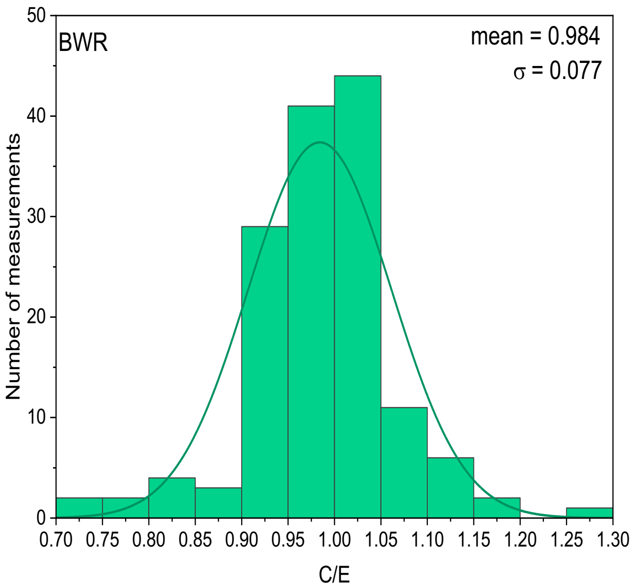
Experimental Decay Heat Data Used for Validation

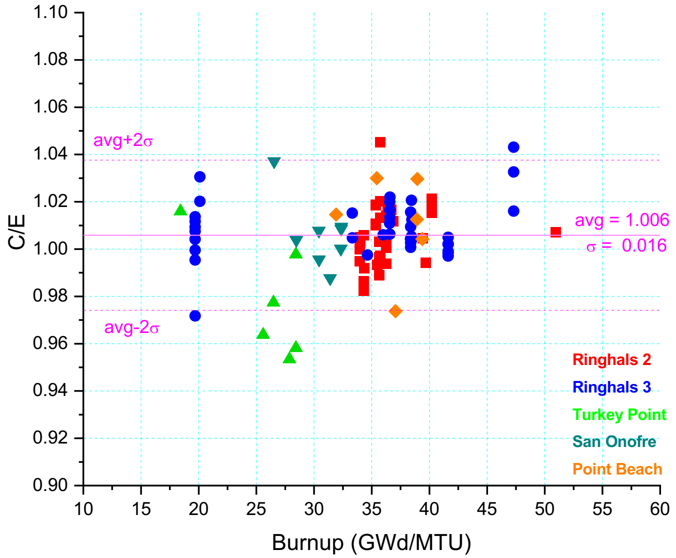
236 full assembly measurements for PWRs and BWRs

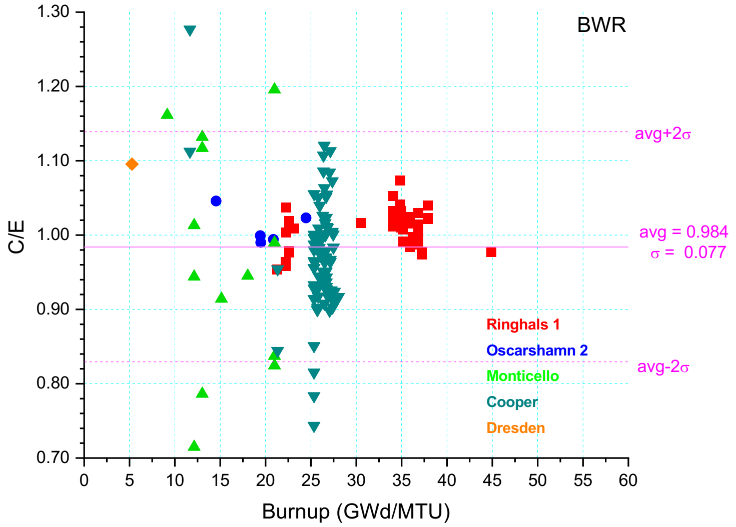
Reactor type	Reactor name	Assembly lattice	Burnup (GWd/MTU)	Cooling time (years)	Enrichment (wt % ^{235}U)	Measurement laboratory	No. of measured assemblies/ measurements	Exp. relative uncertainty (%)
PWR	Point Beach 2	14×14	31.9–39.4	4.5	3.4	GE-Morris	6/6	4.7
	San Onofre 1	15×15	26.5–32.4	3.0–8.2	3.9 – 4.0	GE-Morris	8/8	4.7
	Turkey Point 3	14×14	18.4–28.4	2.4–5.7	2.6	GE-Morris	4/6	5.0 – 10.0
	Ringhals 2	15×15	34.0–51.0	15.9–26.7	3.1 – 3.3	Clab	18/33	2.3 – 3.0
	Ringhals 3	17×17	19.7–47.3	12.9–25.9	2.1 – 3.4	Clab	16/38	2.2 – 4.1
BWR	Cooper	7×7	11.7–28.0	2.3–7.2	1.1 – 2.5	GE-Morris	54/81	4.7
	Dresden 2	7×7	5.3	8.1	2.1	GE-Morris	1/1	4.7
	Monticello	7×7	9.2–21.0	9.7–11.2	2.3	GE-Morris	6/13	4.7
	Oskarshamn 2	8×8	14.5–24.5	20.3–26.7	2.2	Clab	5/5	4.2 – 7.5
	Ringhals 1	8×8	21.3–44.7	12.6–23.6	2.3 – 2.9	Clab	17/45	2.5 – 5.1
Total			5.3–51.0	2.4 – 26.7	1.1 – 4.0		135/236	

Results: Decay Heat in PWR and BWR Fuel Assemblies









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G. Ilas, I. C. Gauld, and G. Radulescu, *Validation of new depletion capabilities and ENDF/B-VII data libraries in SCALE*, Annals of Nuclear Energy, vol. 46, p.43-55 (2012). https://doi.org/10.1016/j.anucene.2012.03.012

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Publicly-available documents can be accessed via OSTI. See https://www.ornl.gov/scale/references Depletion and Decay

Additional information

https://www.ornl.gov/scale/references

SCALE/ORIGEN Sensitivity Demo

Oak Ridge National Laboratory
February 1, 2024

Will Wieselquist

New SCALE/ORIGEN sensitivity calculation in SCALE 6.3 (2023)

- Based on linear perturbation theory for the change in a response due to a parameter α

$$R(\alpha) = R(\alpha_0) + \left.\frac{\partial R}{\partial \alpha}\right|_{\alpha_0} (\alpha - \alpha_0) + \cdots,$$

- Relative change of that response to input is given as *S*

$$S \equiv \left.\frac{\partial R}{\partial \alpha}\right|_{\alpha_0} \cdot \frac{\alpha_0}{R(\alpha_0)}$$

- Sensitivity coefficient can be calculated with inner product of the forward solution *N(t)* with adjoint *N*(t)*

$$S = \frac{\alpha_0}{R(\alpha_0)} \int_0^T dt N^*(t) \cdot \frac{\partial A}{\partial \alpha} \cdot N(t) \Rightarrow S = \frac{\alpha_0}{R(\alpha_0)} \left(\left.\frac{\partial R}{\partial \alpha}\right|_{\alpha_0} + \int_0^T dt N^*(t) \cdot \frac{\partial A}{\partial \alpha} \cdot N(t) \right)$$

SCALE 6.3 Nuclide Response

SCALE 7.0 General Response (e.g. decay heat)

Sensitivity of fission product Rh102m to nuclear data in commercial power reactor neutron energy spectrum

- This simple model calculates the sensitivity of Rh102m to all nuclear data
- Rh102m has a half-life of ~1300 days
- Interesting because total neutron induced destruction rate (in this system) is similar to decay rate

```
=origen

% Forward case with 1 gram of U235 irradiated at
% constant flux for 1000 days.
case(1){
  lib{ file="${DATA}/arplibs/w17_e50.f33" pos=10 }
  mat{ load{ file="${INPDIR}/origami1.f71" pos=1 } }
  time=[ 20I 52 1040 ]
  power=[ 22R 40 ]
}


% Perturbation theory sensitivity calc for Rh102m.
sens{
  case=1
  response{
    iso=[rh102m=1.0] type=NUCLIDE step=LAST
  }
  threshold=1e-2
  dp_verify{ nrank=3 nrank_pert=1.001 }
}

end
```

SCALE/ORIGEN input file

Sensitivity of fission product **Rh102m** to nuclear data in commercial power reactor neutron energy spectrum

- Output tabulates all reaction and decay channels that have sensitivity above user-defined threshold, here 0.8%

- This data could be used to create a “low-order model” for how changes in nuclear data would affect the prediction of a specific nuclide in this reactor type

- Interpretation examples
  1. Increasing Rh103 (n,2n) reaction by 1% leads directly to ~1% more Rh102m
  2. Increasing U238 (n,gamma) by 1% leads to more minor actinides which leads to 0.4% more fission product Rh102m
  3. Reaction product pathways can be tricky: the model is **constrained** such that increasing yield of daughter Rh102m from (n,2n) decreases yield of Rh102—the value of 0.63% is due to the nonequal probabilities of ground or metastable daughter

```
Reaction Channels
-------------------------------------------------------
| Nuclide ID |      Reaction      | Adjoint Sens. Coeff. |
-------------------------------------------------------
|      45103 |               n,2n |          1.00095e+00 | Example 1
|      92238 |            n,gamma |          3.95961e-01 | Example 2
|      92235 |            fission |          3.57099e-01 |
|      45103 |            n,gamma |         -2.66811e-01 |
|    1045102 |            n,gamma |         -2.22104e-01 |
|      94239 |            fission |          2.12464e-01 |
-------------------------------------------------------

Reaction Products
--------------------------------------------------------------------
|   Parent   |      Reaction      |  Daughter  | Adjoint Sens. Coeff. |
--------------------------------------------------------------------
|      45103 |               n,2n |    1045102 |          6.31710e-01 | E
|      45103 |               n,2n |      45102 |         -6.31710e-01 | x
|      92235 |            fission |      41103 |          2.28124e-01 | a
|      94239 |            fission |      42103 |          1.87227e-01 | m
|      92235 |            fission |      42103 |          1.68355e-01 | p
|      94239 |            fission |      41103 |          1.32866e-01 | l
--------------------------------------------------------------------   e
                                                                       3
Decay Channels
-------------------------------------------------------
| Nuclide ID |     Decay Mode     | Adjoint Sens. Coeff. |
-------------------------------------------------------
|    1045102 |              beta+ |         -1.31826e-01 |
|      44103 |              beta- |          8.55690e-02 |
-------------------------------------------------------
```

SCALE/ORIGEN output excerpt

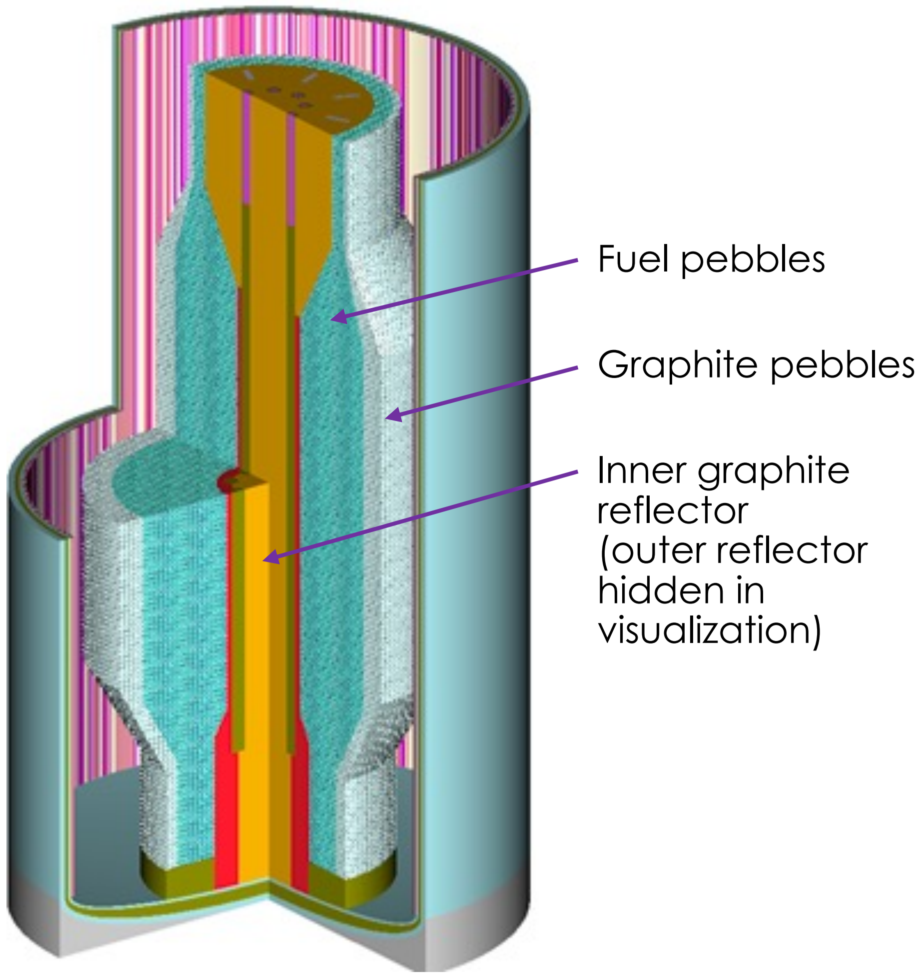
TRITON Reactor Physics Calculations

Oak Ridge National Laboratory
February 1, 2024

Rike Bostelmann

TRITON Overview

- SCALE's flexible reactor physics sequence for 1D, 2D, and 3D depletion calculations of detailed models
- Major input:
  - Material compositions
  - Detailed geometry
  - Neutron transport settings
  - Depletion settings (power, time, etc.)
- Key output as a function of fuel burnup:
  - Fuel inventory (detailed composition)
  - Collapsed 1-group cross sections (F33 files)
  - Mixture-specific neutron flux and power
  - Multiplication factor



SCALE model of a pebble-bed fluoride salt cooled high temperature reactor (FHR)

SCALE Reactor Physics Calculations
The Physics

3 fundamental parts:

	Inputs	Process	Outputs
Cross section processing in case of multigroup calculations	• Cross Section Library • Material Concentrations • Geometry • Temperature	Cross Section Processing	MG Cross sections
Multigroup (MG) or continuous-energy (CE) neutron transport	• MG or CE Cross sections • Material Concentrations • Geometry	MG or CE Transport	• k-effective • Flux-dependent QOIs
Depletion	• Material Concentrations • Material Transition Matrices • Power level • Time step	Depletion/ Decay	New Material Concentrations

Automatic execution of these parts through SCALE's control sequence **TRITON**

Introduction to SAMPLER

Oak Ridge National Laboratory
February 1, 2024

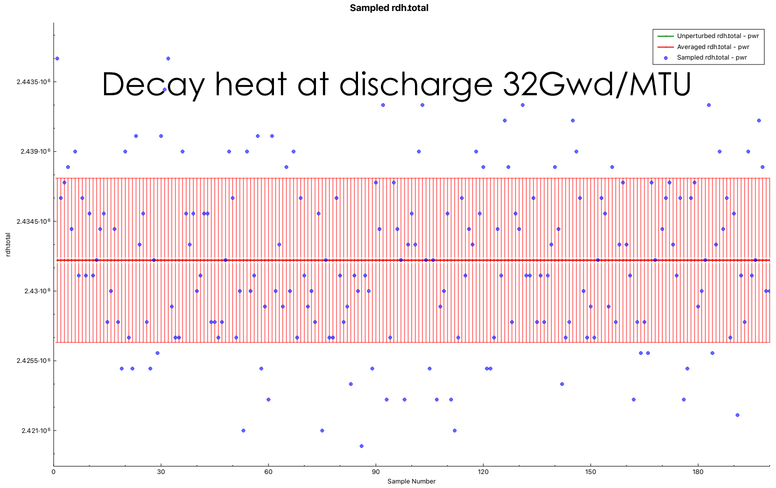
Ugur Mertyurek

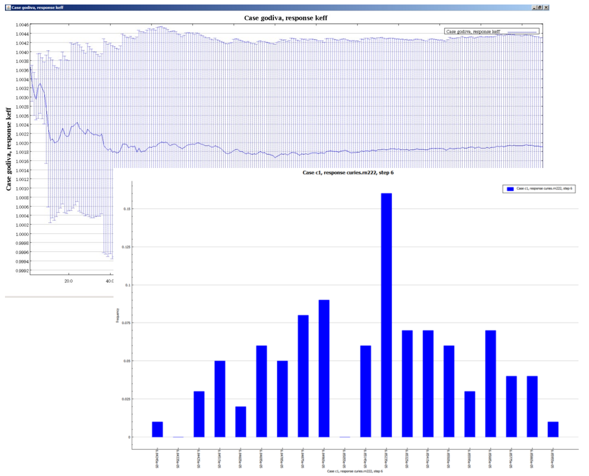
W. A. Wieselquist, F. Bostelmann, M. L. Williams, F. Havlůj, R. A. Lefebvre, W. Zwermann, D. Wiarda, M. T. Pigni, I. C. Gauld, M. A. Jessee, J. P. Lefebvre, K. J. Dugan, and B. T. Rearden

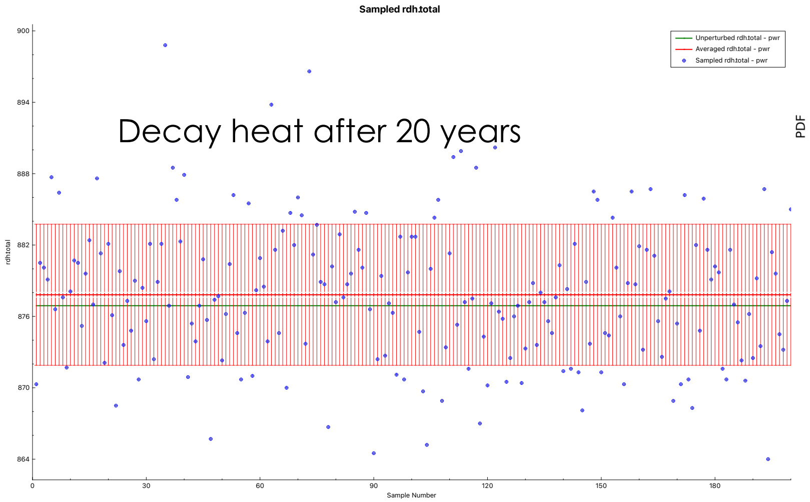
Sampler: A Module for Statistical Uncertainty Analysis with SCALE Sequences

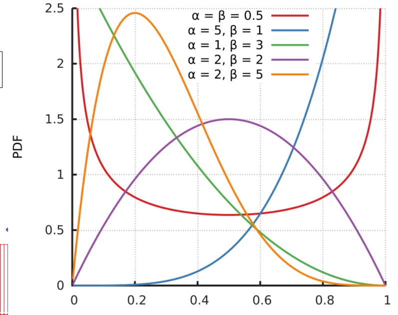
Calculates uncertainty in *any* result of a SCALE computation due to two basic types of uncertainty

- **nuclear data uncertainty**
  - cross sections
  - fission yield
  - decay
  - recoverable energy
  - kinetics
- **input model uncertainty**
  - geometry
  - composition
  - and anything else that appears in an input file









Sampler Input

```
=sampler
  read parameters
     ...
  end parameters

  read case [myCase]
     sequence=polaris/origen/opus
       ...
     end sequence
  end case

  read variable [myVariable]
      ...
  end variable

  read response [myResponse]
    ...
   end response
end
```

Sampler run time parameters: what to perturb, how many samples, libraries etc.

Case : A set of SCALE sequences (any) for your analysis

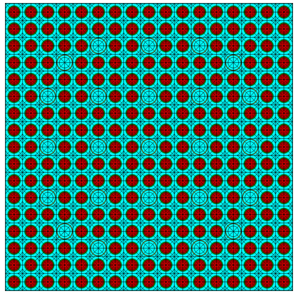
Variable : A variable in your SCALE simulation, that is allowed to be modified by Sampler

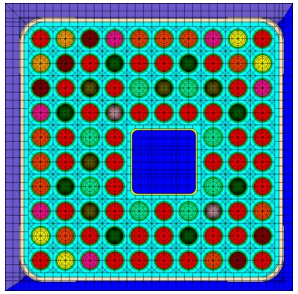
Response : Quantity of interest Sampler is requested to post process

Question:

- **Do PWR and BWR assemblies show similar trends in decay heat with respect to ND ? (are their sensitivities to nuclear data similar ?)**

```
=sampler
read parameters
n_samples=200
perturb_xs=yes
perturb_geometry=no
library="v7-56"
run_cases=no
end parameters

read case [pwr]
sequence=polaris
mat FUEL.1 : c_uox3 10.4
comp c_uox3 : UOX 5.0
pin 1 :  0.4555 0.465  0.5375
      :  FUEL.1 GAP.1 CLAD.1

read case [bwr]
sequence=polaris
mat FUEL.1 : c_uox3 10.4
comp c_uox3 : UOX 5.0
pin 1 :  0.527 0.542  0.615
      :  FUEL.1 GAP.1 CLAD.1

read response [rdh]
type=opus_plt
ndataset=0
nuclides=total end
end response

read analysis[dh_ck]
  type = pearson_corr
  targets = pwr:orig.pu239(8) pwr:orig.cm244(8) pwr:orig.cs134(8) end
  sources = pwr:rdh.total(8) pwr:rdh.total(last) end
end analysis
```





Similarity Index	BWR:discharge	BWR:5yr	BWR:10yr	BWR:20yr
PWR:discharge	0.997	-0.187	-0.261	-0.266
PWR:5yr	-0.144	0.999	0.731	0.459
PWR:10yr	-0.222	0.755	0.997	0.926
PWR:20yr	-0.235	0.479	0.93	0.999

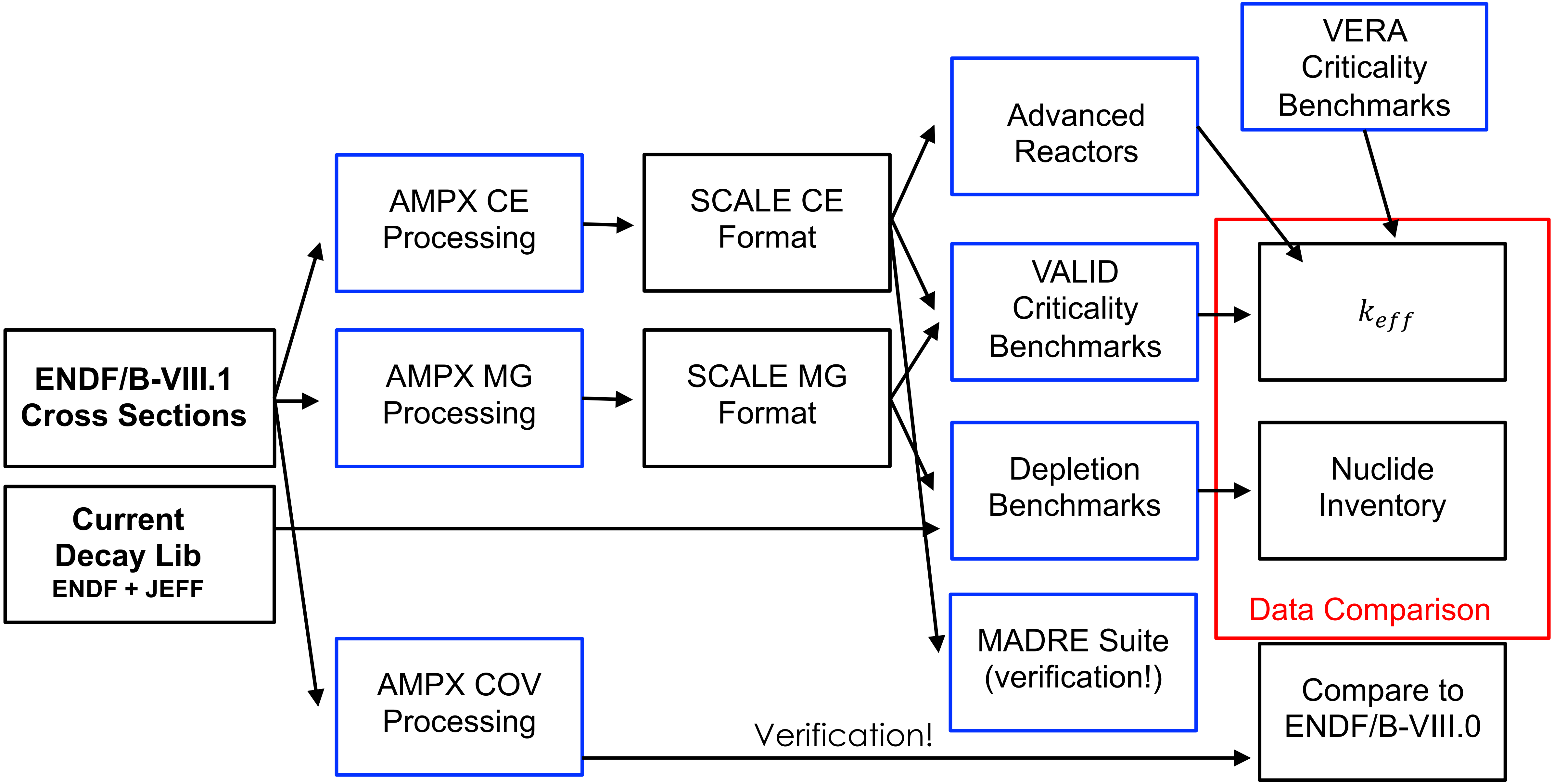
Oak Ridge National Laboratory

Path to Automated Validation of ENDF/B-VIII.1

Oak Ridge National Laboratory
February 1, 2024

Jesse Brown, Kang Seog Kim, Rike Bostelmann, Germina Ilas

ENDF-8.1 Validation Methods Supporting NRC



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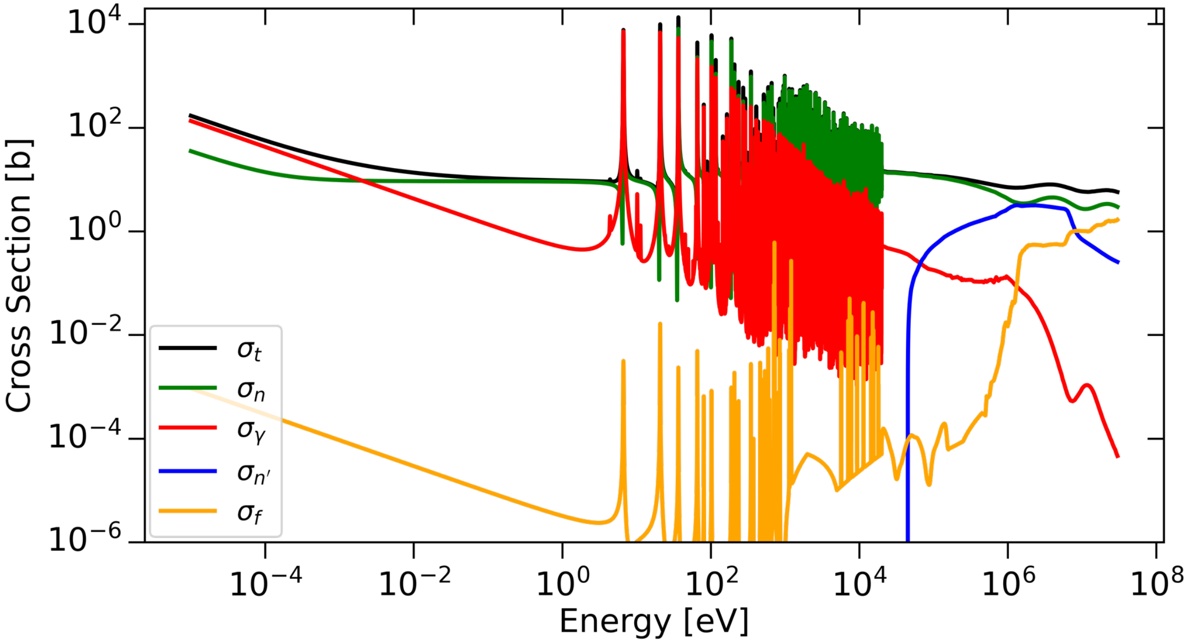
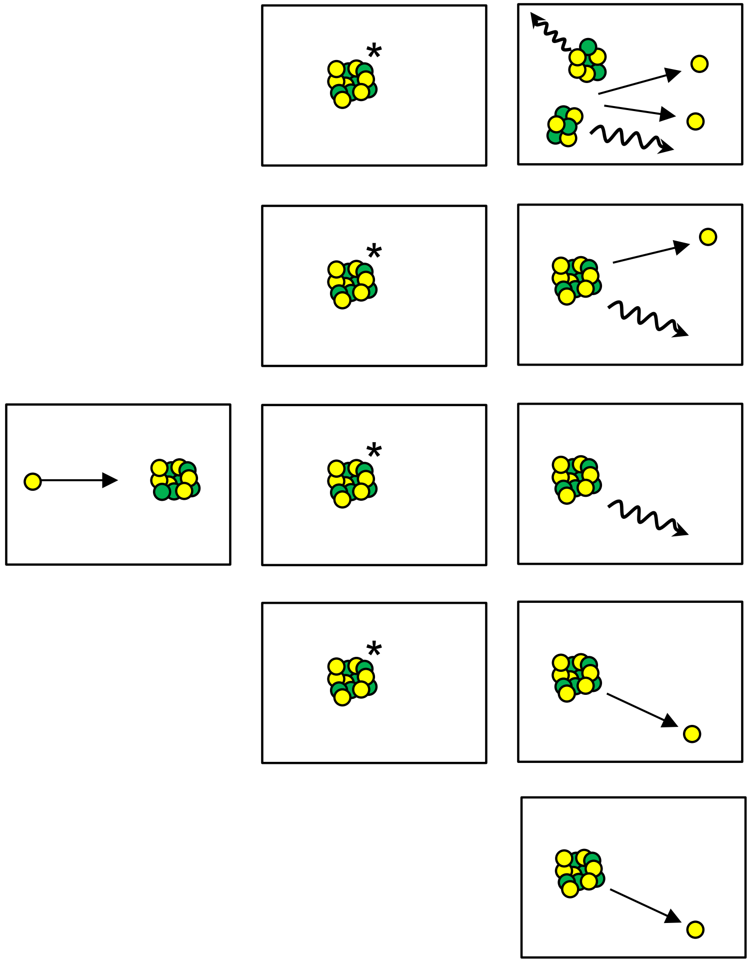
National Laboratory

Nuclear Reactions

^{238}U





$${}^{A}_{Z}N(n,f)$$

$${}^{A}_{Z}N(n,n')\,{}^{A}_{Z}N$$

$${}^{A}_{Z}N(n,\gamma)\,{}^{A+1}_{Z}N$$

$${}^{A}_{Z}N(n,n)\,{}^{A}_{Z}N$$

$${}^{A}_{Z}N(n,n)\,{}^{A}_{Z}N$$

etc.

*compound

Validation & Verification

Use many different application spaces

- Criticality benchmarks (VALID criticality benchmarks)
- Reactor Criticality (BWR, PWR, Advanced Reactors)
- Depletion Radiochemical Assay (RCA) Data
- Depleted Fuel Reactivity (VERA Suite)

ORIGEN Nuclear Data

- **Decay data (ENDF/B-VII.1)**
  - ~2600 decay transitions allowed with T ½ (> 1 ms)
  - Decay branching fractions β^-, β^+, EC, α, IT, $\beta^-\beta^-$, β^-n, SF, n, β^-α
  - Transitions to ground and excited states
  - Recoverable energy from decay (α, β, γ)
- **Neutron reaction cross section data (JEFF-3.1/A)**
  - ~800 nuclides (ENDF/B has ~400)
  - ~13000 neutron-induced reactions
  - Expanded reaction types supported (ENDF/B in red)

    (n,2n), (n,3n), (n,f), (n,nα), (n,n3α), (n,2nα), (n,3n α), (n,np), (n,n2α), (n,2n2α), (n,nd), (n,nt), (n,n ^{3}He), (n,nd2α), (n,nt2α), (n,4n), (n,g), (n,p), (n,d), (n,t), (n,^{3}He), (n,α), (n,2α), (n,3α), (n,2p), (n,pα), (n,t2α), (n,d2α), (n,n')
  - Isomeric transitions, e.g. Am-241 -> Am-242m

- **Fission product yields (ENDF/B-VII.0)**
  - 30 actinides: ^{227,228,232}Th, ^{231}Pa, $^{232-238}$U, $^{238-242}$Pu, ^{241,242m,243}Am, ^{237,238}Np, $^{242-246,248}$Cm, ^{249,252}Cf, and ^{254}Es
  - Data are from England and Rider compilations
  - Energy-dependent yields tabulated at
    - Thermal fission: 0.0253 eV
    - Fast fission: 500 keV
    - High energy fission: 14 MeV
  - Actual yields are interpolated using the mean energy of neutrons causing fission

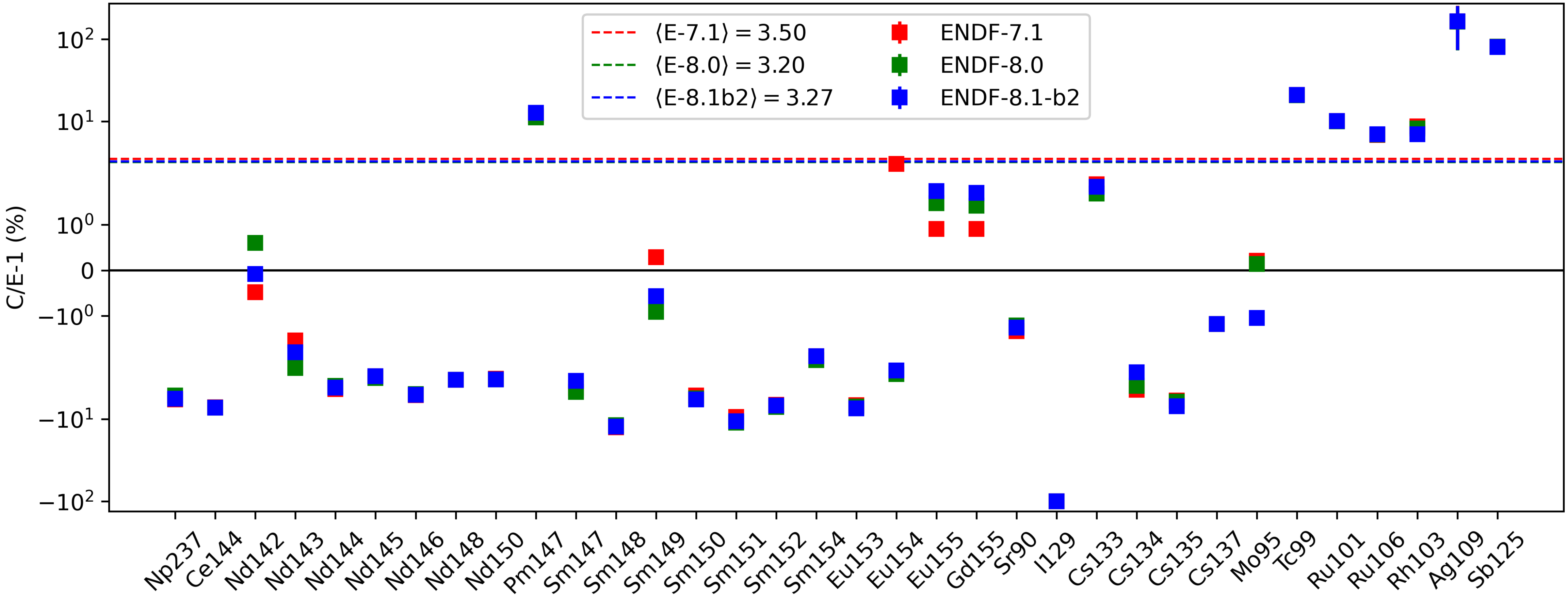
SCALE/ORIGEN team evaluates new nuclear data and corrects/reports errors for downstream users
Example from ENDF/B-VII.0

Issue: *^{234}Th beta decay daughter incorrectly assigned as ^{234}Pa instead of isomer ^{234m}Pa*

Impact: *order of magnitude difference in gamma spectra for ^{238}U decay*

Validation: TRITON example

Goesgen PWR, GGU1 sample, UO_2 fuel, ~70 GWd/ Actinides



Impact of Nuclear Data on Advanced Energy Systems Safety and Operation

New project funded by DOE ND Program, FY24 – FY26

Oak Ridge National Laboratory
February 1, 2024

Germina Ilas

Our Team

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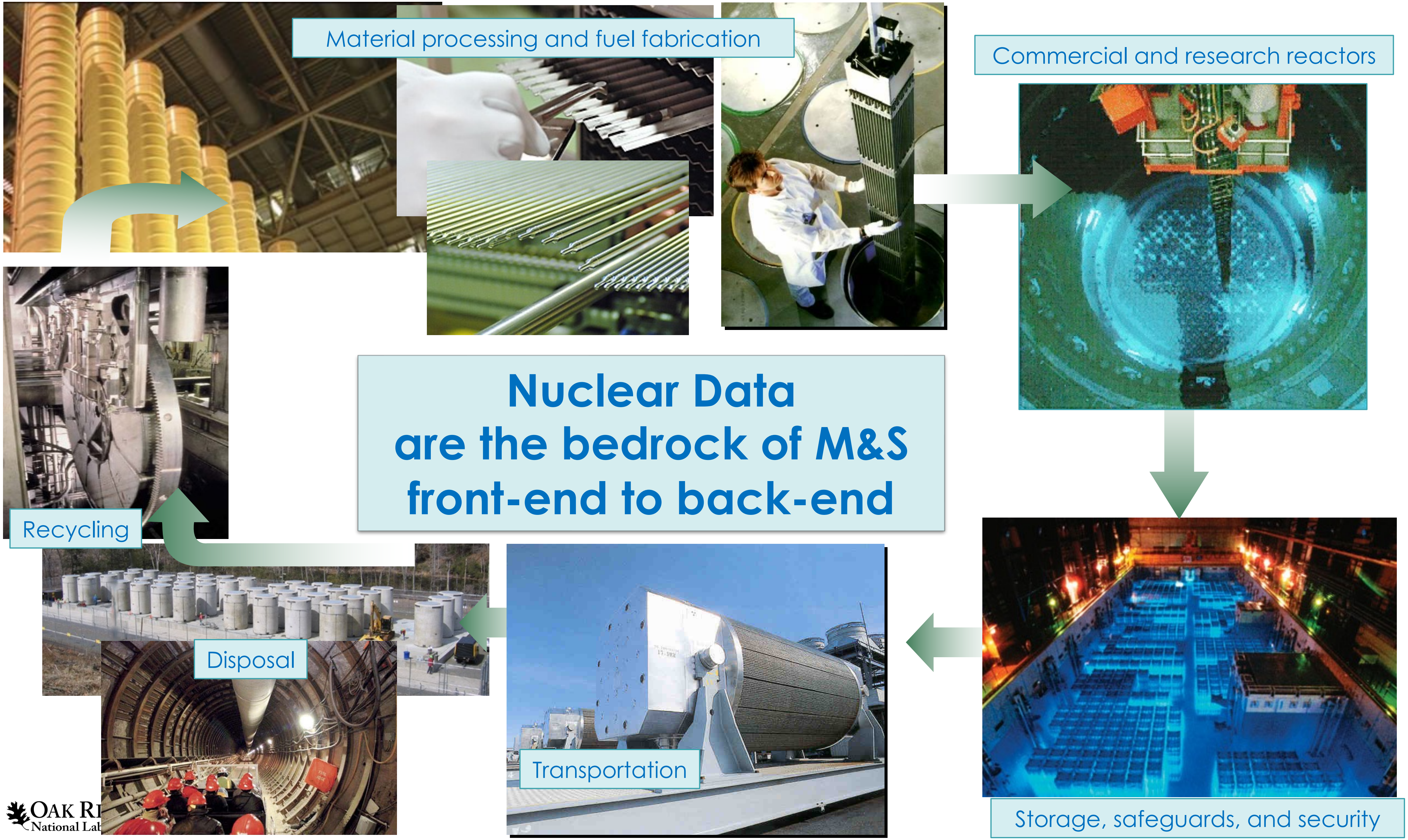
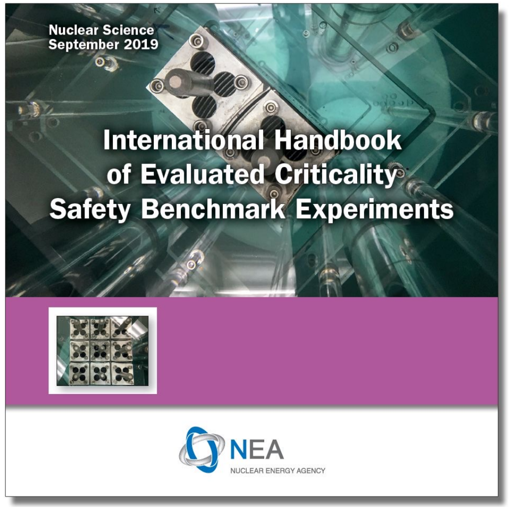

Material processing and fuel fabrication
Commercial and research reactors
Nuclear Data
are the bedrock of M&S
front-end to back-end
Recycling
Storage, safeguards, and security
Transportation
Disposal

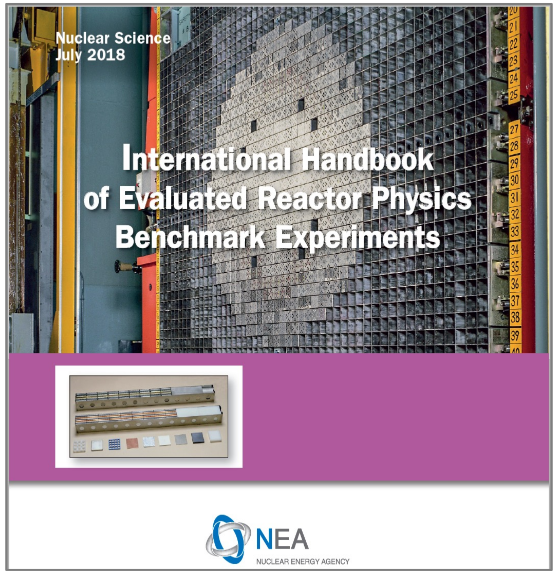
Resources to assess nuclear data impacts for advanced reactors are very limited compared to LWRs

A large diversity of resources and knowledge documented over the past 60 years of commercial operational and experimentation is available for LWR assessments.



over 600 criticality benchmarks

over 160 reactor benchmarks

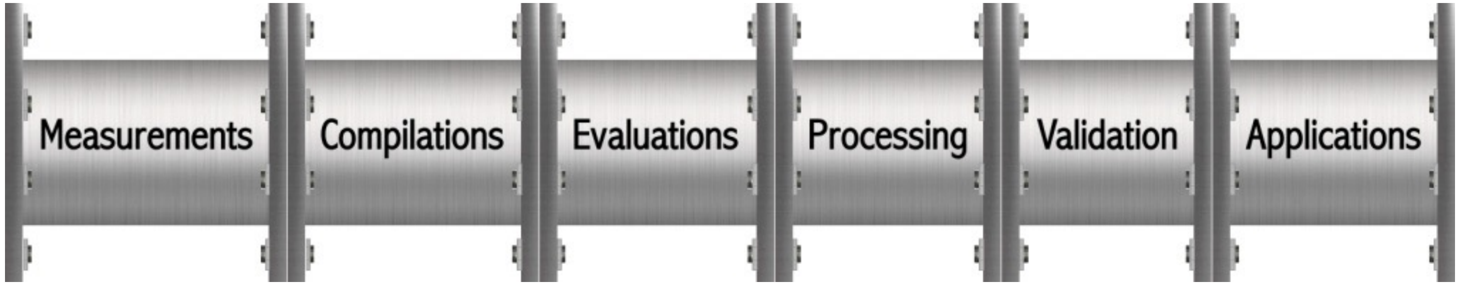


Seven IRPhE benchmarks are relevant to advanced reactors configurations. None of them include measurement data for **reactor key metrics as a function of fuel burnup during reactor operation.**

Clear need for a benchmark model resource to assess nuclear data impacts for advanced reactors beyond integral metrics like k_{eff} and beyond fresh fuel

Overarching Goal of this project

- **Facilitate identifying** nuclear data deficiencies and needs in the US Nuclear Data Program databases that have the most impact on advanced nuclear energy systems' safety and operation
- **Develop resources** for enabling end-user-driven, application-driven improvements in the nuclear data pipeline to address these needs



Steps towards achieving the overarching goal

1. Formulate extended advanced reactor benchmark models with irradiated fuel → **Benchmark model resource to assess nuclear data impacts as function of fuel burnup**
2. Assess nuclear data impacts for advanced reactor key metrics and develop sensitivity coefficients of key nuclides and nuclear data → **Sensitivity data file (SDF) resource**
3. Investigate nuclear data needs for advanced reactors by quantifying uncertainties of key metrics due to nuclear data uncertainties → **Key metrics uncertainty resource**
4. Demonstrate approach to improve critical steps in nuclear data pipeline, for rapid testing and evaluation of NNDC nuclear data and associated data processing tools

Questions ?