

Validation with SCALE: How to Connect Paper Reactors with Reality

SCALE Workshop

PHYSOR 2024
San Francisco, CA
April 21, 2024

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



U.S. DEPARTMENT OF
ENERGY

Goals

1. Explore the key capabilities of the SCALE code system for neutron transport, depletion, uncertainty quantification, and sensitivity analysis
2. Gain practical insight into using SCALE for validation analyses as accepted by US regulators
3. Learn how to perform similarity assessments, how to determine biases, and how to identify validation gaps
4. See SCALE's graphical user interface Fulcrum, in action to create and validate input files, visualize 2D and 3D geometries, and explore various result files

Agenda

1. Intro to validation **(30 min)**
2. Criticality safety validation for HTGR pebble transport **(40 min)**
3. Reactor physics validation for MSR **(40 min)**
4. Sampling-based uncertainty, sensitivity, similarity **(40 min)**
5. Nuclide and decay heat similarity **(40 min)**

Interrupt us to ask questions! 😊

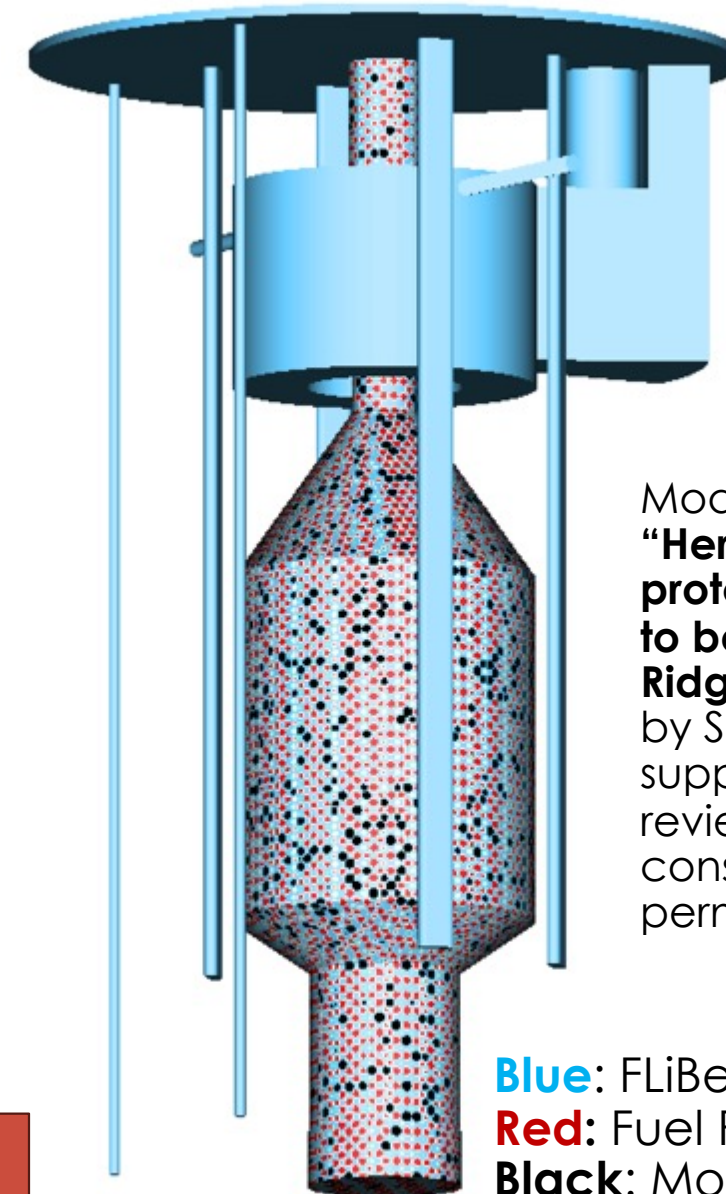
We'll take 5-minute breaks as needed

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/power 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 capabilities in SCALE

- **Perturbation theory-based sensitivity methods** generate sensitivity coefficients of outputs like critical eigenvalue, k_{eff} , to 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 ^7Li (n,γ) cross section uncertainty • Significant update from ENDF/B-VII.0 to VII.1 in the ^6Li (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 $^{135\text{m}}\text{Xe}$ • No thermal scattering data are available for salts (e.g., FLiBe) • No graphite thermal scattering data uncertainties are available • Large ^7Li (n,γ) cross section uncertainty • Significant update from ENDF/B-VII.0 to VII.1 in the ^6Li (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).

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
 - Open-source **code** (subset)
<https://code.ornl.gov/scale/code/scale-public>
 - Open-source SCALE **models**
<https://code.ornl.gov/scale/analysis>

SCALE Team

Director
Will Wieselquist

Leadership Team

Production Coordinator
Rob Lefebvre
Shane Hart (*Deputy, Release Coordinator*)

User Support Coordinator
Germina Ilas

Sponsor Representatives
Seth Johnson, HPC
B.J. Marshall, NCSP
Ugur Mertiyurek, NRC

Advisors
Matt Jessee, NEAMS Reactor Physics Lead
Bob Grove, Section Head, Nuclear Software Development
Doug Bowen, Section Head, Radiation Shielding & Criticality
Jordan McDonnell, AMPX lead

Project Management
Marsha Henley

Logistics
Sandra Poarch

Product Owners

AMPX	Jordan McDonnell
CSAS	Kursat Bekar
DATA	Jesse Brown
FULCRUM	Rob Lefebvre
MAVRIC	Cihangir Celik
OMNIBUS	Seth Johnson
ORIGAMI	Steve Skutnik
ORIGEN	B.K. Jeon
POLARIS	Matt Jessee
SAMPLER	Ugur Mertiyurek
STDCOMP	Rob Lefebvre*
TRITON	Rike Bostelmann
TSUNAMI	Jordan McDonnell*
VADER	BJ Marshall
XSPROC	Kang Seog Kim

*Interim owner

Dev/Testing/Analysis

Arzu Alpan	Brandon Langley
Goran Arbanas	Tara Pandya
Jin Whan Bae	Douglas Peplow
Mark Baird	Marco Pigni
Elliot Biondo	Georgeta Radulescu
Chris Chapman	Joel Risner
Eva Davidson	Kat Royston
Gregory Davidson	Jose S. Perez
Mathieu Dupont	Alex Shaw
Rabab Elzohery	Ben Taylor
Tom Evans	
Tarek Ghaddar	
Travis Greene	
Steven Hamilton	
Donny Hartanto	
Briana Hiscox	
Jianwei Hu	
Alex Lang	

NRC Projects Office

Program Manager
Bruce Bevard
Business Ops Manager
Lindsey Aloisi

NCSP Management

NCSP Execution Manager
Doug Bowen
Business Systems
Marsha Henley

Validation background



Definitions

- **Validation** is defined as **comparing your calculations to reality** with the goal of estimating code bias and bias uncertainty,
 - typically presented as a C/E-1 (%) with C the calculation and E the experiment/measurement
 - Yields combined on quality of nuclear data, models, and code
- **Verification** is defined as the things we do to understand correctness without a measurement
 - Code-to-code comparisons
 - Comparisons to analytic solution
- **How can you prove that your data+code+methods+models can assess the safety of a paper reactor before it is built?**

Validation + Similarity!

US regulations for criticality safety

Regulations require maintaining criticality safety under all conditions!

- 10 CFR 70.61 – Subcritical under normal and credible abnormal conditions
- 10 CFR 70.64 – Double contingency principle
- 10 CFR 70.24 – Criticality monitoring
- 10 CFR 71.55 - Single packages.
 - 10 CFR 71.55(b): subcritical considering water in-leakage
 - 10 CFR 71.55(d): subcritical under normal conditions of transport (NCT)
 - 10 CFR 71.55(e): subcritical under hypothetical accident conditions (HAC)
- 10 CFR 71.59 – Package arrays.
 - Subcritical under NCT and HAC
 - Limiting number of packages under NCT or HAC used to determine Criticality Safety Index (CSI) to control package accumulation on conveyance

Proving sub-criticality requires validation!

- ANS 8.1 - *Nuclear Criticality Safety In Operations With Fissionable Materials Outside Reactors*:
 - **Validation** shall be performed by comparison to critical experiments, and the **area of applicability for the validation should be established from this comparison**
 - Establish:
 - Applicability of experiments
 - Code bias and bias uncertainty
 - Trending analysis
- ANS 8.24 - *Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations*
- NUREG/CR-6698 - *Guide for Validation of Nuclear Criticality Safety Computational Methodology*
- NUREG/CR-5661 - *Recommendations for Preparing the Criticality Safety Evaluation of Transportation Packages*
- NUREG/CR-6361 - *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*
- International Criticality Safety Benchmark Evaluation Project (ICSBEP):
 - Descriptions of over 5,000 laboratory critical experiments
 - Grouped by fissile media, physical form, and neutron energy where most fissions occur
 - Many experiments representative of <5% enriched UO_2 LWR fuel; less for enrichment range of 5-20%; much less for key systems of interest (e.g., TRISO, low moderation UF_6)

So we need validation, but why similarity?

- *Can you validate graphite-moderated fuel transportation with water-moderated critical experiments?*
- **Similarity** assessment relates your case to the available validation suite to find the specific experiments/measurements that are **applicable**
- **Applicability** means that the bias PDF ($C/E - 1$) calculated from that subset will be indicative of your system

Goal for Future SCALE:

- Comprehensive, automated validation
 - radiation shielding
 - isotope production
 - criticality safety
 - spent fuel applications
- Robust capabilities for **sensitivity** and **similarity**
- Provide the community with a **reference solution** compared to actual measurements for data + method + implementation

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Criticality Safety Validation

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Learning goals

- Understand SCALE's tools for neutron transport (CSAS), sensitivity to k_{eff} (TSUNAMI-3D), and similarity assessment (TSUNAMI-IP)
- Understand when to use which tool for different assessment needs
- Understand a demonstration of the above tools with the Versa-Pac fuel transport canister

Overview

- CSAS: SCALE sequences that compute k_{eff} of a system with 3D Monte Carlo neutron transport
- TSUNAMI-3D: SCALE sequences that compute the k_{eff} sensitivities to nuclear data
- TSUNAMI-IP: SCALE sequence that performs uncertainty quantification and similarity assessment

CSAS sequence description



CSAS5/6 Sequences

- Automatically set up the input for each functional module that is called in the sequence
- Automated cross-section processing (multigroup only)
 - Simple 1-D cell description
- 3-D criticality calculation using KENO V.a (CSAS5), KENO-VI (CSAS6), or Shift (CSAS5-Shift or CSAS6-Shift)
- SCALE 6.3 contains Shift as an alternative Monte Carlo transport solver in place of KENO
 - Shift is intended to replace KENO in future releases

TSUNAMI-3D sequences



Overview

- TSUNAMI-3D: SCALE sequences that compute the k_{eff} sensitivities to nuclear data
- Input is largely the same as CSAS
- TSUNAMI-3D-K5 uses KENO V.a for transport solution, TSUNAMI-3D-K6 uses KENO-VI, and TSUNAMI-3D-K5-Shift or TSUNAMI-3D-K6-Shift uses Shift
- Can assess uncertainty in k_{eff} by utilizing the nuclear covariance data

TSUNAMI-3D: Continuous Energy



CE TSUNAMI-3D Sensitivity Methods

Eigenvalue Sensitivity Calculations

- IFP Method (KENO or Shift) (cet=2)
- CLUTCH Method (KENO only) (cet=1)

Iterated Fission Probability Method

- The Iterated Fission Probability (IFP) method calculates adjoint-weighted tallies using the notion that the importance of an event is proportional to the population of neutrons present in the system during some future generation.
- In practice, the IFP method can require storing reaction rate tallies for a significant number of generations.
- In CE TSUNAMI-3D, the IFP method is used by setting: **cet=2**
- The number of “latent generations” is set using the **cfp=#** parameter.

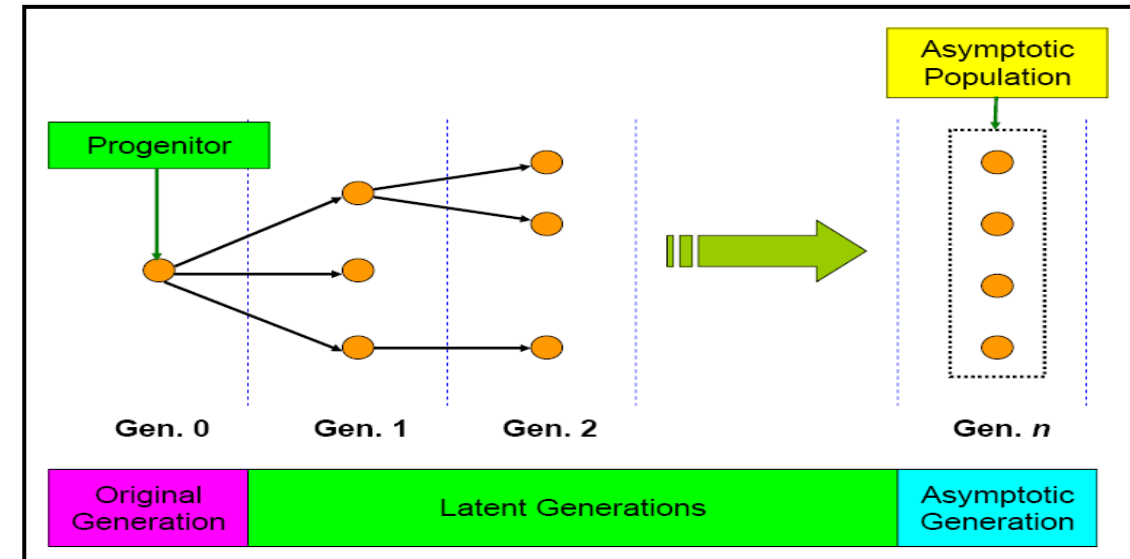


Illustration of the IFP process. Image courtesy of Brian Kiedrowski.

How Many Latent Generations Do We Need?

- IFP calculations should use somewhere between 2 and 20 latent generations to obtain accurate sensitivities
 - In practice, most simulations require between 5 and 10 latent generations.
- Memory footprint of SCALE IFP calculations increases with the number of latent generations
 - Users should use enough latent generations to obtain accurate sensitivity coefficients, but also as few as possible to minimize the simulation's memory footprint
 - Confirm results with direct perturbations!

CE TSUNAMI-3D Summary

- CE TSUNAMI-3D contains two methods for calculating eigenvalue sensitivity coefficients
- CE TSUNAMI-3D usually does not require as much input as multigroup TSUNAMI-3D, and calculates sensitivity coefficients in a single forward simulation
- The IFP sensitivity method (**cet=2**) requires inputting some number of latent generations (**cfp=#**)
 - Between 2 and 20 latent generations is recommended – 5 to 10 is generally sufficient

TSUNAMI-IP: Tool for similarity assessment



Criticality Code Validation with TSUNAMI

- Some questions TSUNAMI analysis is intended to answer:
 - Which experiments should I use to validate my application?
 - Is there a quantitative basis for generating a reactivity allowance for a validation weakness or gap?
 - Is there any appropriate basis for extrapolating information from existing experiments to applications where no similar experiments exist?
- TSUNAMI-IP performs
 - Benchmark experiment selection
 - Uncertainty analysis

Propagation of Cross Section Uncertainties

- Chain rule allows for propagation of cross section uncertainty (i.e., covariance) to quantify the data-induced uncertainty in k_{eff} (σ_k^2)

$$\sigma_k^2 = S C_{aa} S^T$$

Where:

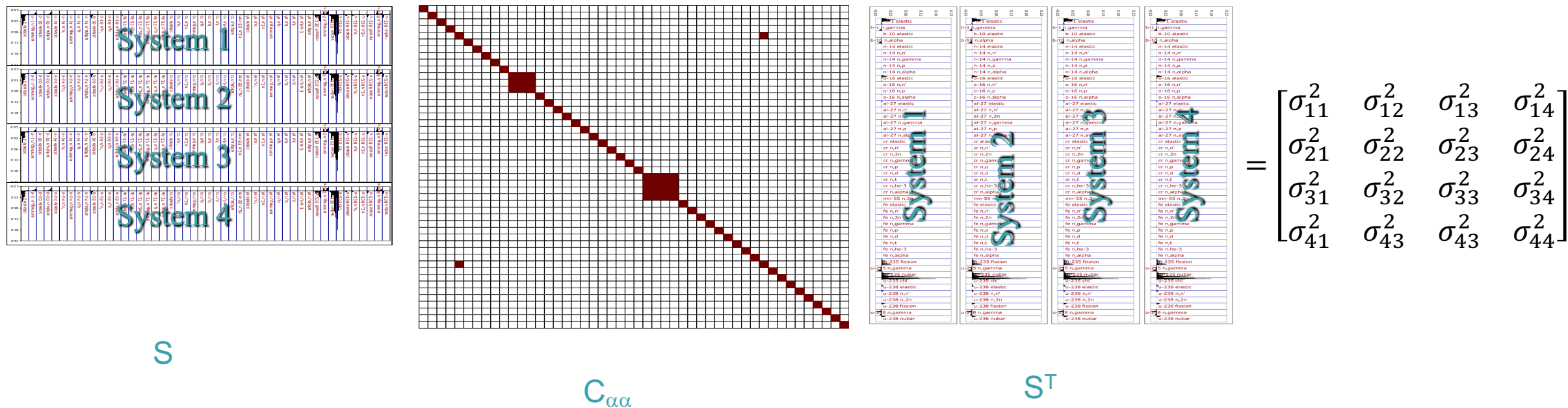
- S is a matrix of all energy-dependent sensitivity data for all systems considered (S^T is transpose)
- C_{aa} is a matrix containing energy-dependent covariance information evaluated for all nuclear data

Use of Uncertainty Information to Assess System Similarity

- “Fundamental theorem of TSUNAMI”: bias is caused by errors in cross section data, which are bounded by cross-section uncertainties
- Systems will have similar computational biases if they have similar sensitivities
 - Uncertainties act like a weighting function
- Comparison must examine nuclide-, reaction-, and energy-dependent data

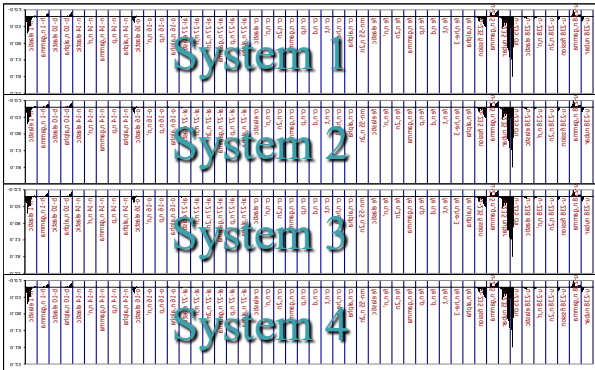
Uncertainty Propagation

- Suppose we have sensitivity information for multiple systems:

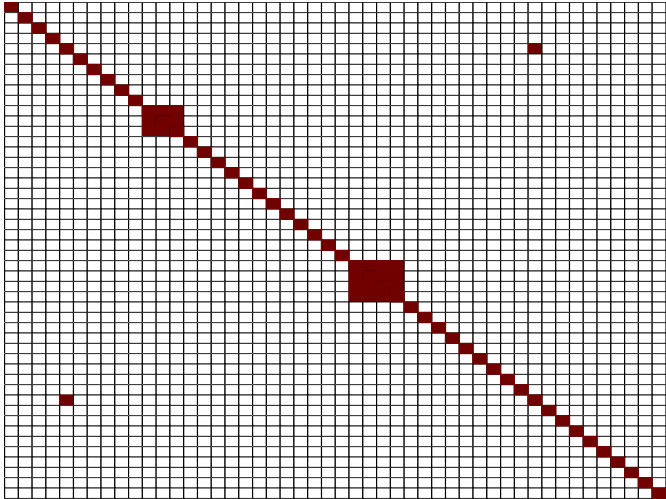


Uncertainty Propagation

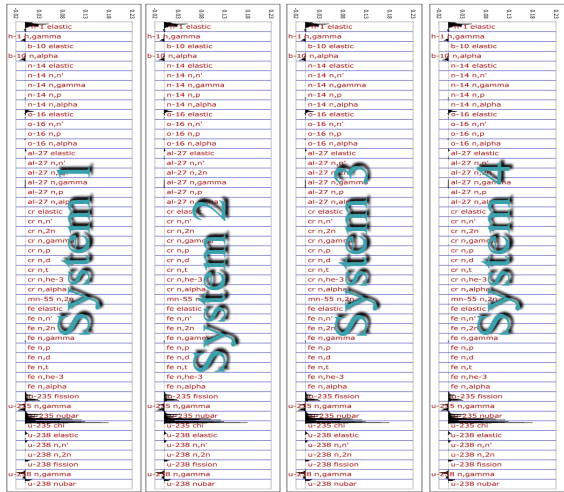
- Suppose we have sensitivity information for multiple systems:



S



C_{αα}



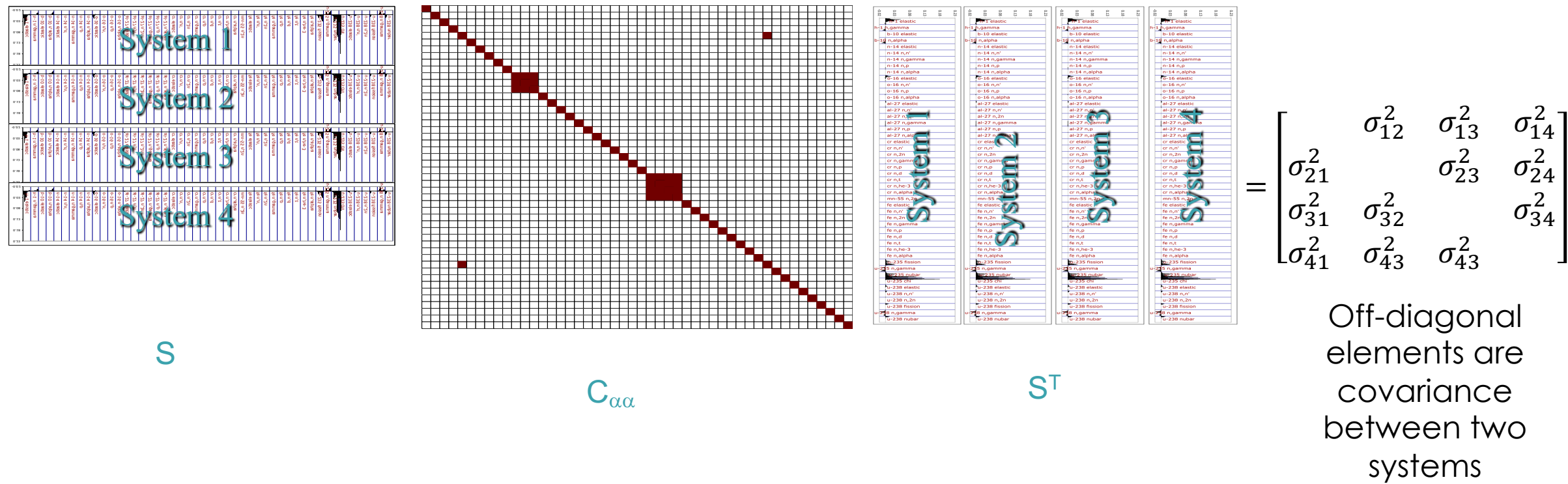
ST

Diagonal elements are variance in each system

$$= \begin{bmatrix} \sigma_{11}^2 & & & \\ & \sigma_{22}^2 & & \\ & & \sigma_{33}^2 & \\ & & & \sigma_{44}^2 \end{bmatrix}$$

Uncertainty Propagation

- Suppose we have sensitivity information for multiple systems:



Correlation Coefficient c_k for System 1 and System 4

$$C_{kk} = \begin{bmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \sigma_{13}^2 & \sigma_{14}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & \sigma_{23}^2 & \sigma_{24}^2 \\ \sigma_{31}^2 & \sigma_{32}^2 & \sigma_{33}^2 & \sigma_{34}^2 \\ \sigma_{41}^2 & \sigma_{42}^2 & \sigma_{43}^2 & \sigma_{44}^2 \end{bmatrix}$$

$$c_k = \frac{\sigma_{41}^2}{\sqrt{\sigma_{11}^2} \sqrt{\sigma_{44}^2}}$$

Integral Index c_k

- c_k is an integral index used to assess similarity
 - Uncertainty-weighted sensitivity profiles between a design system and a criticality experiment
 - What fraction of the data-induced uncertainty is shared by two systems?
 - Correlation coefficient, so normalized from 0 to +1.0
 - +1.0 is exactly the same system while 0 is completely uncorrelated
- Current guidance*:
 - c_k of 0.9 or higher indicates a “highly similar” system
 - c_k between 0.8 and 0.9 are “marginally similar”

*Broadhead, B. L., Rearden, B. T., Hopper, C. M., Wagschal, J. J., and Parks, C. V., “Sensitivity- and Uncertainty-Based Criticality Safety Validation Techniques,” *Nuclear Science and Engineering*, vol 146, pp. 340–366, 2004.

Summary

- S/U-based parameters should be useful in identifying similar benchmark systems
 - Basis for similarity is both sensitivity information and nuclear data uncertainties
- Similarity assessment can be used in trending analyses to determine subcritical limits
- Uncertainty analysis can be used to support determination of margins for validation gaps and weaknesses
- ORNL recommends c_k values greater than 0.8 for inclusion in validation

Validation workshop with Versa-Pac

- Fulcrum introduction
- Versa-Pac workshop

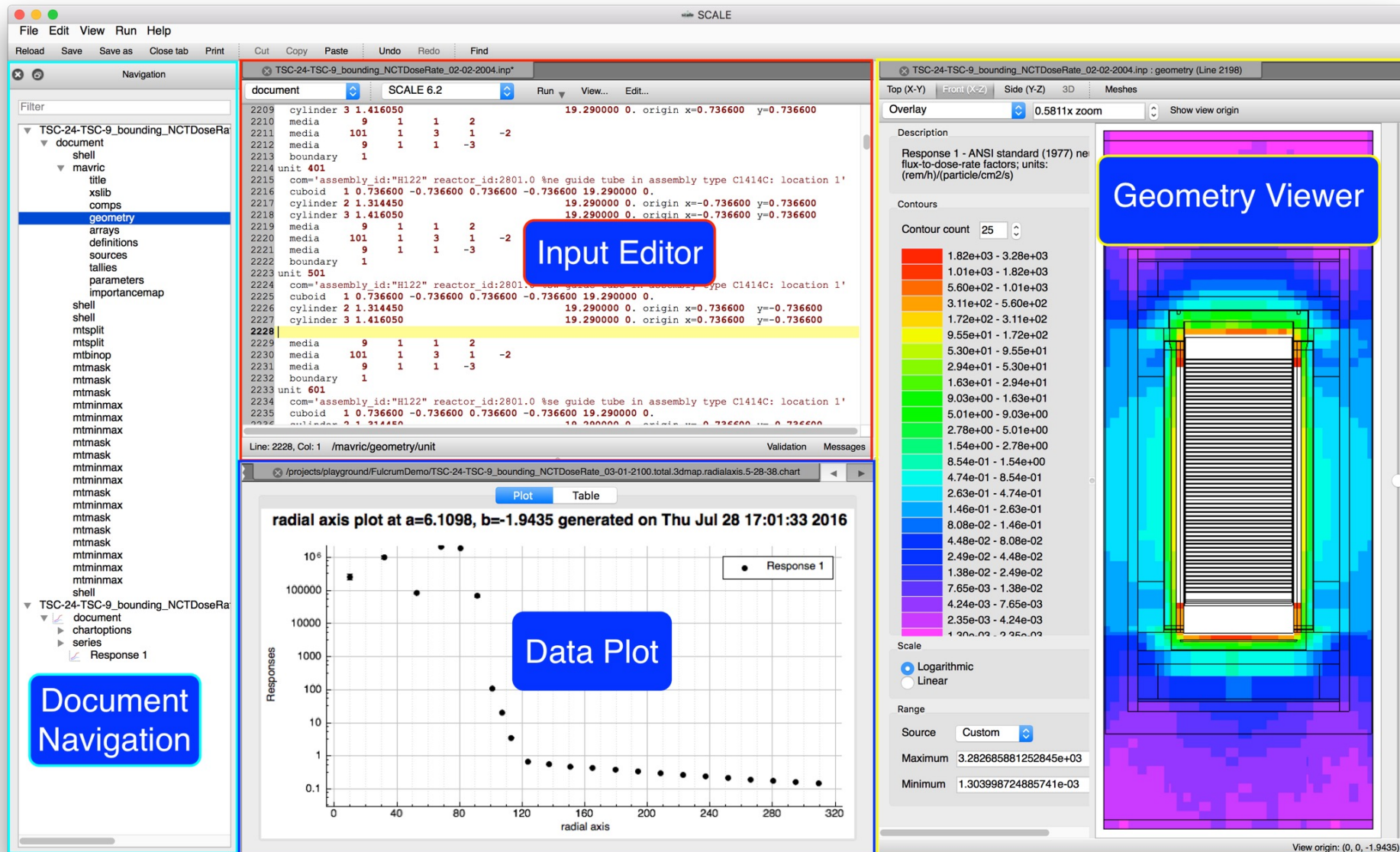


Fulcrum – SCALE's graphical user interface

- Platform-independent!
- GUI and integrated development environment for SCALE input files
- Looks like a text editor but is more powerful, with modular workspaces
- Syntax highlighting and input checking
- Integrated geometry visualization
- Run SCALE directly from Fulcrum
- View screen output in Fulcrum
- Integrated results visualization

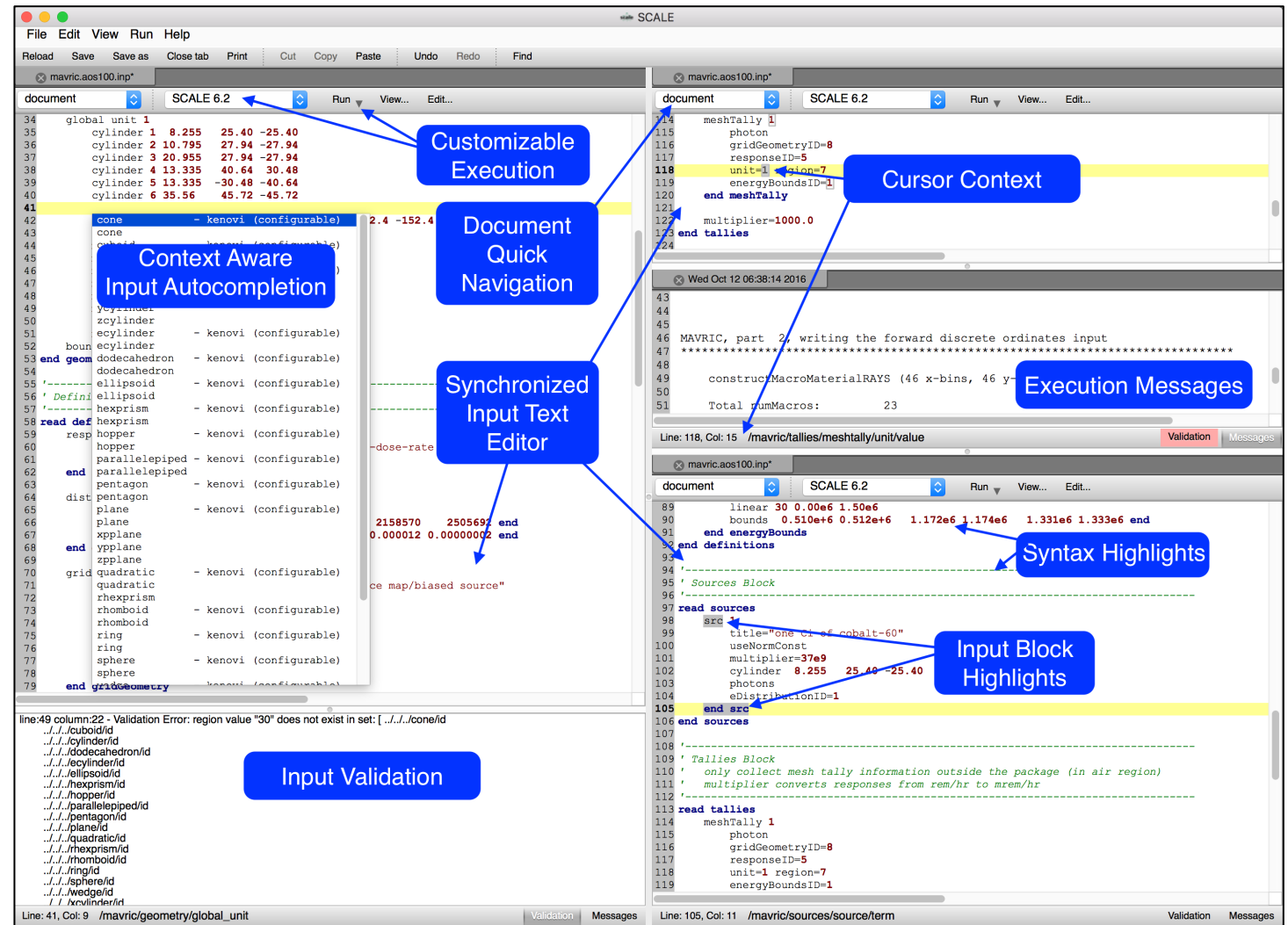


Fulcrum components overview



Fulcrum text editor features | Overview

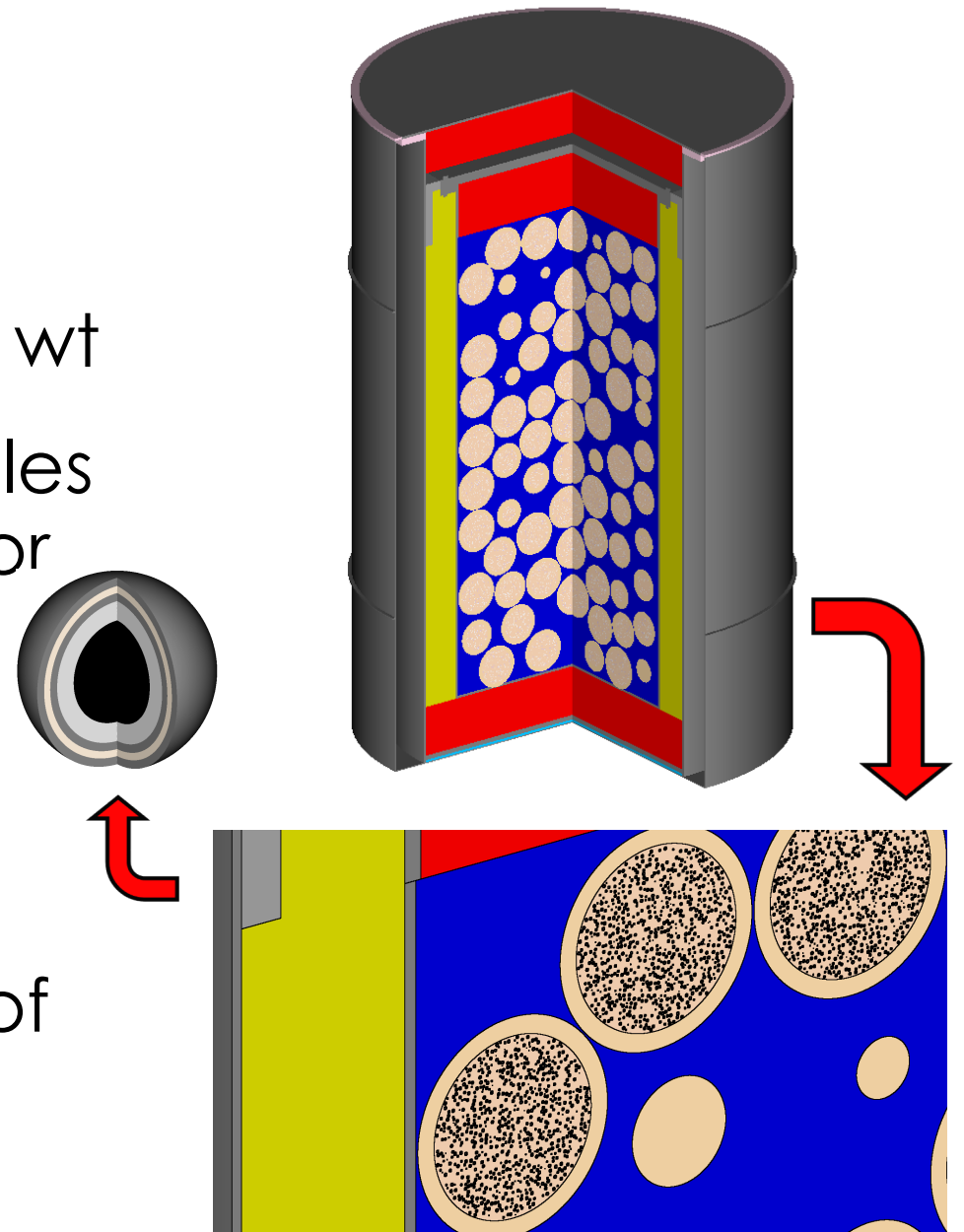
- Customizable execution
- Quick navigation
- Cursor context
- Execution messages
- Input validity checks
- Syntax highlights
- Current block highlight
- Context-aware input auto completion
- Synchronized and split workspaces



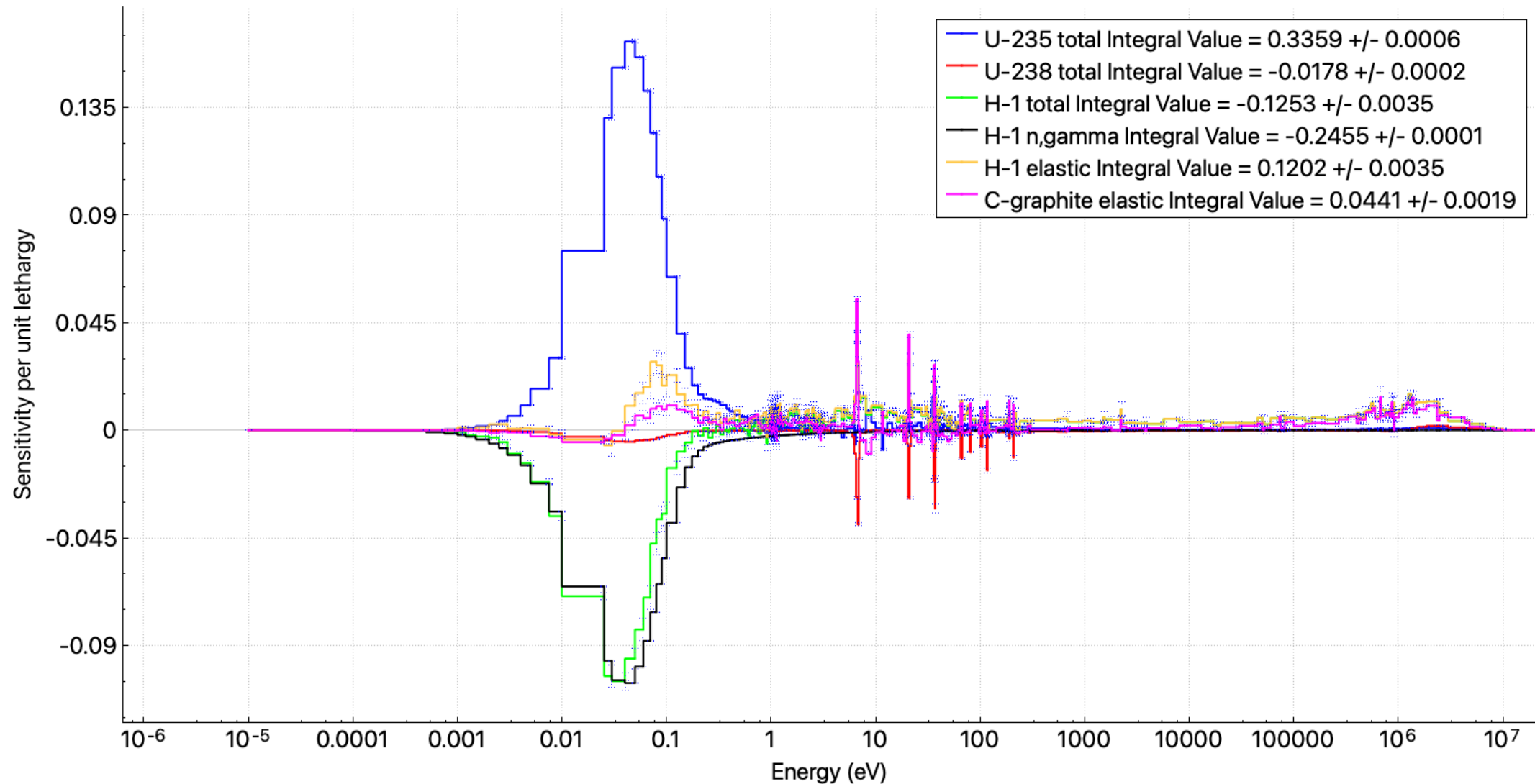
Application

Versa-Pac model

- Licensed to transport ^{235}U up to 100% wt
- Package design based on fuel pebbles from the Pebble Bed Modular Reactor (PBMR) 400 design: TRISO fuel
- Packing fraction of 17%
- ^{235}U enrichment of 20% wt
- Analysis condition is an infinite array of flooded packages



Sensitivity profiles for Versa-Pac



Uncertainty of Versa-Pac

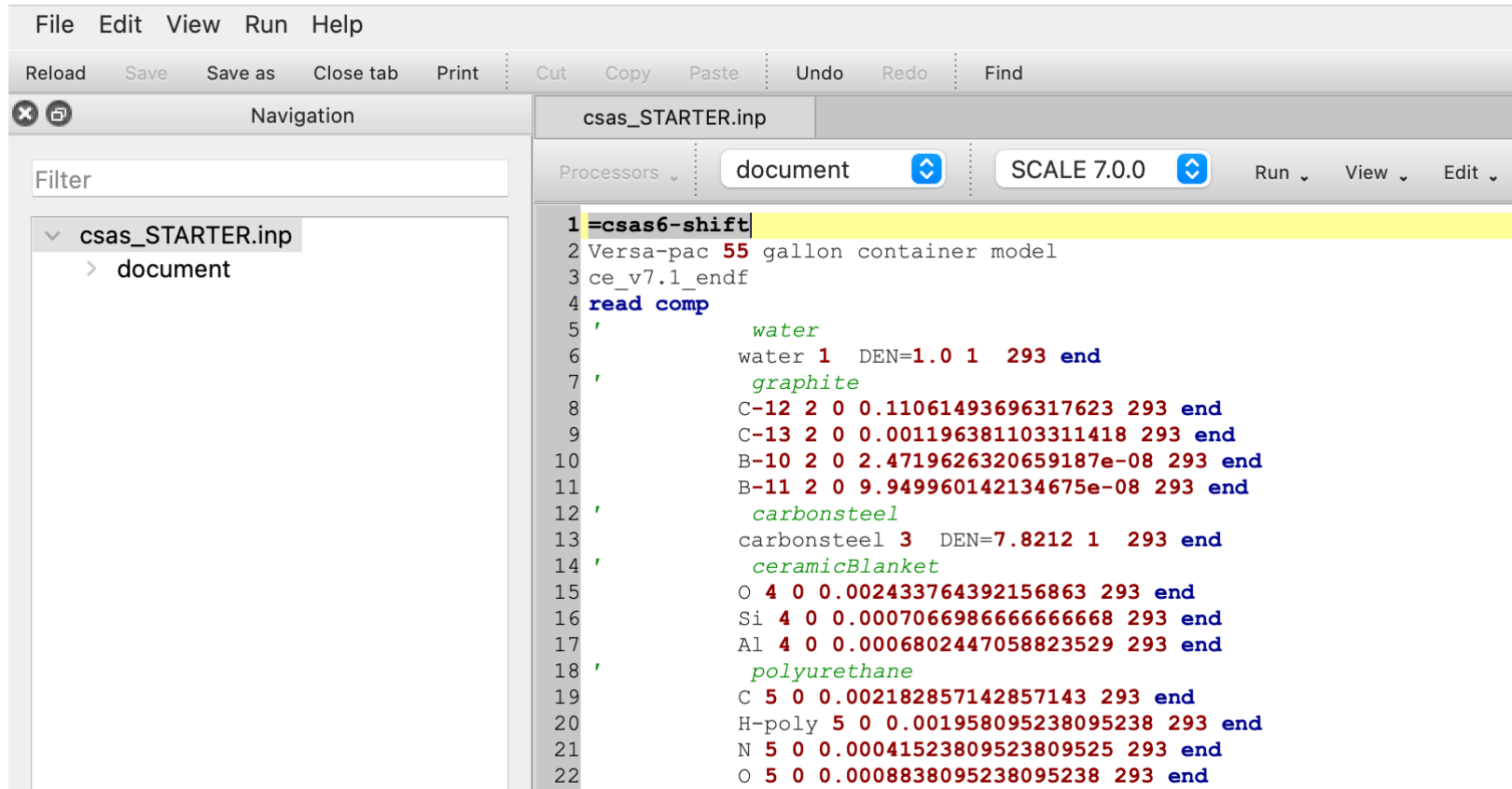
- Data-induced uncertainty is 0.677% $\Delta k/k$
- With 1σ confidence, bias should be bounded by 0.677% $\Delta k/k$
- Top 10 contributors listed
 - Account for more than 99.7% of the data-induced uncertainty

Covariance matrix		% $\Delta k/k$ due to this matrix
Nuclide–reaction	Nuclide–reaction	
^{56}Fe (n, γ)	^{56}Fe (n, γ)	0.400
^{235}U nubar	^{235}U nubar	0.381
^1H (n, γ)	^1H (n, γ)	0.261
^{235}U (n, γ)	^{235}U (n, γ)	0.153
^{235}U (n,fission)	^{235}U (n,fission)	0.150
^{235}U (n,fission)	^{235}U (n, γ)	0.135
^{235}U χ	^{235}U χ	0.128
^{54}Fe (n, γ)	^{54}Fe (n, γ)	0.029
^{238}U (n, γ)	^{238}U (n, γ)	0.028
^1H elastic	^1H elastic	0.028

Available experiments

- Individual benchmark cases from ICSBEP
 - 80 from TSUNAMI-1D (ORNL – ^{233}U)
 - 463 from TSUNAMI-3D (ORNL – ^{233}U or VALID)
 - Thousands of additional cases generated by Ian Hill at OECD/NEA with automated scripts and sample inputs
 - SDFs are believed to be useful for screening
 - Should be checked with DPs and/or regenerated for further use
- 504 benchmark cases provided for this workshop demonstration (combination of VALID and NEA SDFs)

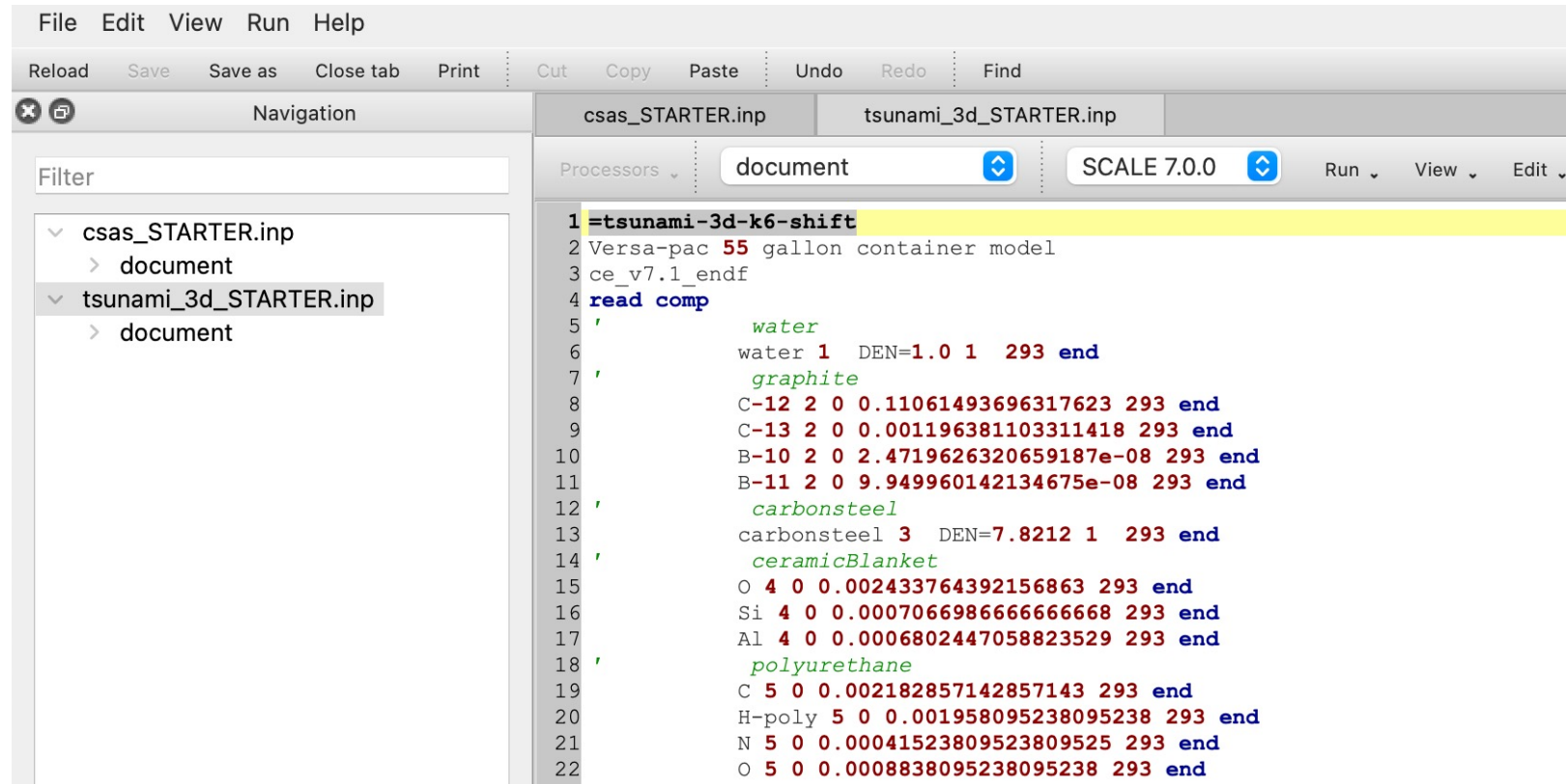
Open csas_STARTER.inp in /PHYSOR_2024/ncs/demo or
c:\PHYSOR_2024\ncs\demo



```
File Edit View Run Help
Reload Save Save as Close tab Print Cut Copy Paste Undo Redo Find
Navigation
Filter
csas_STARTER.inp
  document
1 =csas6-shift
2 Versa-pac 55 gallon container model
3 ce_v7.1_endf
4 read comp
5 '
6   water 1 DEN=1.0 1 293 end
7 '
8   graphite
9   C-12 2 0 0.11061493696317623 293 end
10  C-13 2 0 0.001196381103311418 293 end
11  B-10 2 0 2.4719626320659187e-08 293 end
12  B-11 2 0 9.949960142134675e-08 293 end
13 '
14  carbonsteel
15  carbonsteel 3 DEN=7.8212 1 293 end
16 '
17  ceramicBlanket
18  O 4 0 0.002433764392156863 293 end
19  Si 4 0 0.0007066986666666668 293 end
20  Al 4 0 0.0006802447058823529 293 end
21 '
22  polyurethane
23  C 5 0 0.002182857142857143 293 end
24  H-poly 5 0 0.001958095238095238 293 end
25  N 5 0 0.00041523809523809525 293 end
26  O 5 0 0.0008838095238095238 293 end
```

Run as is for k_{eff} value only.

Open tsunami_3d_STARTER.inp in /PHYSOR_2024/ncs/demo
or c:\PHYSOR_2024\ncs\demo



```
1 =tsunami-3d-k6-shift
2 Versa-pac 55 gallon container model
3 ce_v7.1_endf
4 read comp
5 '
6   water 1 DEN=1.0 1 293 end
7 '
8   graphite
9   C-12 2 0 0.11061493696317623 293 end
10  C-13 2 0 0.001196381103311418 293 end
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18  O 4 0 0.002433764392156863 293 end
19  Si 4 0 0.0007066986666666668 293 end
20  Al 4 0 0.0006802447058823529 293 end
21 '
22  polyurethane
23  C 5 0 0.002182857142857143 293 end
24  H-poly 5 0 0.001958095238095238 293 end
25  N 5 0 0.00041523809523809525 293 end
26  O 5 0 0.0008838095238095238 293 end
```

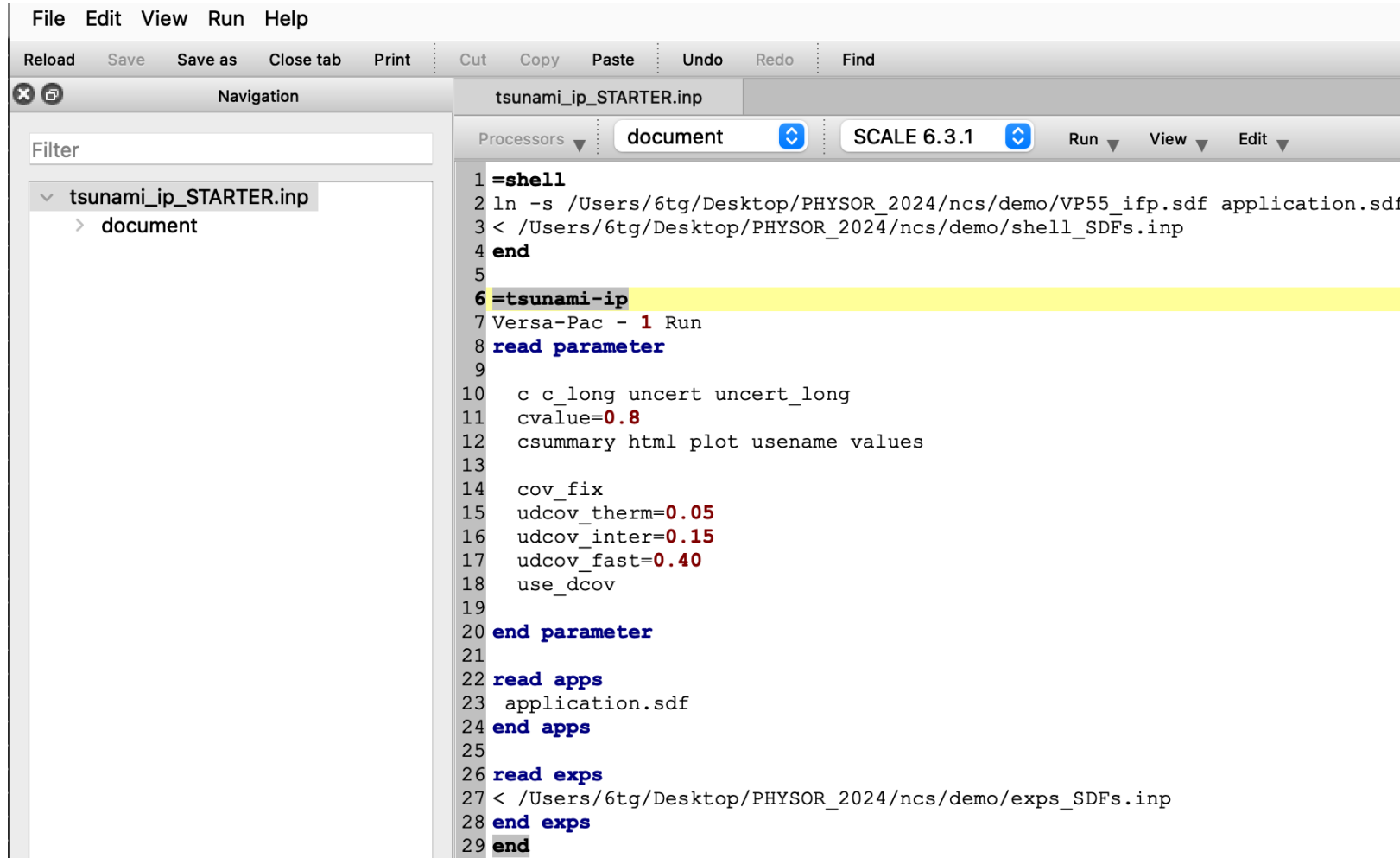
Run as is for sensitivity calculations with IFP-Shift.

Open tsunami_3d_STARTER.inp in /PHYSOR_2024/ncs/demo
or c:\PHYSOR_2024\ncs\demo

```
61 read parameter
62     htm=no
63     flx=no
64     npg=50000
65     gen=1100
66     nsk=100
67     sig=0.00020
68     thc=40
69     cet=2
70     cfp=5
71 end parameter
```

IFP parameters

Open tsunami_ip_STARTER.inp in /PHYSOR_2024/ncs/demo or c:\PHYSOR_2024\ncs\demo



```
File Edit View Run Help
Reload Save Save as Close tab Print Cut Copy Paste Undo Redo Find
Navigation
Filter
tsunami_ip_STARTER.inp
  document
1 =shell
2 ln -s /Users/6tg/Desktop/PHYSOR_2024/ncs/demo/VP55_ifp.sdf application.sdf
3 < /Users/6tg/Desktop/PHYSOR_2024/ncs/demo/shell_SDFs.inp
4 end
5
6 =tsunami-ip
7 Versa-Pac - 1 Run
8 read parameter
9
10 c c_long uncert uncert_long
11 cvalue=0.8
12 csummary html plot username values
13
14 cov_fix
15 udcov_therm=0.05
16 udcov_inter=0.15
17 udcov_fast=0.40
18 use_dcov
19
20 end parameter
21
22 read apps
23 application.sdf
24 end apps
25
26 read exps
27 < /Users/6tg/Desktop/PHYSOR_2024/ncs/demo/exps_SDFs.inp
28 end exps
29 end
```

Parameters

- **c** – compute c_k
- **c_long** – extended edit of c_k
- **uncert** – uncertainty due to covariance data for application and benchmarks
- **uncert_long** – extended edit of uncertainty for application
- **cvalue=0.8** – allow more experiments to be used for analysis (default is 0.9)

```
8 read parameter
9
10 c c_long uncert uncert_long
11 cvalue=0.8
12 csummary html plot username values
13
14 cov_fix
15 udcov_therm=0.05
16 udcov_inter=0.15
17 udcov_fast=0.40
18 use_dcov
19
20 end parameter
```

Output edits

- `csummary` – c_k values that exceed `cvalue` cutoff criteria
- `html (html_p)` – produce HTML output
- `plot` – generate some plots of values
- `username` – use file name to identify SDF files
- `values` – produces tables of values (k_{eff} , c_k , uncert)

```
8 read parameter
9
10 c c_long uncert uncert_long
11 cvalue=0.8
12 csummary html plot username values
13
14 cov_fix
15 udcov_therm=0.05
16 udcov_inter=0.15
17 udcov_fast=0.40
18 use_dcov
19
20 end parameter
```

Covariance data

- `cov_fix` – patch up any remaining holes in covariance data
- `use_dcov` – use default settings for patches
- `udcov_therm` – user-defined uncertainty for thermal data
- `udcov_inter` – user-defined uncertainty for intermediate data
- `udcov_fast` – user-defined uncertainty for fast data

```
8 read parameter
9
10 c c_long uncert uncert_long
11 cvalue=0.8
12 csummary html plot username values
13
14 cov_fix
15 udcov_therm=0.05
16 udcov_inter=0.15
17 udcov_fast=0.40
18 use_dcov
19
20 end parameter
```

Application and experiments paths and data

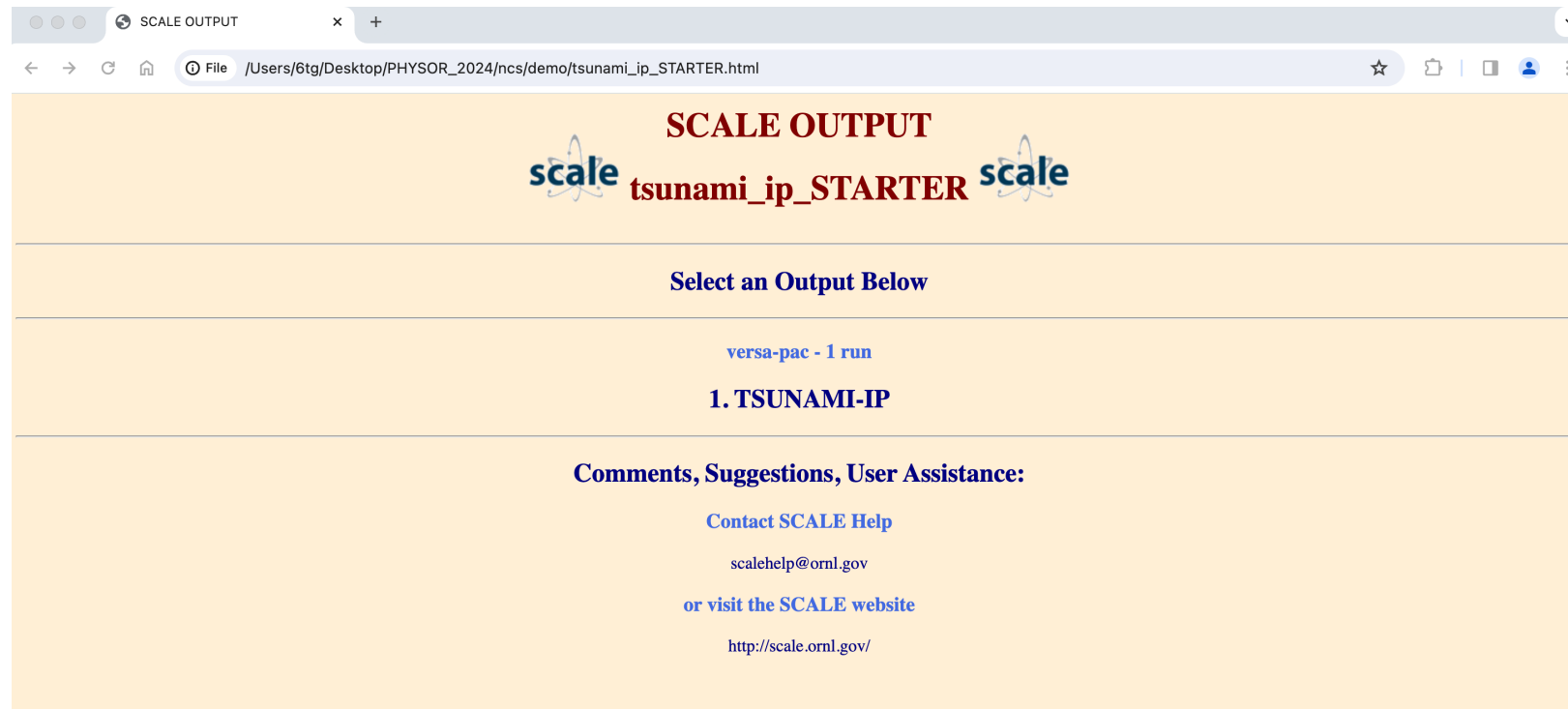
```
File Edit View Run Help
Reload Save Save as Close tab Print Cut Copy Paste Undo Redo Find
Navigation
Filter
tsunami_ip_STARTER.inp
  document
1 =shell
2 ln -s /Users/6tg/Desktop/PHYSOR_2024/ncs/demo/VP55 ifp.sdf application.sdf
3 < /Users/6tg/Desktop/PHYSOR_2024/ncs/demo/shell_SDFs.inp
4 end
5
6 =tsunami-ip
7 Versa-Pac - 1 Run
8 read parameter
9
10 c c_long uncert uncert_long
11 cvalue=0.8
12 csummary html plot username values
13
14 cov_fix
15 udcov_therm=0.05
16 udcov_inter=0.15
17 udcov_fast=0.40
18 use_dcov
19
20 end parameter
21
22 read apps
23 application.sdf
24 end apps
25
26 read exps
27 < /Users/6tg/Desktop/PHYSOR_2024/ncs/demo/exps_SDFs.inp
28 end exps
29 end
```

} Shell
command

"ln -s" is used to link in a file from another location
"<" is used to inject a file from another location

Ready to run TSUNAMI-IP!

TSUNAMI-IP HTML output



Extended uncertainty edit for application shows likely sources of bias

General Information

Messages

Input Data

Results

scale

TSUNAMI-IP - Extended Uncertainty Assessment
versa-pac - 1 run

scale

Application #1
application

the standard deviation of keff (% dk/k) is: 6.771E-01 ± 5.559E-03 percent

contributions to uncertainty in keff (% dk/k) by individual energy covariance matrices:

Values colored Blue represent default covariance data

Values colored RoyalBlue represent default covariance data used to correct zeros or large values in some groups

Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
⁵⁶ Fe n,gamma	⁵⁶ Fe n,gamma	4.0022E-01 ± 6.3462E-05
²³⁵ U nubar	²³⁵ U nubar	3.8051E-01 ± 3.8810E-05
¹ H n,gamma	¹ H n,gamma	2.6147E-01 ± 8.3909E-06
²³⁵ U n,gamma	²³⁵ U n,gamma	1.5296E-01 ± 5.5957E-06
²³⁵ U fission	²³⁵ U fission	1.5031E-01 ± 1.5267E-05
²³⁵ U fission	²³⁵ U n,gamma	1.3527E-01 ± 6.7802E-06
²³⁵ U chi	²³⁵ U chi	1.2754E-01 ± 5.5580E-03
⁵⁴ Fe n,gamma	⁵⁴ Fe n,gamma	2.9049E-02 ± 3.9156E-07
²³⁸ U n,gamma	²³⁸ U n,gamma	2.7836E-02 ± 3.9592E-07
¹ H elastic	¹ H elastic	2.7654E-02 ± 5.2962E-06

Applications

Application #1
application

Integral index values – All c_k values are here

General Information

Messages

Input Data

Results

- Global Integral Indices
 - Integral Index Values
 - Integral Indices Plot
 - Integral Indices Summary
 - Integral Indices Summary Plot
 - c_k Summary
- Nuclide-Reaction Specific Integral Indices
 - Extended c_k Edit
- Penalty and Uncertainty Assessment
 - Extended Uncertainty Assessment

TSUNAMI-IP - Integral Index Values
versa-pac - 1 run

Integral Indices for All Experiments in Relation to All Applications

Values colored Blue exceed cutoff value

Values colored Red are maximum for each application

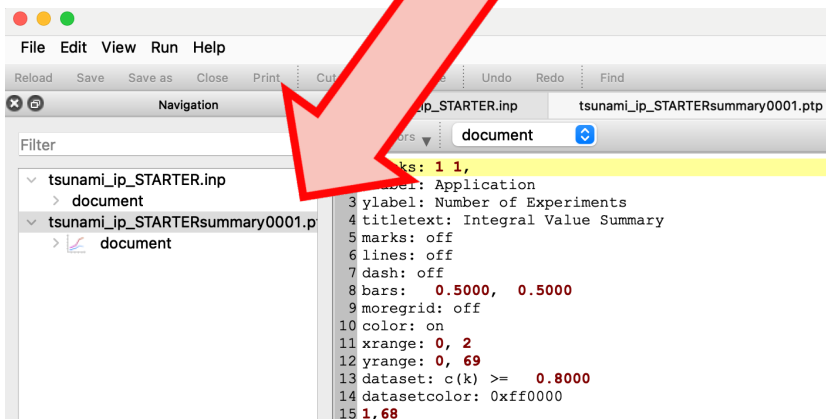
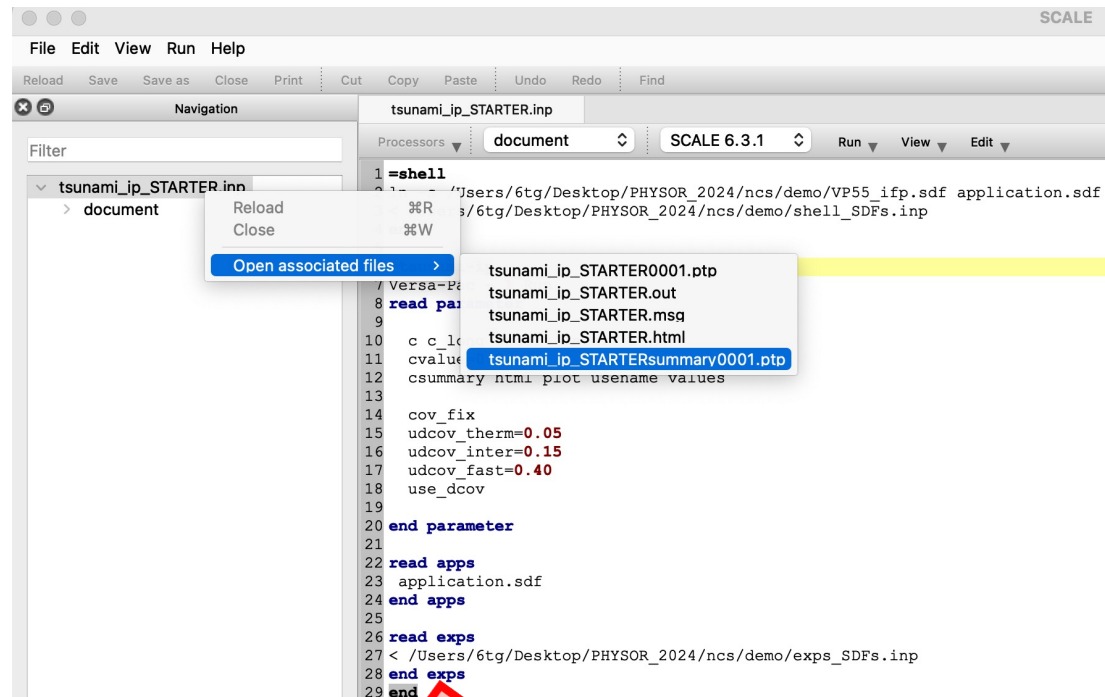
Application #1 application

NUMBER	EXPERIMENT	Type	Format	Value	Xsec Uncert	$c_k \uparrow$
346	LEU-COMP-THERM-028-017_KENO_ENDF-B-VII.0---238-Group_SENS	keff	Relative	9.9699E-1 ± 2.3700E-4	6.00984E-1 ± 2.6923E-5 % dk/k	0.9370 ± 0.0114
347	LEU-COMP-THERM-028-018_KENO_ENDF-B-VII.0---238-Group_SENS	keff	Relative	9.9765E-1 ± 2.2500E-4	6.21327E-1 ± 2.9682E-5 % dk/k	0.9277 ± 0.0135
345	LEU-COMP-THERM-028-016_KENO_ENDF-B-VII.0---238-Group_SENS	keff	Relative	9.9681E-1 ± 2.2700E-4	6.57620E-1 ± 3.4737E-5 % dk/k	0.9081 ± 0.0166
161	IEU-COMP-THERM-002-003	keff	Relative	1.0049E+0 ± 9.9000E-5	6.69821E-1 ± 6.2990E-5 % dk/k	0.9004 ± 0.0219
348	LEU-COMP-THERM-028-019_KENO_ENDF-B-VII.0---238-Group_SENS	keff	Relative	9.9650E-1 ± 2.4100E-4	6.59643E-1 ± 3.4501E-5 % dk/k	0.8969 ± 0.0158
344	LEU-COMP-THERM-028-015_KENO_ENDF-B-VII.0---238-Group_SENS	keff	Relative	9.9679E-1 ± 2.3300E-4	6.84005E-1 ± 3.8165E-5 % dk/k	0.8959 ± 0.0177
163	IEU-COMP-THERM-002-005	keff	Relative	9.9960E-1 ± 1.0000E-4	6.79182E-1 ± 6.5324E-5 % dk/k	0.8946 ± 0.0224
341	LEU-COMP-THERM-028-012_KENO_ENDF-B-VII.0---238-Group_SENS	keff	Relative	9.9483E-1 ± 2.4600E-4	6.16937E-1 ± 3.5237E-5 % dk/k	0.8898 ± 0.0144
349	LEU-COMP-THERM-028-020_KENO_ENDF-B-VII.0---238-Group_SENS	keff	Relative	9.9415E-1 ± 2.3500E-4	6.53579E-1 ± 2.9706E-5 % dk/k	0.8813 ± 0.0132
162	IEU-COMP-THERM-002-004	keff	Relative	1.0019E+0 ± 1.0000E-4	6.79155E-1 ± 5.7295E-5 % dk/k	0.8807 ± 0.0229
164	IEU-COMP-THERM-002-006	keff	Relative	9.9602E-1 ± 1.0000E-4	6.90410E-1 ± 6.1190E-5 % dk/k	0.8736 ± 0.0236
448	LEU-COMP-THERM-090-007_KENO_ENDF-B-VII.0---238-Group_SENS	keff	Relative	1.0002E+0 ± 3.7300E-4	7.24110E-1 ± 2.1195E-5 % dk/k	0.8647 ± 0.0170
447	LEU-COMP-THERM-090-006_KENO_ENDF-B-VII.0---238-Group_SENS	keff	Relative	9.9949E-1 ± 3.4700E-4	7.21516E-1 ± 1.9766E-5 % dk/k	0.8637 ± 0.0167
443	LEU-COMP-THERM-090-002_KENO_ENDF-B-VII.0---238-Group_SENS	keff	Relative	1.0005E+0 ± 3.6500E-4	7.29391E-1 ± 2.1011E-5 % dk/k	0.8626 ± 0.0170

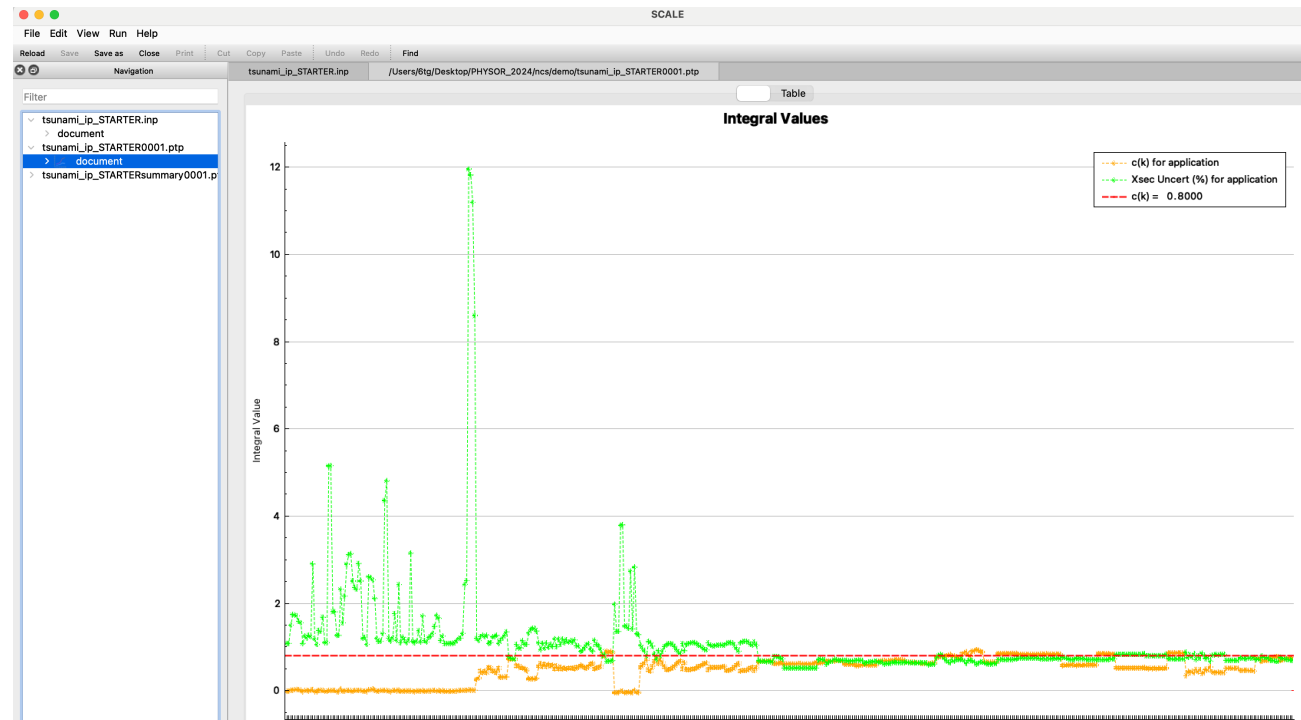
Applications

- Application #1 application

Plot of c_k values and uncertainties



Double click!



On your own

- Examine similarity of additional experiments to the application
 - c_k values
 - Extended c_k values
 - Fulcrum sensitivity plots

Similarity assessment for a molten salt reactor

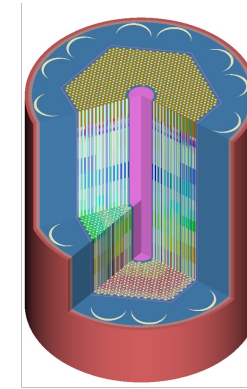
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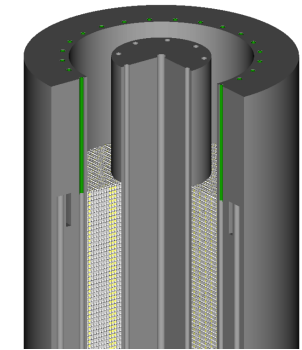
U.S. DEPARTMENT OF
ENERGY

Similarity assessments for advanced reactors

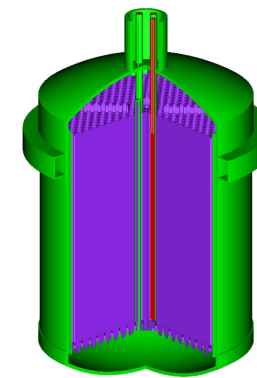
- Beyond criticality of transportation packages, similarity assessments for reactors can be of value:
 - Identify existing operation experience of similar systems
 - Adopt understanding of neutronics behavior
 - Design experiments with high similarity to target full scale design
 - Especially relevant for gaps in operation experience
 - Confirm adequateness of surrogate models, for example, to support:
 - Nuclear data assessments
 - Calculation of quantities such as system-average inventory generation
 - Method development



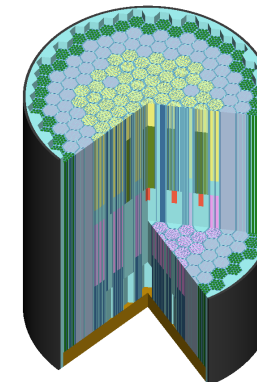
INL Design A
(Heat pipe reactor)



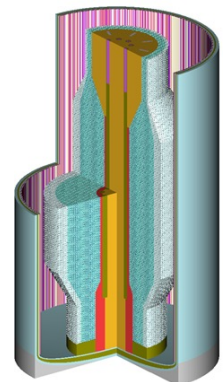
PBMR-400
(High temperature gas-cooled reactor)



MSRE (Molten salt reactor)



ABTR (Sodium-cooled fast reactor)



UCB Mark 1 (Fluoride salt-cooled high temperature reactor)

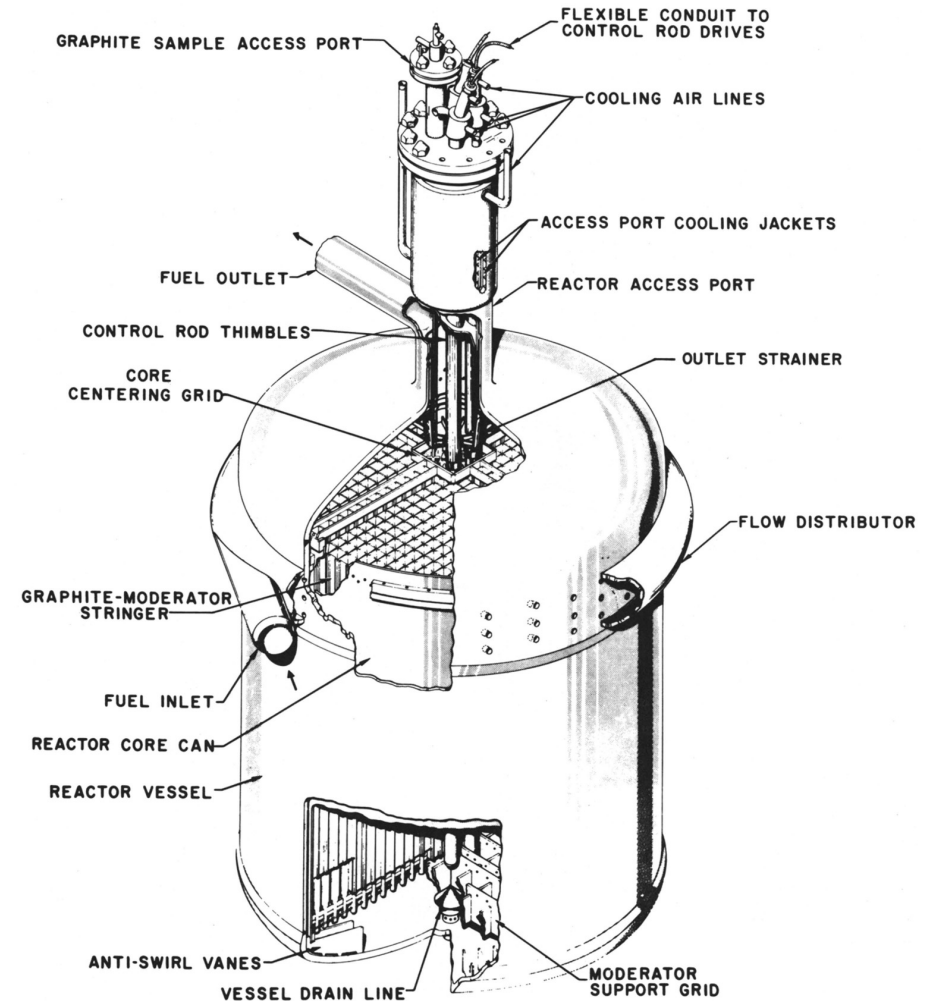
SCALE non-LWR models and citations:
<https://code.ornl.gov/scale/analysis/non-lwr-models-vol3>

Validation with SCALE: similarity assessment for a MSR

Molten Salt Reactor Experiment (MSRE)

- First large-scale, long-term, high-temperature experiment performed using a fluid fuel salt, graphite moderator, and new nickel-based alloys in a reactor environment
- Operated from 1965 to 1969 at ORNL, first with ^{235}U enriched fuel, later with ^{233}U fuel
- Initial critical experiment recently included in the OECD/NEA International Handbook of Reactor Physics Experiments*
- ORNL technical reports discuss design and operation

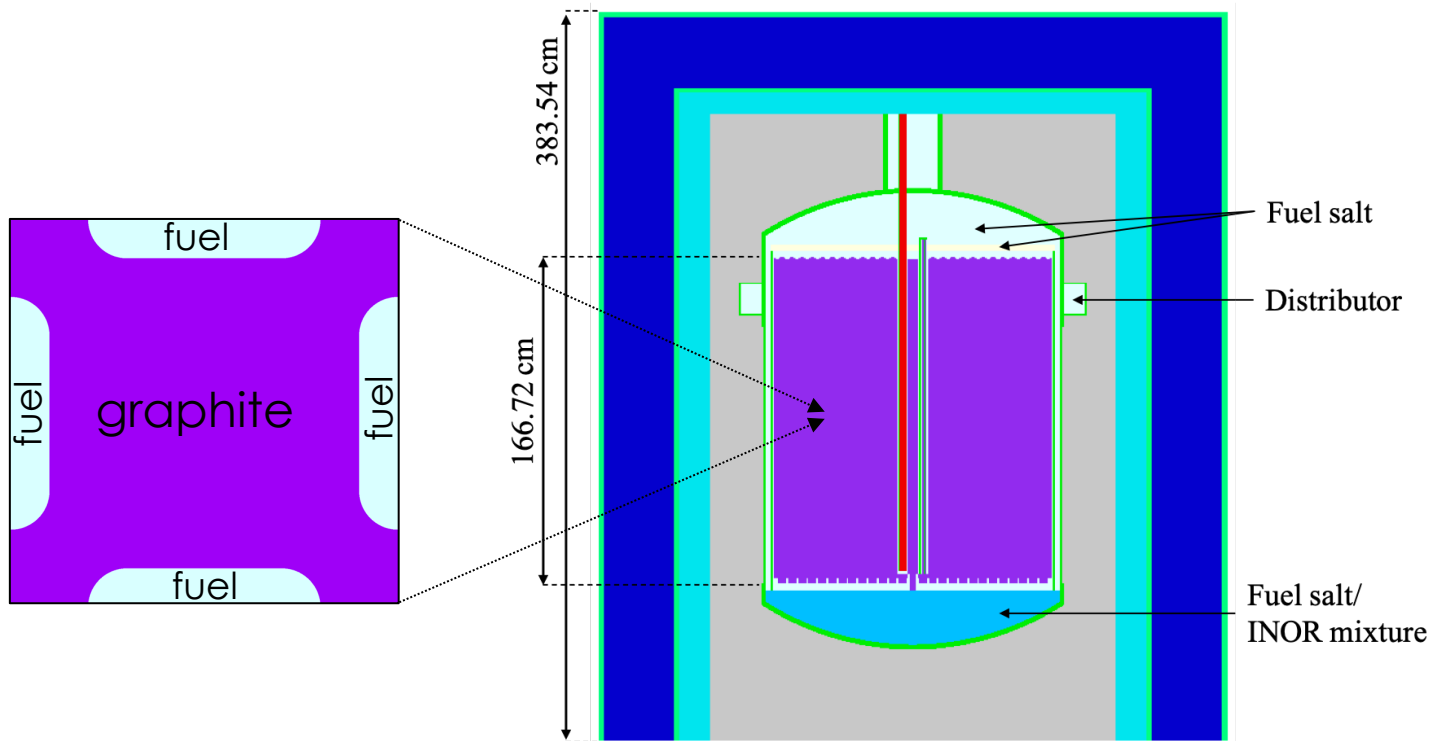
Description	Value
Power	10 MWth (initial criticality) / 8 MWth (operation)
Fuel/coolant	$\text{LiF-BeF}_2\text{-ZrF}_2\text{-UF}_2$
Enrichment	34.5 wt.% ^{235}U
Moderator	Graphite
Structure	Nickel-based alloys



MSRE reactor vessel*

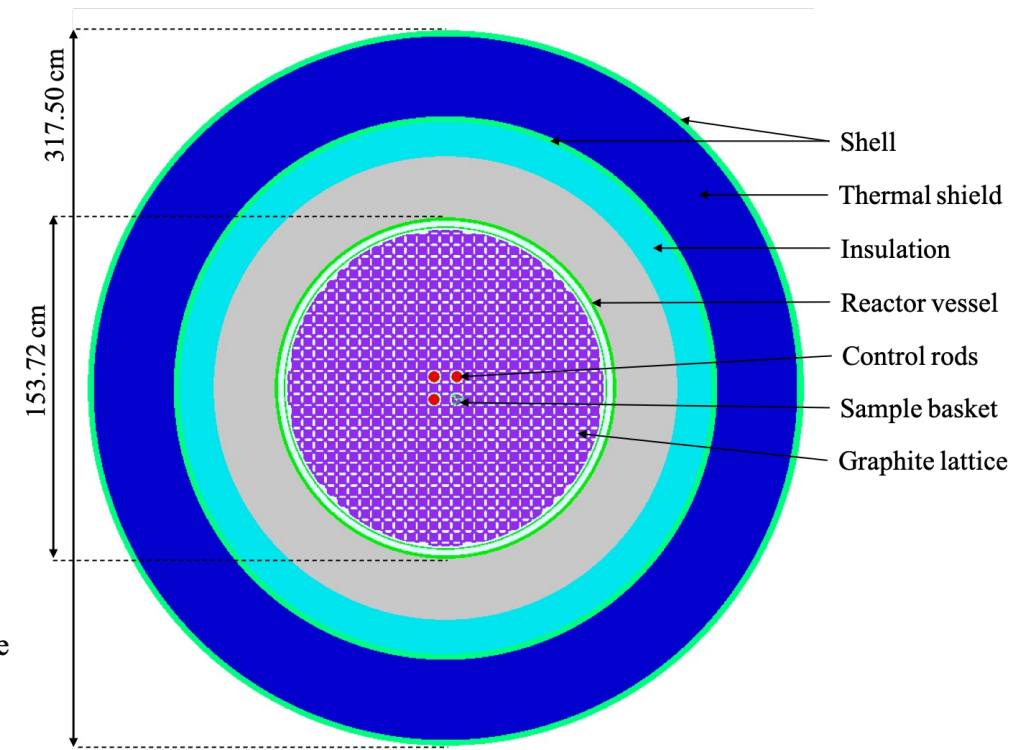
SCALE MSRE full core model

- SCALE core model developed based on zero-power first critical experiment with ^{235}U from the OECD/NEA International Handbook of Reactor Physics Experiments*



**Cross section of
graphite stringer**

YZ-cut through SCALE 3D model



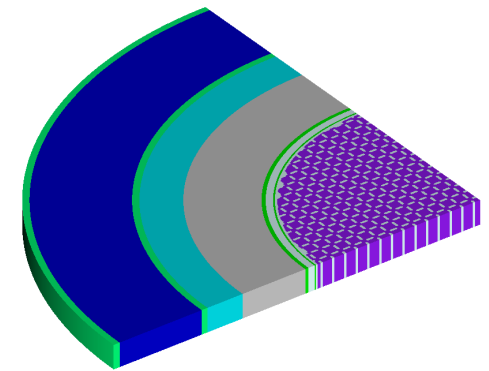
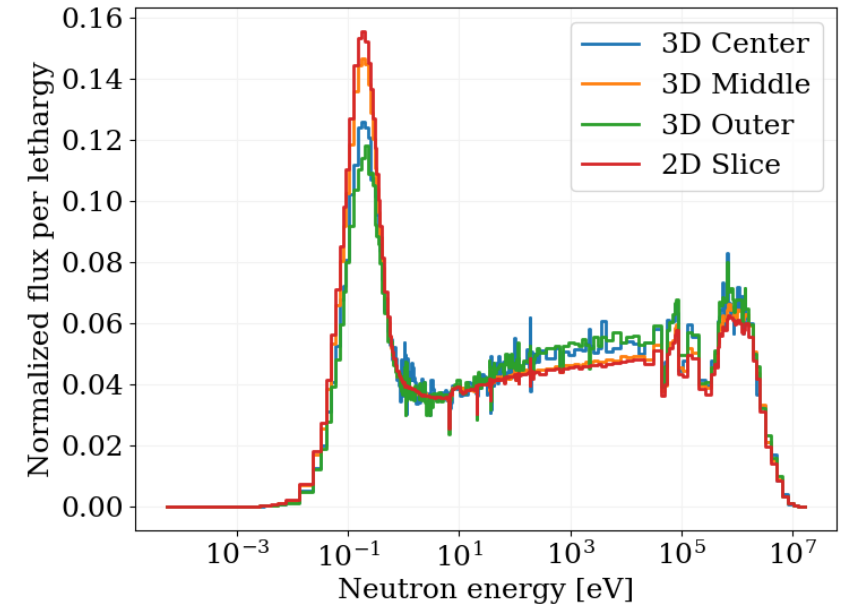
XY-cut through SCALE 3D model

Workshop: Similarity assessment for MSRE

1. Create a TSUNAMI input by using the provided neutron transport model on an axial slice through the MSRE core, and generate an SDF file
 - a) Sequence “=tsunami-3d-k6-shift” (or “tsunami-3d-k6” in SCALE 6.2)
 - b) Parameters “cet=2”, “cfp=5”
2. Create a TSUNAMI-IP input to calculate c_k of the MSRE with the VALID experiments
3. Answer the questions:
 - a) Why do you think the use of an axial slice model is justified for the current analysis? How could you obtain confidence in this decision?
 - b) Which VALID experiments show the greatest similarity with MSRE?
 - c) What can you conclude from this analysis on the availability of validation data for this kind of reactor?

Solution (1/3)

- Question: Why do you think the use of an axial slice model is justified for the current analysis? How could you obtain confidence in this decision?
 - The slice model provides representative spectral conditions through radial leakage and a representative moderator-to-fuel ratio
 - The flux spectra between the axial slice and the full 3D model axial midline are similar
 - **Better than a mere flux comparison is the analysis of similarity coefficients E and C_k :**
 - $E = 0.9966 \pm 0.0033$ (E is the cosine of the angle between the two sensitivity vectors for the analyzed systems)
 - $C_k = 0.9836 \pm 0.0137$ (C_k is a measure of the similarity of the systems in terms of related uncertainty)
 - Impact: For a similarity assessment with experiments and for a quick analysis of the impact of nuclear data uncertainties, the axial slice model provides an adequate surrogate model



SCALE "2D" slice model

Solution (2/3)

- Question: Which VALID experiments show the greatest similarity with MSRE?
 - None of the experiments show a c_k greater than 0.9
 - Greatest obtained $c_k = 0.668 \pm 0.019$
 - Experiments with largest c_k : LCT-10, LCT-17, LST-2 show c_k between 0.65-0.67
 - LCT: low enriched, compact, thermal spectrum
 - LST: low enriched, solution, thermal spectrum

EXPERIMENT NUMBER	EXPERIMENT	c_k VALUE ↑
266	leu-comp-therm-010-006	0.6680 ± 0.0185
265	leu-comp-therm-010-005	0.6665 ± 0.0164
267	leu-comp-therm-010-007	0.6600 ± 0.0206
303	leu-comp-therm-017-013	0.6570 ± 0.0149
411	leu-sol-therm-002-002	0.6563 ± 0.0234
268	leu-comp-therm-010-008	0.6563 ± 0.0211
297	leu-comp-therm-017-007	0.6561 ± 0.0141
302	leu-comp-therm-017-012	0.6560 ± 0.0146
296	leu-comp-therm-017-006	0.6560 ± 0.0138
295	leu-comp-therm-017-005	0.6555 ± 0.0135
272	leu-comp-therm-010-012	0.6553 ± 0.0205
304	leu-comp-therm-017-014	0.6545 ± 0.0150
301	leu-comp-therm-017-011	0.6542 ± 0.0143
294	leu-comp-therm-017-004	0.6541 ± 0.0123
298	leu-comp-therm-017-008	0.6539 ± 0.0151
412	leu-sol-therm-002-003	0.6538 ± 0.0224
292	leu-comp-therm-017-002	0.6528 ± 0.0159

Solution (3/3)

- Question: What can you conclude from this analysis on the availability of validation data for this kind of reactor?
 - Validation basis for molten salt fueled systems is very thin
 - Including MSRE in database of critical benchmark experiments would contribute to closing validation gap*
 - More experiments are needed to expand validation base for MSR reactivity calculations

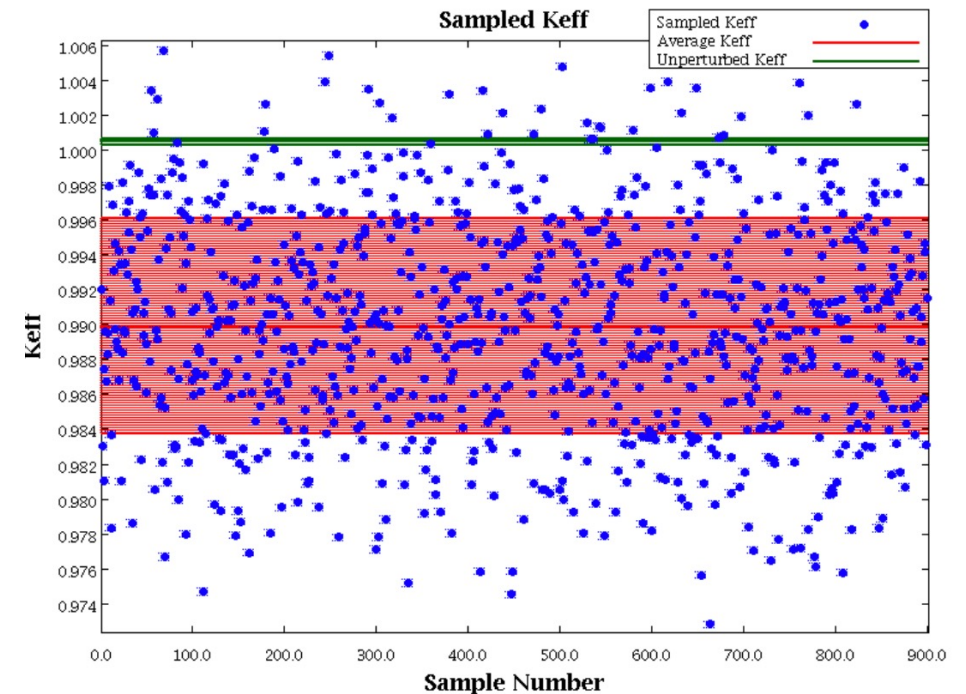
Emerging capabilities in Sampler

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Sampler: Statistical Uncertainty Analysis with SCALE

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 parameter uncertainty
 - geometry
 - composition
 - and anything else that appears in an input file



Sources of Sampler Nuclear Data Uncertainty

- Cross section covariances:

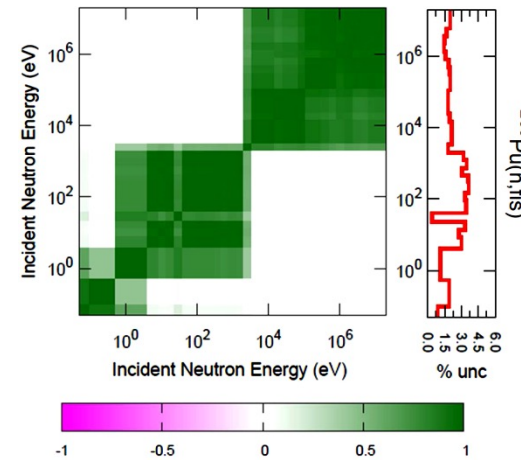
SCALE ENDF/B-VII.1,VIII.0 supplemented by other sources

- Fission product yield:

SCALE fission Standard deviations from ENDF/B-VII; correlations generated by combining independent and cumulative yields

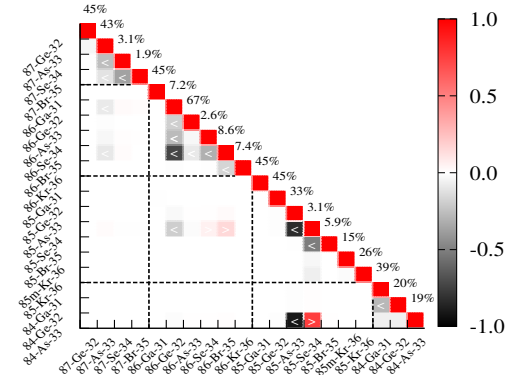
- Decay data:

ENDF-VII.1 modified to include branching correlations due to constraint that branch sum=1.0

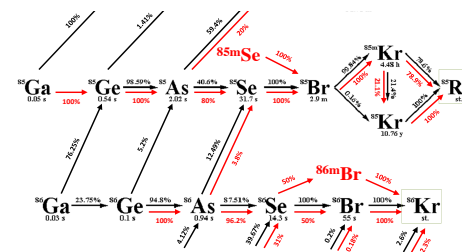


Pu^{239} fission covariance

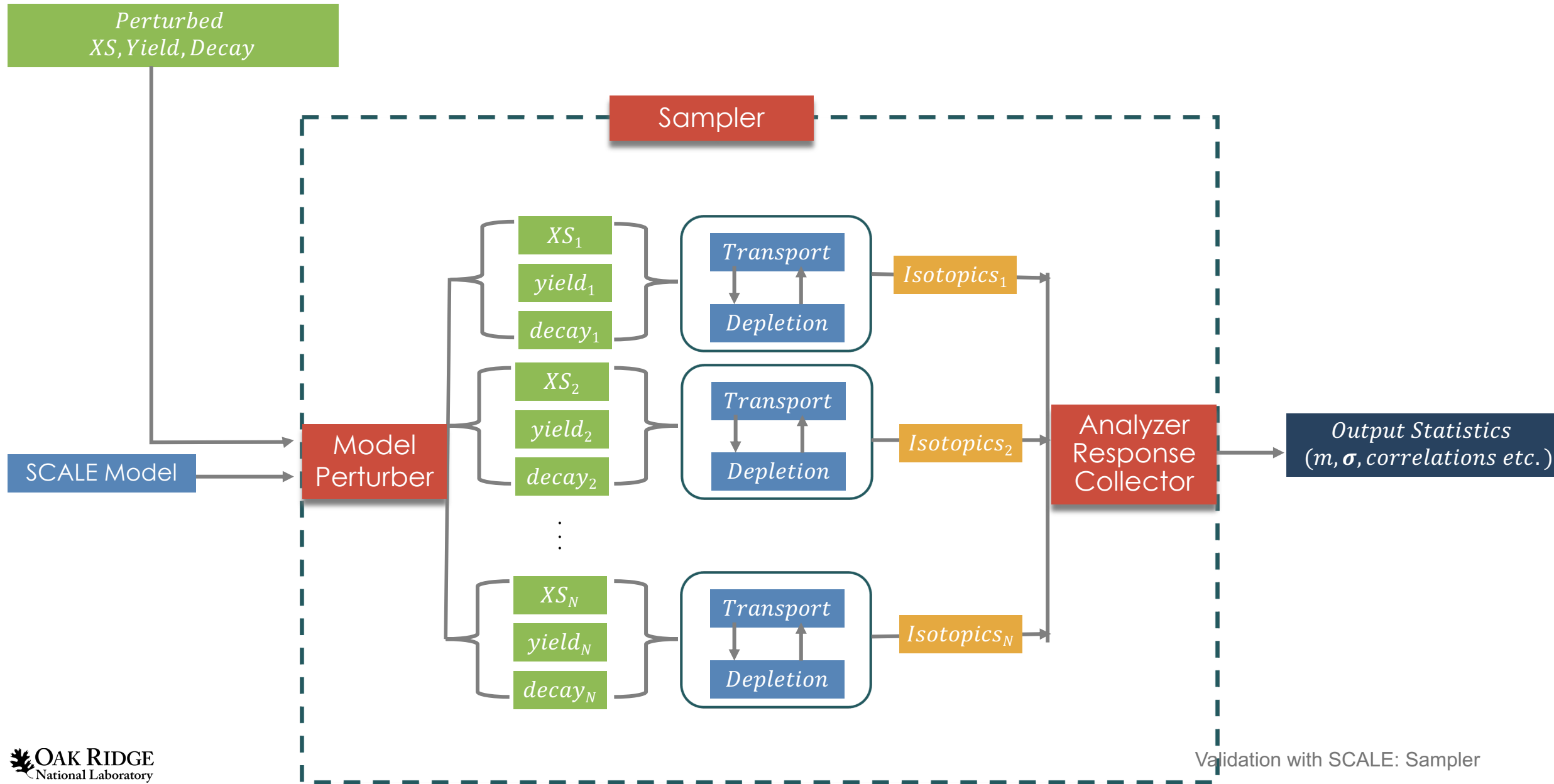
Fission yield covariance



Mass A=85-87 yields



UQ Calculations with Coupled Transport/Depletion



Variables: Example Input

- Placeholders are variable IDs inside #{}, e.g., #{NORMAL}
- **Must have perturb_geometry=yes**
- It is defined inside the case it applies or outside of all cases with a cases card
- Using *shell* as a sequence is an easy way to test the sampling process

```
=sampler
  read parameters
    n_samples = 5
    perturb_bondarenko = no
    perturb_pointwise = no
    perturb_xs = no
    perturb_geometry = yes
    force_run = yes
  end parameters

  read case[c1]
    sequence=shell
    echo NORMAL= #{NORMAL}
    echo UNIFORM= #{UNIFORM}
  end sequence
end case

read variable[NORMAL]
  distribution=normal
  minimum=-2 value=-1 maximum=0 stddev=2
  cases=c1 end
end variable

read variable[UNIFORM]
  distribution=uniform
  minimum=-2 value=-1 maximum=0
  cases=c1 end
end variable
end
```

Responses

- Collects quantities of interest from the perturbed SCALE cases

```
read response[NAME]  
  type=TYPE  
  [type-specific-params]  
end variable
```

- TYPE
 - **grep** – general expression from the text output file
 - **origen_nuclides** – concentrations from the F71 file
 - **stdcmp** – standard composition files
 - **opus_plt** – data from an OPUS-generated PLT file
 - **triton** – TRITON homogenized cross-sections (xfile016)
 - **variables** – the geometry perturbation sampled values

Post-processing

- Analysis Block (New in SCALE 6.3)

- Allows users to analyze relationship between selected user defined case dependent responses
 - any response type at any depletion step/index
 - target vs. sources one to many, many to one, many to many

- **Current analysis types :**

- pearson_corr (c_k)
- covariances
- correlation_matrix
- covariance_matrix
- r2 (sensitivity index)

read analysis [analysis_name]

type = analysis_type

target = tresponse1, tresponse2 ... end

sources = sresponse1, sresponse2 ... end

end analysis

Post-processing

- Analysis Block Types

- pearson_corr

- pearson correlation coefficient (similarity index) calculation between each responses

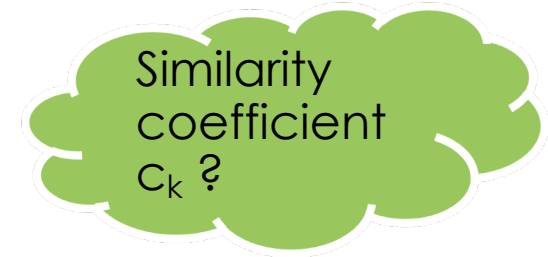
```
read analysis [do_they_have_same_sensitivity]
```

```
type = pearson_corr
```

```
targets = mycase1:app.u-238(0)
```

```
sources = mycase2:exp.u-235(last) mycase2:ex.pu-239(last) end
```

```
end analysis
```



- cor(mycase1:app.u-238(0), mycase2:exp.u-235(last))
cor(mycase1:app.u-238(0), mycase2:ex.pu-239(last))

Question 1:

- If we have a BWR pin critical experiment, can we use it for PWR pin validation? (Is a BWR pin similar to a PWR pin with respect to nuclear data uncertainties ?)
- TSUNAMI-1D vs Sampler c_k (*pwrpin-tsunami.inp*, *bwrpin-tsunami.inp*, *tsunami-ip_bwr-pwr.inp*)

```
=tsunami-1d
pwr-pincell
v7-56
read comp
uo2 1 0.95 900 92235 4.0 92238 96.0 end
zirc2 2 1 595 end
h2o 3 den=0.7042 1 600 end
end comp
read celldata
  multiregion cylindrical right_bdy=white end
1 0.4180
2 0.4796
3 0.711 end zone
end celldata
read geometry
cylindrical white reflected end
1 0.4180
2 0.4796
3 0.711
end geometry
read sams
prtmp
end sams
end
```

```
=tsunami-1d
bwr-pincell
v7-56
read comp
uo2 1 0.95 900 92235 4.0 92238 96.0 end
zirc2 2 1 600 end
h2o 3 den=0.46 1 600 end
end comp
read celldata
  multiregion cylindrical right_bdy=white end
1 0.4470
2 0.5131
3 0.7315 end zone
end celldata
read geometry
cylindrical white reflected end
1 0.4470
2 0.5131
3 0.7315
end geometry
read sams
prtmp
end sams
end
```

```
=tsunami-ip
TSUNAMI-IP input
read parameter
c c_long uncert uncert_long csummary html
plot username values
cvalue=0.7 cov_fix use_dcov penalty penlong
lg uslstats uslsummary
end parameter
read exps
/Users/u2m/Workfolder/physor/bwrpin-tsunami.sdf
end exps
read apps
/Users/u2m/Workfolder/physor/pwrpin-tsunami.sdf
end apps
end
```

What is the c_k ?

Question 1:

- If we have a BWR pin critical experiment, can we use it for a PWR pin validation? (Is a BWR pin similar to a PWR pin with respect to its response to nuclear data uncertainties ?)
- Tsunami-1D vs Sampler c_k (*pwrpin-xsdrn.inp*, *bwrpin-xsdrn.inp*, *sampler_bwr-pwr.inp*)

```
=csas1
pwr-pincell
v7-56
read comp
uo2 1 0.95 900 92235 4.0 92238 96.0 end
zirc2 2 1 600 end
h2o 3 den=0.7042 1 600 end
end comp
read celldata
  multiregion cylindrical right_bdy=white end
1 0.4180
2 0.4796
3 0.711 end zone
end celldata
end
```

```
=csas1
bwr-pincell
v7-56
read comp
uo2 1 0.95 900 92235 4.0 92238 96.0 end
zirc2 2 1 600 end
h2o 3 den=0.46 1 600 end
end comp
read celldata
  multiregion cylindrical right_bdy=white end
1 0.4470
2 0.5131
3 0.7315 end zone
end celldata
end
```

```
=sampler
read parameters
n_samples=100
perturb_xs=yes
perturb_geometry=no
library="v7-56"
run_cases=yes
end parameters

read case [bwr]
import="/Users/u2m/Workfolder/physor/bwrpin-xsdrn.inp"
end case

read case [pwr]
import="/Users/u2m/Workfolder/physor/pwrpin-xsdrn.inp"
end case

read response[kinf]
  type = grep
  regexp = ":xsdrn.lambda:"
end response

read analysis[k_ck]
  type = pearson_corr
  targets = pwr:kinf end
  sources = bwr:kinf end
end analysis

end
```

What is c_k ?

```
response_table.analysis.k_ck.csv
response_table.dynamic.1.avg.csv
response_table.dynamic.1.stddev.csv
response_table.dynamic.1.val.csv
response_table.dynamic.2.avg.csv
response_table.dynamic.2.stddev.csv
response_table.dynamic.2.val.csv
```

Question 2:

- If TSUNAMI and Sampler give the same answer, why do we need Sampler?
- We can't answer the following questions with TSUNAMI
 - a. Can you validate your code's BWR fuel ^{239}Pu prediction using a PWR fuel experiment ?
 - b. Is the similarity we observed between BWR and PWR fuel preserved for depleted fuel?
 - c. Do geometry changes in your BWR fuel shipping cask design effect your validation ?
- Any study that requires investigation responses other than k-eff, depletion or non-linear responses, require capabilities beyond TSUNAMI methodology.
- We will be using Polaris sequence for faster depletion.

Question 2 a-b:

- Sampler depletion similarity study: bwr-polaris.inp, pwr-polaris.inp, sampler_pwr-bwr-depl.inp

```
=polaris
lib "xn56v7.1"
sys BWR
geom FuelNode1 : ASSM 1 1.295
basis ALL=no FUEL.1=yes
shield ALL=N FUEL=P
deplete FUEL=YES
%opt CRITSPEC Method="P1"

mat CAN.1 : ZIRC4
mat CLAD.1 : ZIRC4

mat FUEL.1 : c_uox4
comp c_uox4 : UOX 4.0 refdens=10.4

pin 1 : 0.4470 0.5131
      : FUEL.1 CLAD.1
pinmap
1
state ALL : temp=560
      FUEL : temp=900
      COOL : temp=600 dens=0.46
power 25
dt 60 60 60 60 60
opt CRITSPEC Mode='none'
end
```

```
=polaris
lib "xn56v7.1"
sys PWR
geom FuelNode1 : ASSM 1 1.26
basis ALL=no FUEL.1=yes
shield ALL=N FUEL=P
deplete FUEL=YES
%opt CRITSPEC Method="P1"

mat CAN.1 : ZIRC4
mat CLAD.1 : ZIRC4

mat FUEL.1 : c_uox4
comp c_uox4 : UOX 4.0 refdens=10.1

pin 1 : 0.4180 0.4796
      : FUEL.1 CLAD.1
pinmap
1
state ALL : temp=600
      FUEL : temp=900
      COOL : temp=600 boron= 600.0 dens=0.7042
power 25
dt 60 60 60 60 60
opt CRITSPEC Mode='none'
end
```

```
=sampler
read parameters
n_samples=100
perturb_xs=yes
perturb_geometry=no
library="v7-56"
run_cases=yes
end parameters

read case [bwr]
import="/Users/u2m/Workfolder/physor/bwr-polaris.inp"
end case

read case [pwr]
import="/Users/u2m/Workfolder/physor/pwr-polaris.inp"
end case

read response[kinf]
type = grep
regexp = "Transport:[[:space:]]k-eff[[:space:]]=[[:space:]]+:scale.number:"
regexp = ":scale.number:"
end response

read response [nuc]
type = origen_nuclides
nuclides = pu-239 end
mixture = 10
end response

read analysis[k_ck]
type = pearson_corr
targets = pwr:kinf(all) end
sources = bwr:kinf(all) end
end analysis

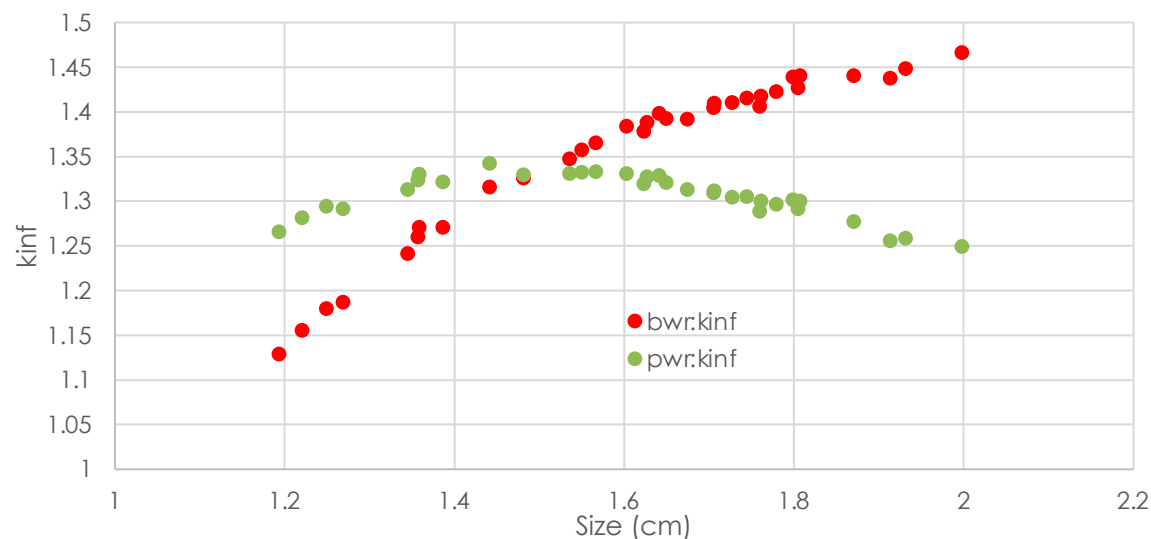
read analysis[Pu_ck]
type = pearson_corr
targets = pwr:nuc.pu239(all) end
sources = bwr:nuc.pu239(all) end
end analysis

end
```

How does c_k change with depletion ?

Question 2c:

- Sampler geometry and nuclear data similarity study: sampler-pwr-bwr-cask.inp



Does container size have any effect on similarity ?

```
=sampler
read parameters
n_samples=50
perturb_xs=yes
perturb_geometry=yes
library="xn56v7.1"
run_cases=yes
end parameters

'BWR case-----
read case [bwr]
sequence=polaris
lib "xn56v7.1"
sys BWR
geom FuelModel : ASSM 1 #{pitch}
mat FUEL.1 : c_uox4
comp c_uox4 : UOX 4.0 refdens=10.4
pin 1 : 0.4470 0.5131
        : FUEL.1 CLAD.1
state ALL : temp=560 FUEL : temp=900 COOL : temp=600 dens=0.46
opt CRITSPEC Mode='none'
end sequence
end case

'PWR case-----
read case [pwr]
sequence=polaris
lib "xn56v7.1"
sys PWR
geom FuelModel : ASSM 1 #{pitch}
mat FUEL.1 : c_uox4
comp c_uox4 : UOX 4.0 refdens=10.1
pin 1 : 0.4180 0.4796
        : FUEL.1 CLAD.1
state ALL : temp=600 FUEL : temp=900 COOL : temp=600 boron= 600.0 dens=0.7042
opt CRITSPEC Mode='none'
end sequence
end case

'Container radius -----
read variable[pitch]
distribution=uniform
minimum = 1.1
maximum = 2.0
cases=bwr pwr end
end variable

read response[pitch]
type = variables
data = pitch end
end response

'request Sampler to pick keff
read response[kinf]
type = grep
regexp = "Transport:[[:space:]]k-eff[[:space:]]=[[:space:]]+:scale.number:"
regexp = ":scale.number:"
end response

'request Sampler to analyze similarity
read analysis[k_ck]
type = pearson_corr
targets = pwr:kinf end
sources = bwr:kinf end
end analysis
end
```

Validation with SCALE: Sampler

Emerging capabilities in SCALE for HBU/non-LWR nuclide inventory and decay heat sensitivity and uncertainty analysis

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



U.S. DEPARTMENT OF
ENERGY

Goals

- Summarize current validation basis for nuclide inventory and decay heat
- Explore capabilities in SCALE that enable uncertainty quantification and sensitivity analysis for depletion problems – nuclide inventory and decay heat estimation - with
 - **Sampler**
 - **ORIGEN**
- Learn how to apply these capabilities to perform similarity assessments, determine uncertainties, and identify effect of nuclear data for nuclide inventory and decay heat estimation
- See SCALE's graphical user interface Fulcrum in action to explore various result files

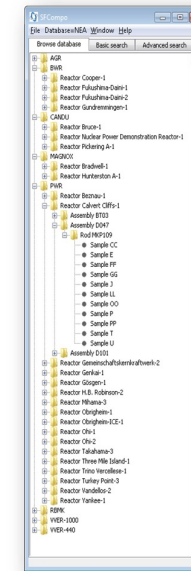
Validation + Similarity!

Validation basis for nuclide inventory and decay heat



Experimental data for nuclide inventory validation in LWRs

- **Destructive radiochemical assay (RCA) data of spent nuclear fuel in SCALE validation basis**
 - 129 PWR samples
 - 77 BWR samples
- **Public resources for validation data**
 - OECD/NEA Spent Fuel Composition Database SFCOMPO <https://www.oecd-nea.org/sfcompo/>
- **Commercial programs for validation data**
 - MALIBU international program (to be publicly released in 2024)
 - REGAL international program, gadolinia fuel (ongoing)
- **Ongoing US experimental programs**
 - at ORNL, jointly funded by DOE and NRC
 - 16 high-burnup PWR fuel samples: 9 completed measurements, 7 ongoing



Diverse information is provided!

Not only the initial nuclide composition of the sample, but detailed assembly and reactor operating conditions.

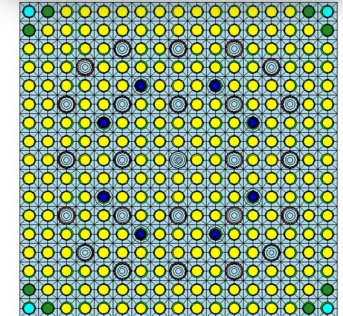
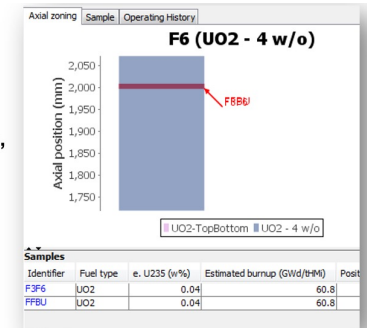
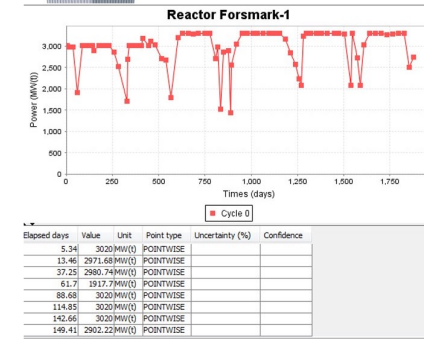
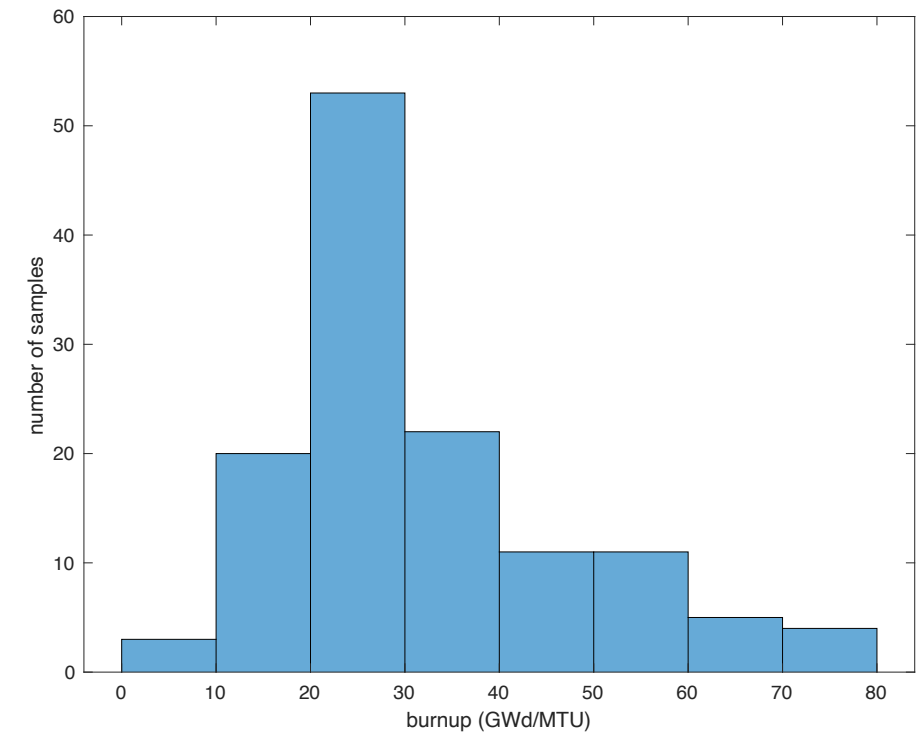
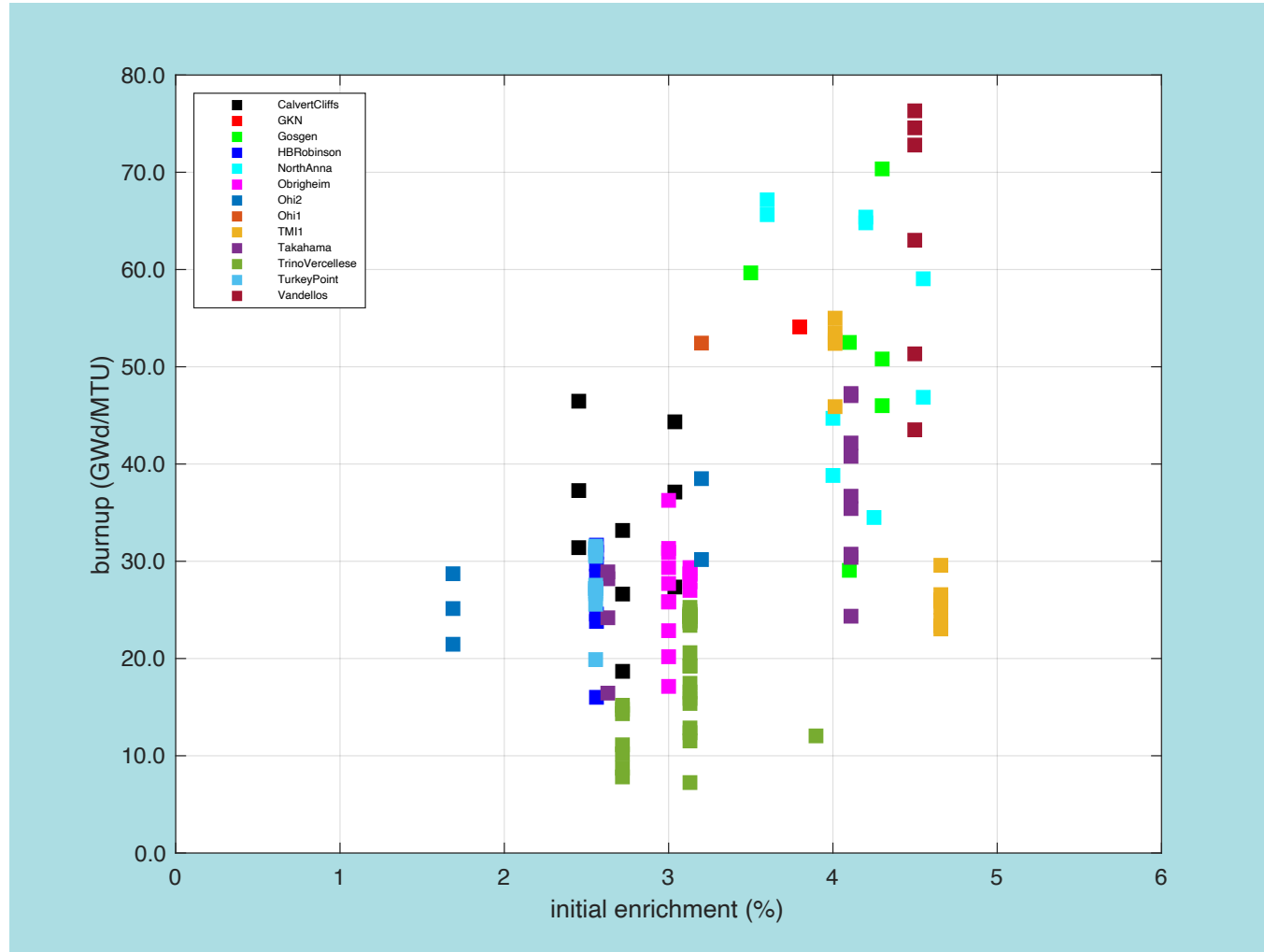


Illustration of SFCOMPO GUI features

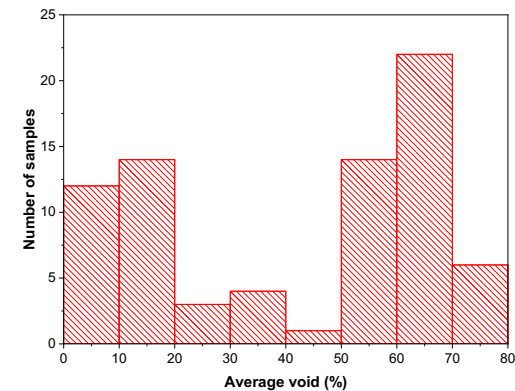
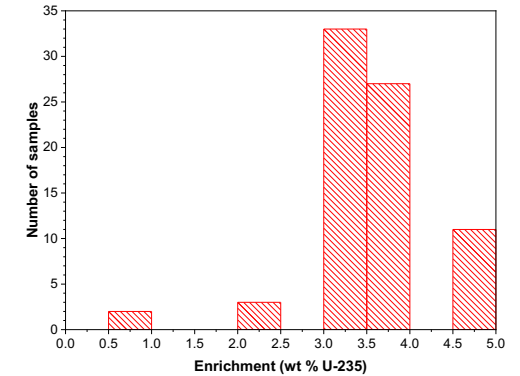
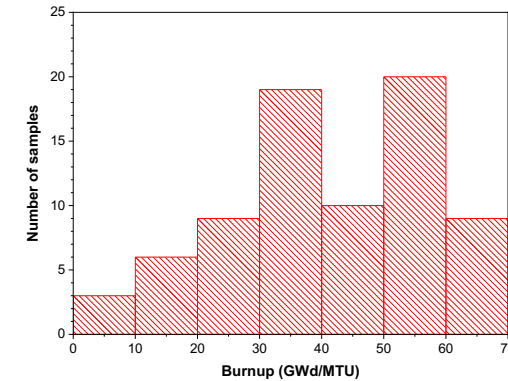
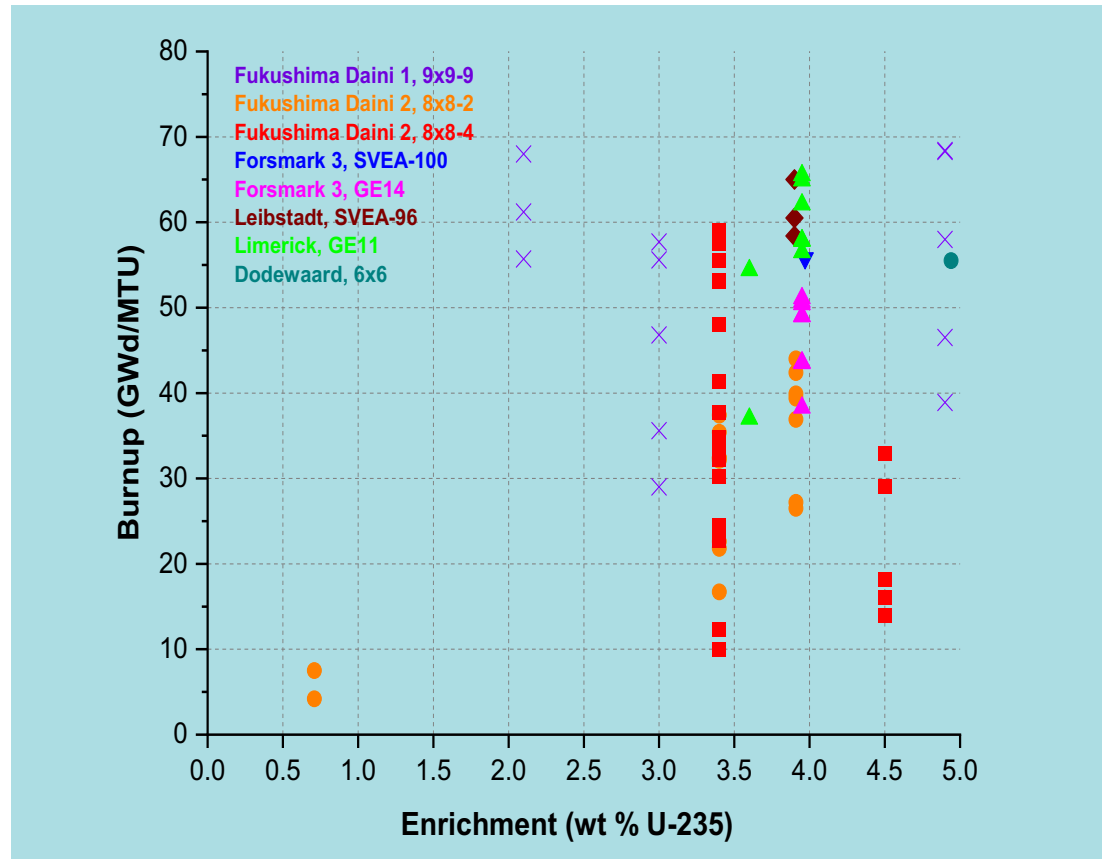
Characteristics of measured PWR spent fuel

burnup and enrichment coverage

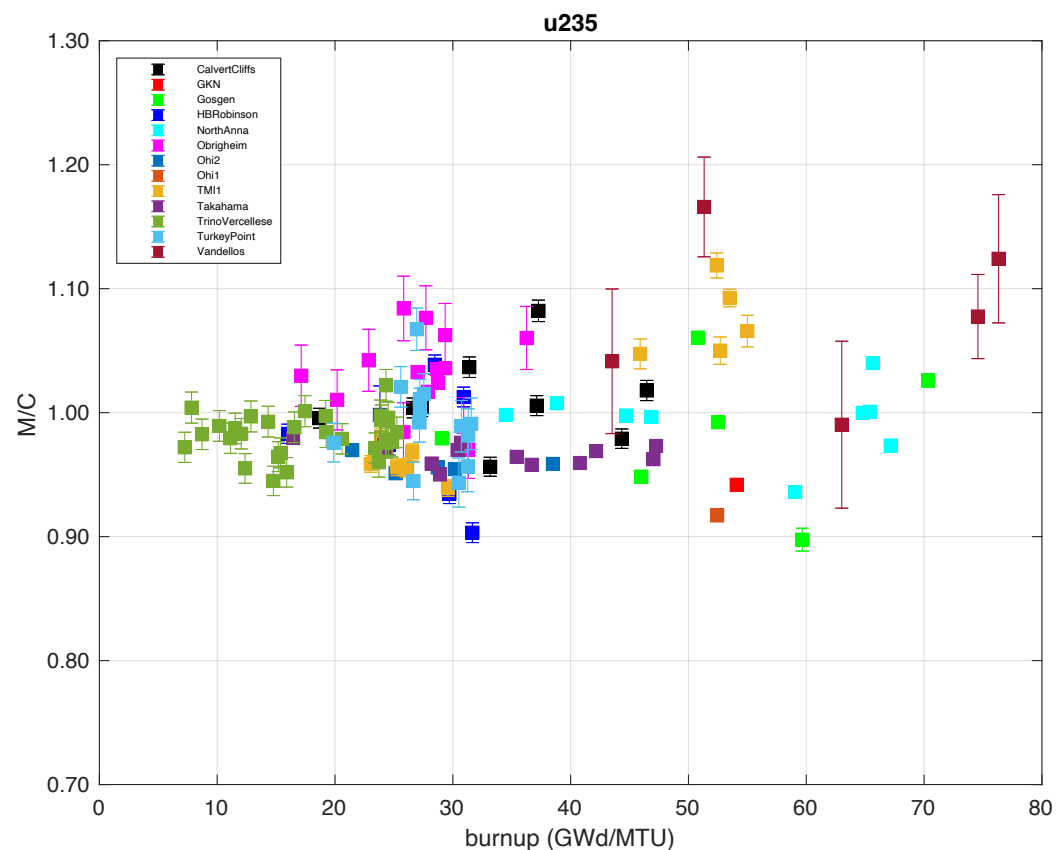


Characteristics of measured BWR spent fuel

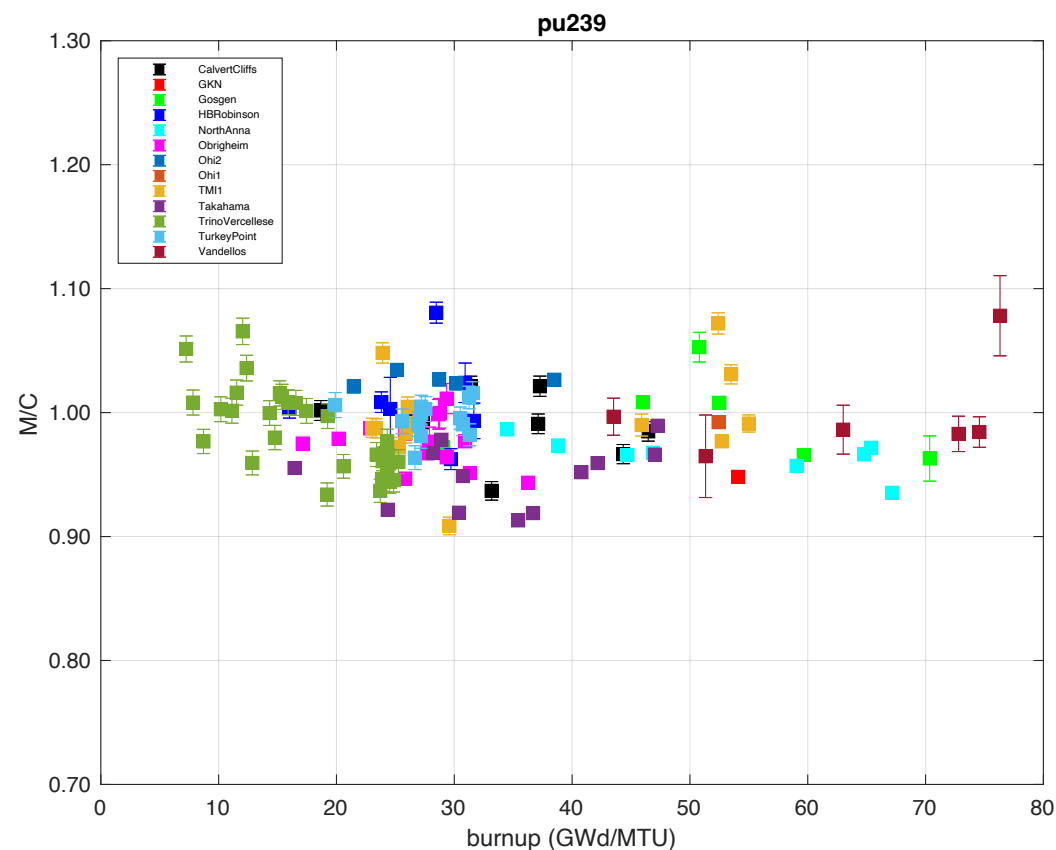
burnup, enrichment, and average void fraction coverage



Example of validation results for PWR fuel: ^{235}U and ^{239}Pu



M/C bias (bias uncertainty)
< 40 GWd/t 0.9883 (0.0383)
40 - 80 GWd/t 1.0121 (0.0829)



M/C bias (bias uncertainty)
< 40 GWd/t 0.9855 (0.0371)
40 - 80 GWd/t 0.9864 (0.0452)

measured-to-calculated concentration ratio (NUREG/CR-7303, 2023)

Experimental data for decay heat validation in LWRs

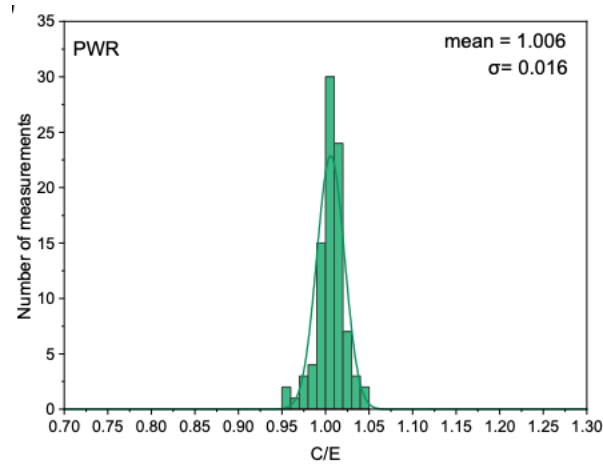
full assembly measurements

Reactor type	Reactor name	Assembly lattice	Burnup (GWd/MTU)	Cooling time (years)	Enrichment (% ²³⁵ U)	Measurement laboratory	No. of measured assemblies	No. of 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

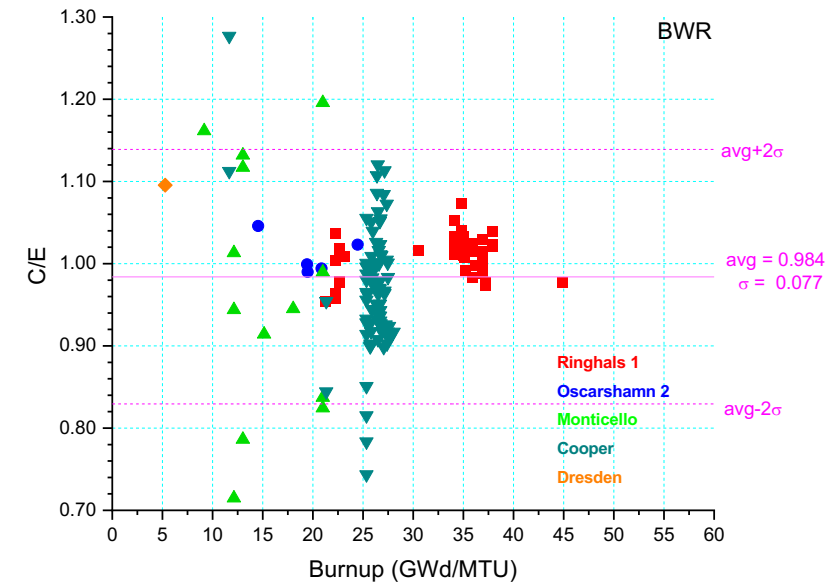
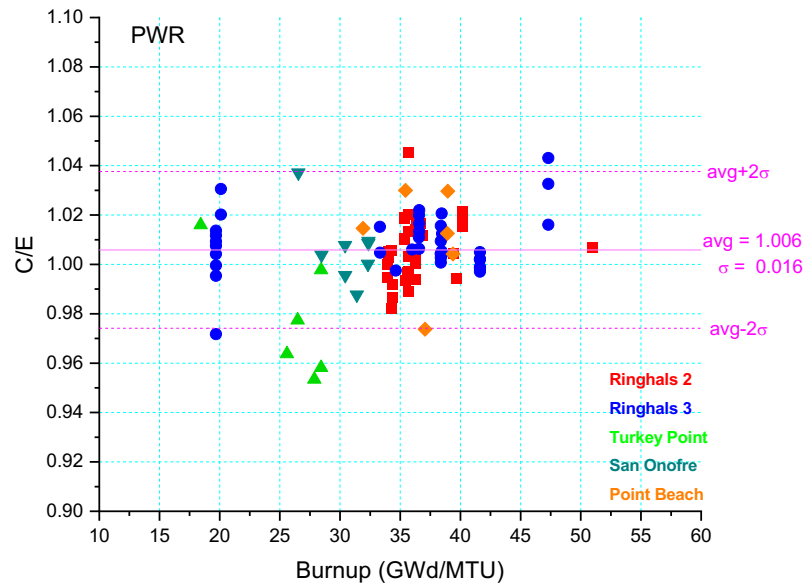
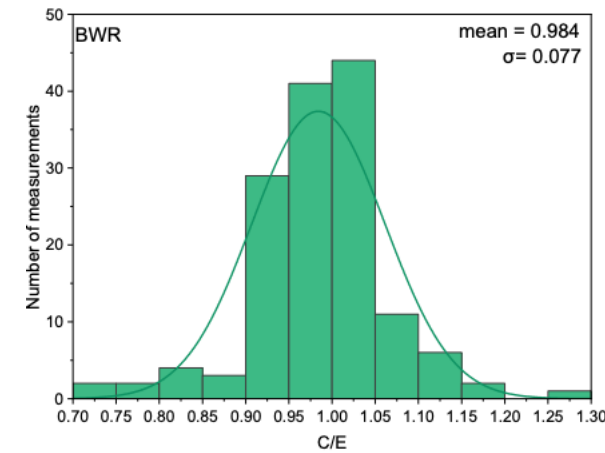
Table shows data as used in the [SCALE 6.2.4 validation report](#)

Decay heat calculation–experiment comparison vs. burnup

PWR



BWR



Source: [SCALE 6.2.4 validation report](#)

Validation data for HALEU/HBU nuclide inventory and decay heat are not available

- Nuclide inventory validation data available for LWR UO_2 spent fuel is limited to initial fuel enrichments $< 5.0\%$ and burnups $< 80 \text{ GWd/t}$
 - SFCOMPO, the world's largest resource of RCA experimental data for spent nuclear fuel, includes data for 750 samples selected from UOX or MOX fuel irradiated in 44 reactors, for more than 90 nuclides. However, no measurement data are included over 5% (UOX) and 80 GWd/t.
 - Potential data for validating, at least in part, depletion methods, are [available](#) from a series of experiments performed in a research reactor spectrum: at ATR (INL), for fuel qualification purposes. Included samples of: U-Mo at 19.8% enrichment; TRISO UOX compacts at 9.6%, 14%, and 19.8% enrichment.
- Decay heat validation data available for LWR UO_2 spent fuel is limited to assembly-average initial enrichments $< 4.0\%$ and burnups $< 51 \text{ GWd/t}$
 - Very few (high-quality) data available for cooling times < 5 years, relevant for validation of fission products contribution to decay heat.
 - No experimental data available for MOX fuel assemblies.

New sensitivity capability in ORIGEN



Implementation is based on Depletion Perturbation Theory (DPT)

- Sensitivity coefficient S can be mathematically obtained via DPT as :

$$S = \frac{\alpha_0}{R(\alpha_0)} \int_0^T dt N^*(t) \cdot \frac{\partial A}{\partial \alpha} \cdot N(t)$$

in SCALE 6.3

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

in SCALE 7.0

where

$$R = \int_0^{t_i} dt R(\sigma, N, \varphi_i, \varphi_i^*)$$

response

$$R(\alpha) = R(\alpha_0) + \left. \frac{\partial R}{\partial \alpha} \right|_{\alpha_0} (\alpha - \alpha_0) + \dots, \quad \text{sensitivity coefficient } S \text{ for a change in input parameter } \alpha \text{ in response } R$$

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

$$\frac{dN}{dt} = \bar{\mathbf{A}} \cdot \mathbf{N}(t) = (\bar{\boldsymbol{\lambda}} + \boldsymbol{\phi}(t)\bar{\boldsymbol{\sigma}}(t))\mathbf{N}(t) \quad \text{transmutation equation solved by ORIGEN}$$

Sensitivity coefficients in SCALE 6.3 (for nuclide response only)

Sensitivity coefficient: the relative change in response per change in a parameter α

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

1. **Total decay loss** sensitivity: α = change in a nuclide's total decay constant.
2. **Decay channel** sensitivity: α = change in specific decay channels (e.g., α -decay).
3. **Decay yield** sensitivity: α = change in a decay yield; for example, the fraction of γ -decays that result in the ground state daughter versus a metastable daughter.
4. **Total reaction loss** sensitivity: α = change in a nuclide's total loss cross section.
5. **Reaction channel** sensitivity: α = change in specific reaction channels (e.g. (n, γ)).
6. **Reaction yield** sensitivity: α = change in a reaction yield (e.g., fission product yields).

Sensitivity capabilities in ORIGEN can help answering these types of questions

- Which nuclides and which nuclear data are affecting decay heat prediction for a given fuel burnup ?
- For an ORIGEN depletion calculation based on ENDF/B-VII.1 nuclear data, what is the effect of the new ENDF/VIII.1 nuclear data ?
- Which are the top nuclides contributing to radioactivity in a spent fuel pool at a given time after fuel placement into the pool, and how are their sensitivities changing with increasing decay times ?
- ^{226}Ra is used as a target material to produce medical isotopes (e.g., $^{225}\text{Ac}/^{213}\text{Bi}$ for treating leukemia). What is the sensitivity of ^{226}Ra after 9-day irradiation of 1 mg? What are the primary contributors to the build-up of by-products ?
- ...and much more

ORIGEN sensitivity input block

```
=origen
case (ID) {
...
}
sens{
  case = ID
  response{
    %iso=[pu238=1.0 u238=1.0]
    type=DECAYHEAT % or NUCLIDE
    step=2
  }
  integration = average % optional
  threshold = 1e-2
  dp_verify{
    nrank = 3
    nrank_pert=1.001
  }
}
end
```

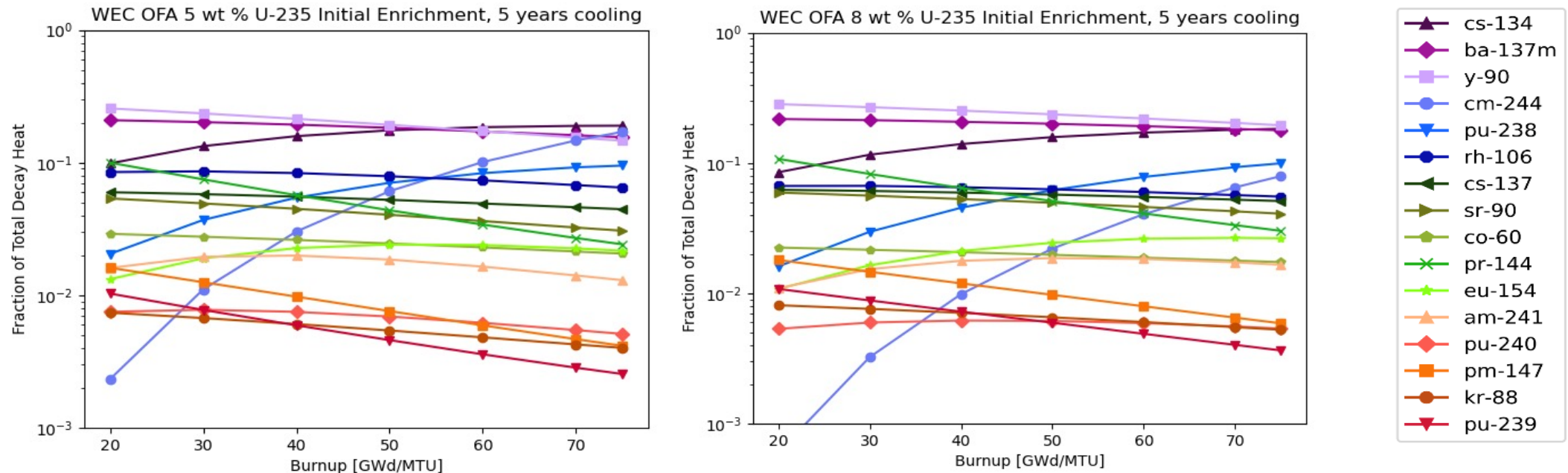
- **case** load from the previous case (ID) for the sensitivity calculations
- **response**
 - *iso* array: list of id=multiplier. If not specified, multiplier is set to 1.0 for all isotopes (useful for total decay heat)
 - *type* : response type
 - NUCLIDE: Nuclide concentration (in SCALE 6.3)
 - **DECAYHEAT**: Decay heat (in SCALE 7.0)
 - *step* : Timestep index
- **integration** method for sensitivity calculation (optional) – trapezoidal/**average**(default)/interp
- **threshold** for sensitivity coefficients
- **dp_verify** direct perturbation (DP)
 - *nrank* : to limit the number of DP calculations
 - *nrank_pert* : relative perturbed amount for DP calculation

See [Section 5.1.5.2.13](#) of the SCALE manual for details

Example: Decay heat for a W17x17 typical fuel assembly

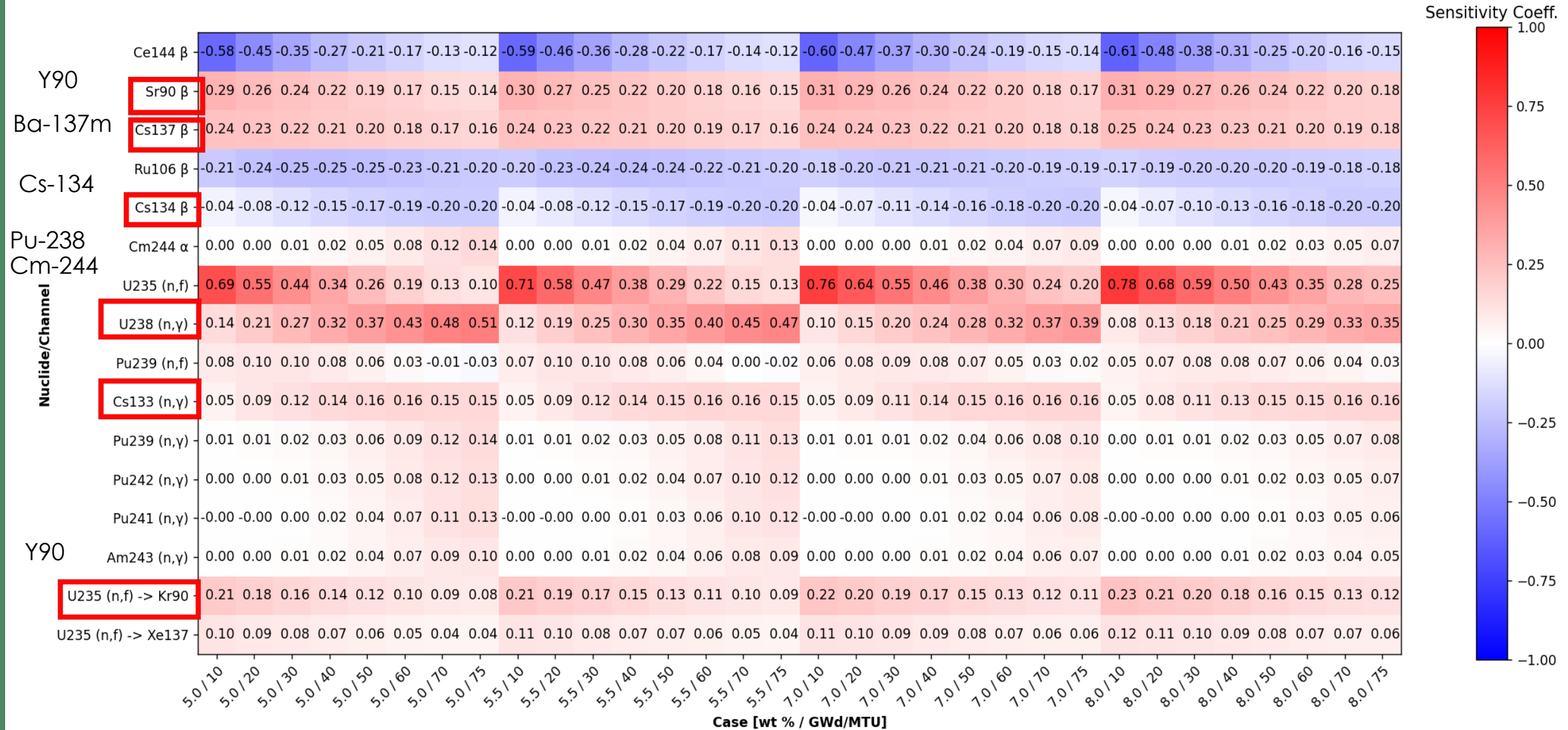
top contributing nuclides for 5% and 8% enrichment, burnup 0-80 GWd/t, 5-year cooling time

- For 8 % enrichment overall: top three contributors are ^{90}Y , ^{134}Cs , and $^{137\text{m}}\text{Ba}$
- For 5 % enrichment at HBU: ^{244}Cm is the 2nd top contributor, ^{90}Y is the 4th top contributor, while contribution of ^{244}Cm decreases with increased enrichment
- ^{238}Pu has notable impact on the total decay heat at HBU



Source: A. Alpan et al., ORNL/TM-2023/2938

Decay heat sensitivity analysis results for W17x17 fuel



- Behavior of decay heat can be explained with the sensitivity analysis!

What is happening in SCALE 7.0 (under development)

- Add more response types (e.g., decay heat, fuel cycle)
- Generate Sensitivity Data Files (SDFs) for ORIGEN
- Couple within neutron transport codes (Polaris/TRITON)
- Expand usage to various types of applications
 - decay heat benchmarks
 - nuclide inventory benchmarks

Demo: PWR fuel pin vs PBR fuel cell

- Similarities and sensitivities



PWR fuel pin vs PBR fuel cell: nuclide inventory and decay heat

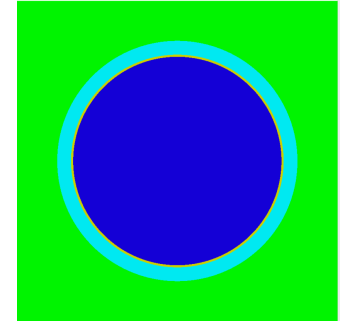
Given two simple depletion models for generic PWR and PBR fuel cells, address the following questions:

- Is uncertainty due to nuclear data in decay heat for PWR fuel different from that of PBR fuel, for the same burnup?
- Are uncertainties due to nuclear data in the indicated nuclides for PWR fuel different from those for PBR fuel, at 80 GWd/t burnup?
- Is the PWR and PBR decay heat similarity index changing with burnup?
- What are the top nuclear data contributors to uncertainty in decay heat for PWR and PBR fuel at 80 GWd/t, relative to the indicated nuclides ?
- What are the top nuclear data contributors to uncertainty in ^{239}Pu in PWR and PBR fuel at 80 GWd/t, relative to the indicated nuclides ?

t-depl depletion model for PWR fuel pin

```
=t-depl parm=(bonami,addnux=4)
PWR pin example, deplete to 80 GWd/MTU
'*****
*** Transport library ***
'*****
v7-56
'*****
*** Material composition data ***
'*****
read comp
uo2 1 0.95 923 92235 4.0 92238 96.0 end
zirc2 2 1 595 end
h2o 3 den=0.7135 1 579 end
boron 3 den=0.7135 653e-06 579 end
n 4 den=0.00125 1 595 end
end comp
'*****
*** Unit cell data (for XSPROC) ***
'*****
read celldata
  latticecell squarepitch pitch=1.4300 3
                        fuel=0.9294 1
                        gapd=0.9484 4
                        cladd=1.0719 2 end
end celldata
'*****
*** Depletion data ***
'*****
read depletion
1
end depletion
'*****
*** Burn data ***
'*****
read burndata
  power=40.0 burn=2000 nlib=20 end
end burndata
'*****

'*****
*** NEWT transport model ***
'*****
read model
PWR pin example
read parm epsilon=1e-3 end parm
read materials
mix=1 pn=1 com='fuel' end
mix=2 pn=1 com='clad' end
mix=3 pn=2 com='water' end
mix=4 pn=0 com='gap' end
end materials
read geom
global unit 1
com='fuel rod'
cylinder 10 0.4647
cylinder 20 0.4742
cylinder 30 0.53595
cuboid 40 4p0.715
media 1 1 10
media 4 1 20 -10
media 2 1 30 -20
media 3 1 40 -30
boundary 40 4 4
end geom
read bounds
all=refl
end bounds
end model
'*****
end
```

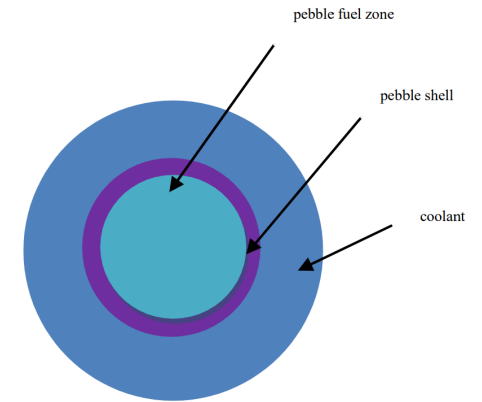


TRITON model for PWR fuel pin (2D)

t-depl-1d depletion model for PBR fuel cell

```
t-depl-1d parm=(bonami,addnux=4)
PBR cell example, deplete to 80 Gwd/MTU
*****
*** Transport library ***
*****
v7-56
*****
*** Material composition data ***
*****
read comp
'fuel kernel
'comp U_C0.5 O1.5 from Table 1, ANL-GenIV-075 (2006)
'density 10.5g/cc from Table 1, ANL-GenIV-075 (2006) and
'      Table 2, INEEL_EXT-03-00870 (2003)
'enrichment 7% from Table 2, INEEL_EXT-03-00870 (2003)
u-235      1 0 1.65259E-3 1200 end
u-238      1 0 2.19558E-2 1200 end
o-16       1 0 3.54126E-2 1200 end
c          1 0 1.18942E-2 1200 end
'buffer
'density 1.0g/cc from Table 4, INEEL_EXT-03-00870 (2003)
c-graphite 2 0 5.01833E-2 1200 end
'2nd fuel coating - inner pyrolytic carbon
'density 1.9g/cc from Table 4, INEEL_EXT-03-00870 (2003)
c-graphite 3 0 9.53483E-2 1200 end
'3rd fuel coating - SiC
c          4 0 4.80734E-2 1200 end
si-28      4 0 4.43381E-2 1200 end
si-29      4 0 2.25128E-2 1200 end
si-30      4 0 1.48403E-2 1200 end
'4th fuel coating - outer pyrolytic carbon
'density 1.9g/cc from Table 4, INEEL_EXT-03-00870 (2003)
c-graphite 5 0 9.53483E-2 1200 end
'graphite matrix
'density 1.25g/cc from Table 1, ANL-GenIV-075 (2006)
c-graphite 6 0 6.02200E-02 1200 end
'pebble shell
'density assumed the same as for the graphite matrix
c-graphite 7 0 6.02200E-02 1200 end
'helium temperature average of inlet and outlet (250 and
'      700C) from INEEL_EXT-03-00870 (2003), Table 2, p.22
'helium pressure 6.0 MPa from INEEL_EXT-03-00870 (2003),
'      Table 2, p.22
'helium density calculated using ideal gas law
he-4       8 den=3.86088e-3 1.0 748.15 end
end comp
*****
'heavy metal loading of about 7g/pebble and # particles
' per pebble 11200 from Table 2, INEEL_EXT-03-00870 (2003)
' fuel kernel radius was inferred 0.025cm based on these
' fuel coating thickness from Table 1, ANL-GenIV-075 (2006)
' coolant radius around a pebble was inferred based on data
' in Table 2, INEEL_EXT-03-00870 (2003)
' core diameter 3m, core height 9.4m, 360,000 fuel pebbles
```

```
read celldata
doublehet fuelmix=10 end
gfr=0.025 1
coatr=0.035 2
coatr=0.039 3
coatr=0.0425 4
coatr=0.0465 5
numpar=11200
matrix=6 end grain
pebble sphtriangp right bdy=white
hpitch=3.195417 8
fuels=2.5
cladr=3.0 7 end
end celldata
*****
read depletion
1 end
end depletion
*****
read burndata
power=80 burn=1000 nlib=20 end
end burndata
*****
read model
NGNP pebble cell
read parm
sn=32
end parm
read materials
mix=10 end
mix=7 end
mix=8 end
end materials
read geom
geom=sphere
rightBC=white
leftBC=reflected
zoneIDs 10 7 8 end zoneIDs
zoneDimensions 2.5 3.0 3.532019 end zoneDimensions
zoneIntervals 3r20 end zoneIntervals
end geom
'=====
end
```



TRITON model for PBR fuel cell (1D)
[double-heterogeneity of the problem is addressed via the *doublehet* option in XSPROC]

PWR fuel pin vs PBR fuel cell: nuclide inventory and decay heat

- **Strategy:** use Sampler based on the two generic models to calculate:
 - Uncertainty in decay heat due to all nuclear data uncertainties (XS, FP yields, decay data) for burnups up to 80 GWd/t
 - Uncertainty in selected nuclides (^{235}U , ^{239}Pu , ^{240}Pu , ^{241}Pu , ^{244}Cm , ^{148}Nd , ^{149}Sm , ^{133}Cs , ^{134}Cs , ^{137}Cs) due to all nuclear data uncertainties (XS, FP yields, decay data) for burnups up to 80 GWd/t
 - Similarity index of PWR and PBR fuel decay heat for 40 and 80 GWd/t burnups
 - R^2 sensitivity indices for decay heat relative to nuclear data for selected nuclides (^{235}U , ^{235}U , ^{238}Pu , ^{239}Pu , ^{240}Pu , ^{244}Cm , ^{134}Cs , ^{137}Cs , $^{137\text{m}}\text{Ba}$, ^{241}Am , ^{144}Pr , ^{106}Rh , ^{154}Eu , ^{90}Sr , ^{90}Y) for PWR and PBR fuel at 80 GWd/t burnup
 - R^2 sensitivity indices for ^{239}Pu in PWR and PBR fuel at 80 GWd/t burnup, relative to nuclear data for selected nuclides (^{235}U , ^{235}U , ^{237}Np , ^{239}Np , ^{238}Pu , ^{239}Pu , ^{240}Pu , ^{242}Cm , ^{241}Am)

Sampler input: parameter, response, analysis blocks

```
=sampler
read parameters
n_samples=100
library="v7-56"
perturb_xs=yes
perturb_decay=yes
perturb_yields=yes
perturb_geometry=no
run_cases=yes
end parameters
.
```

```
=====
' Define responses and analyses
=====

read response [dh]
  type=opus_plt
  ndataset=1
  nuclides=total end
end response

read response[nuc]
  type=origen_nuclides
  nuclides = u-235 pu-239 pu-240 pu-241 cm-244
             nd-148 sm-149 cs-133 cs-134 cs-137 end
  mixture = 1
end response

read analysis[dh_ck]
  type = pearson_corr
  targets = pwr:dh.total(10) pwr:dh.total(10) pwr:dh.total(20) end
  sources = pbr:dh.total(10) pbr:dh.total(10) pbr:dh.total(20) end
end analysis

read analysis[pu239_ck]
  type = pearson_corr
  targets = pwr:nuc.pu239(10) pwr:nuc.pu239(20) end
  sources = pbr:nuc.pu239(10) pbr:nuc.pu239(20) end
end analysis

read analysis [sens_dh_pwr]
  type = r2
  targets = pwr:dh.total(20) end
  sources = u-235 u-238 pu-238 pu-239 pu-240 cm-244 cs-134 cs-137
             ba-137m am-241 pr-144 rh-106 eu-154 sr-90 y-90 end
end analysis

read analysis [sens_dh_pbr]
  type = r2
  targets = pbr:dh.total(20) end
  sources = u-235 u-238 pu-238 pu-239 pu-240 cm-244 cs-134 cs-137
             ba-137m am-241 pr-144 rh-106 eu-154 sr-90 y-90 end
end analysis

read analysis [sens_nuc_pwr]
  type = r2
  targets = pwr:nuc.pu239(20) end
  sources = u-235 u-238 np-237 np-239 pu-238
             pu-239 pu-240 cm-242 am-241 end
end analysis

read analysis [sens_nuc_pbr]
  type = r2
  targets = pbr:nuc.pu239(20) end
  sources = u-235 u-238 np-237 np-239 pu-238
             pu-239 pu-240 cm-242 am-241 end
end analysis
=====
```

Validation with SCALE: nuclide inventory and decay heat

Validation with SCALE: How to Connect Paper Reactors with Reality

Outlook

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

Goals in review

1. Explore the key capabilities of the SCALE code system for neutron transport, depletion, uncertainty quantification, and sensitivity analysis
2. Gain practical insight into using SCALE for validation analyses as accepted by US regulators
3. Learn how to perform similarity assessments, how to determine biases, and how to identify validation gaps
4. See SCALE's graphical user interface Fulcrum, in action to create and validate input files, visualize 2D and 3D geometries, and explore various result files

Final thoughts

- Comprehensive, automated validation
 - radiation shielding
 - isotope production
 - criticality safety
 - spent fuel applications
- Robust capabilities for **sensitivity** and **similarity**
- Provide the community with a **reference solution** compared to actual measurements for data + method + implementation

Key SCALE Initiatives

1. Invest in production-quality Monte Carlo transport on CAD / combined CAD+CSG
2. Extend similarity assessment capability to new application areas
3. Develop uncertainty and correlation for all input nuclear data
4. Improve front end visualization and model inspection options
5. Integrate Python as an integrated backend for processing results
6. Disseminate all reports/training/models for transparency
7. Automate quality metric calculation and validation suites
8. Improve installation/update experience
9. Add new photonuclear physics and charged particle physics

Presenters Team for today



Germina Ilas



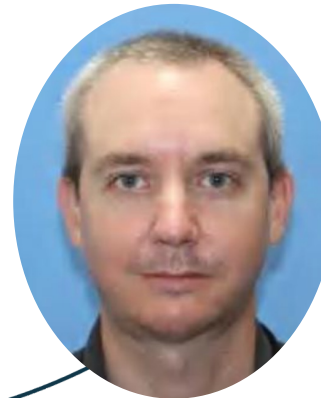
Will Wieselquist



Rike Bostelmann



Ugur Mertюреk



Travis Greene

Useful links

- **Public materials**

- Manual
<https://scale-manual.ornl.gov>
- Reports and journal papers
<https://www.ornl.gov/scale/references>
- Presentations and tutorials
<https://scalemeetings.ornl.gov/>
(under Previous Workshops)
- Open-source **code** (subset)
<https://code.ornl.gov/scale/code/scale-public>
- Open-source SCALE **models**
<https://code.ornl.gov/scale/analysis>

- **Websites**

- SCALE website
<https://www.ornl.gov/scale>
- SCALE users' group workshop
<https://scalemeetings.ornl.gov/>

- **SCALE Help**

- email scalehelp@ornl.gov
- SCALE users' group forum
<https://www.ornl.gov/content/users-group-forum>

Coming soon

2024 SCALE USERS' GROUP WORKSHOP



WHEN

June 5-7, 2024



WHERE

Oak Ridge National
Laboratory (Hybrid)
Building 5100, Room 128

- **Website** <https://scalemeetings.ornl.gov/>
- **Free registration**
- **No SCALE license required to attend technical sessions**
- **15 hands-on tutorials (require SCALE 6.3 or 6.2 license)**
- **Tours of ORNL facilities for in-person attendees**
- **SCALE Open Mic session is waiting for your lightening talk**
- **2023 attendance: 174 participants from 22 countries (138 of them non-ORNL)**