



NUREG/CR-7308

Sensitivity/Uncertainty Methods for Nuclear Criticality Safety Validation

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NRC RES/NMSS Hybrid Technical Workshop on Fuel
Cycle Impacts of High Burnup, Extended
Enrichment, and HALEU Fuel Designs, Featuring an
Overview of ORNL's Capabilities



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NUREG-7308: Outline

- Introduction
- Validation Overview and Previous Guidance
- Sensitivity/Uncertainty (S/U) Analysis
- Case Studies
 - BWR Demo
- Advanced Techniques
- Future Work

Sensitivity/Uncertainty Methods for Nuclear Criticality Safety Validation

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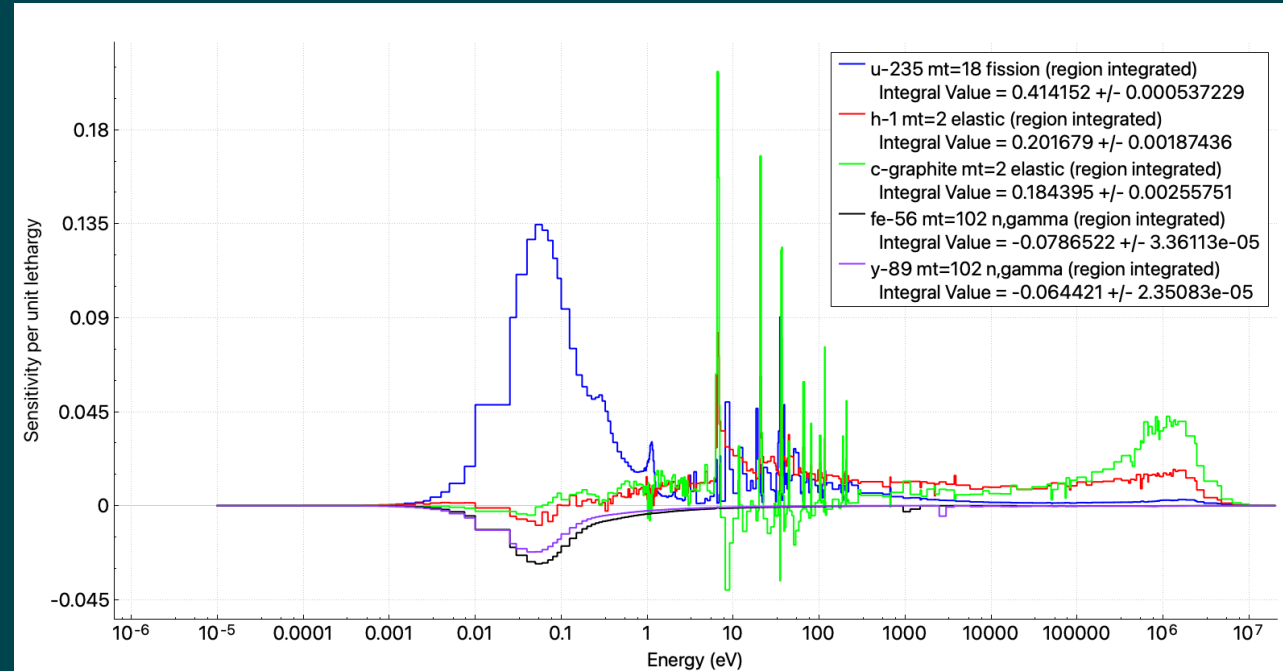
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Introduction

Goal: To provide an up-to-date document on best practices for S/U methods and how the tools should be used by NRC staff and applicants for nuclear criticality safety (NCS) validation

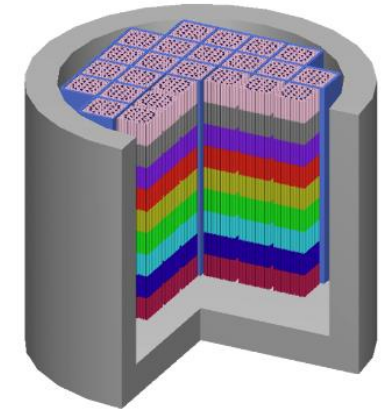
- NCS validation: to ensure that modeling used in evaluations are substantiated against benchmark experiments that are neutronically similar to the application systems
- S/U methods allow for quantifying similarity between systems and estimating bias and bias uncertainties in k_{eff} , as well as estimations of gap penalties for insufficient validations
- Discussion focuses on SCALE TSUNAMI tools/methods; however, general S/U methods are consistent across code packages



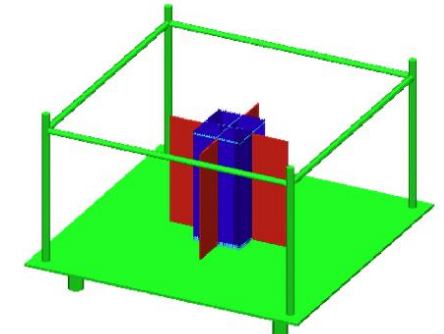
Validation overview

Characterization of Safety Analysis Models

- Characteristics of model drive selection of applicable validation experiments and influence bias and bias uncertainty from trends
 - Nuclear data
 - Production code reliability
 - Uncertainty in benchmark experiments
 - Material compositions
 - Geometry
 - Temperature
 - Reactivity measurement
- Safety analysis models define the boundaries of the required range of parameters (ROP) to be covered in the validation and applicable value(s) for trending parameters (c_k , EALF, etc.)
- The International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook, published by the Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency (NEA), is the best public source for high-quality critical benchmarks



Application



Critical experiment

Previous guidance

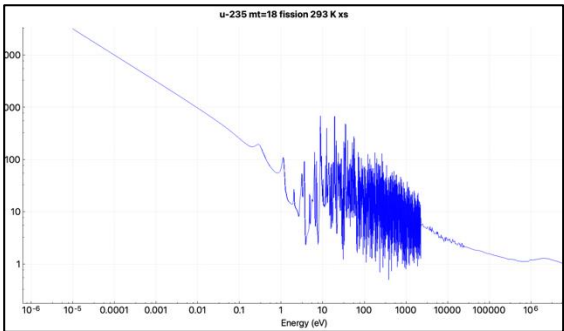
A thorough literature review of previous guidance is given with four recommended sources

1. NUREG/CR-6655 (1999): first S/U methods document for NCS validation
2. Rearden et al., *Nuclear Technology* (2011): detailed description of TSUNAMI and TSUNAMI-IP tools used for validation in SCALE
3. TSUNAMI Primer (2009): step-by-step instructions to generate input files and perform analyses with TSUNAMI (no theory); currently being updated for 2026
4. Jones thesis (2015): TSUNAMI-3D calculation recommendations

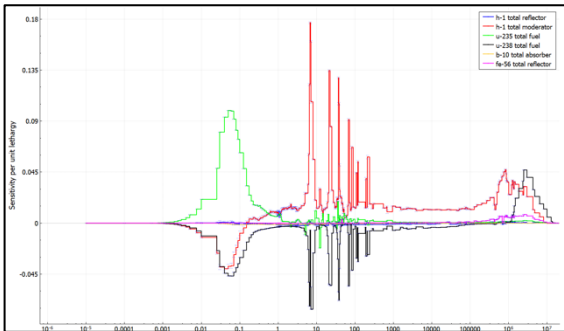
While very useful, these documents are partially outdated and an update (NUREG/CR-7308) was necessary



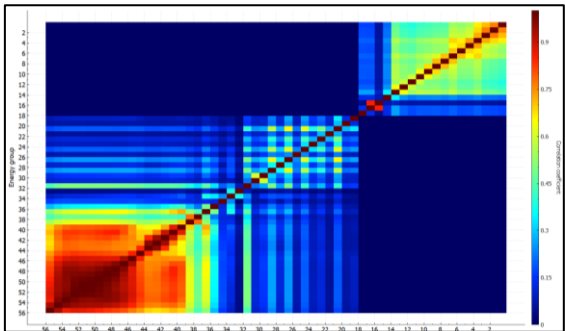
Theoretical aspects of S/U analysis applied to NCS validation



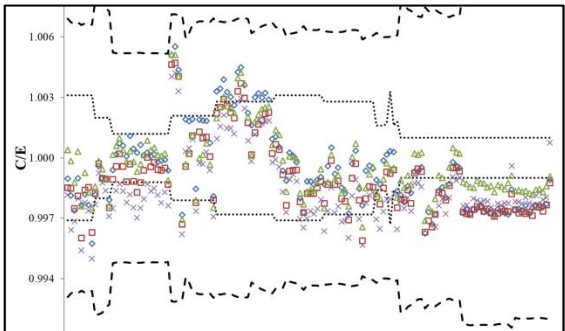
Sensitivity coefficients,
adjoint perturbation theory,
and nuclear data



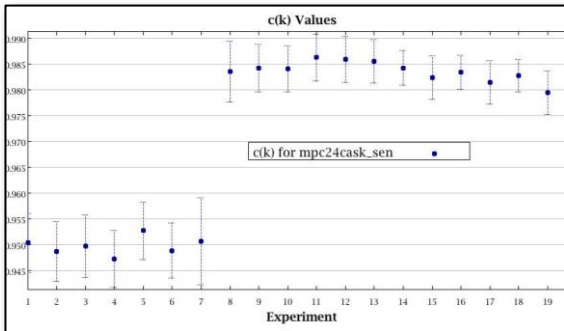
TSUNAMI implementation
of k_{eff} sensitivity methods



Nuclear covariance
data



Uncertainty analysis



Similarity assessment

Sensitivity coefficients

Predict the expected change in a response (k) due to a change in some input parameter (Σ)

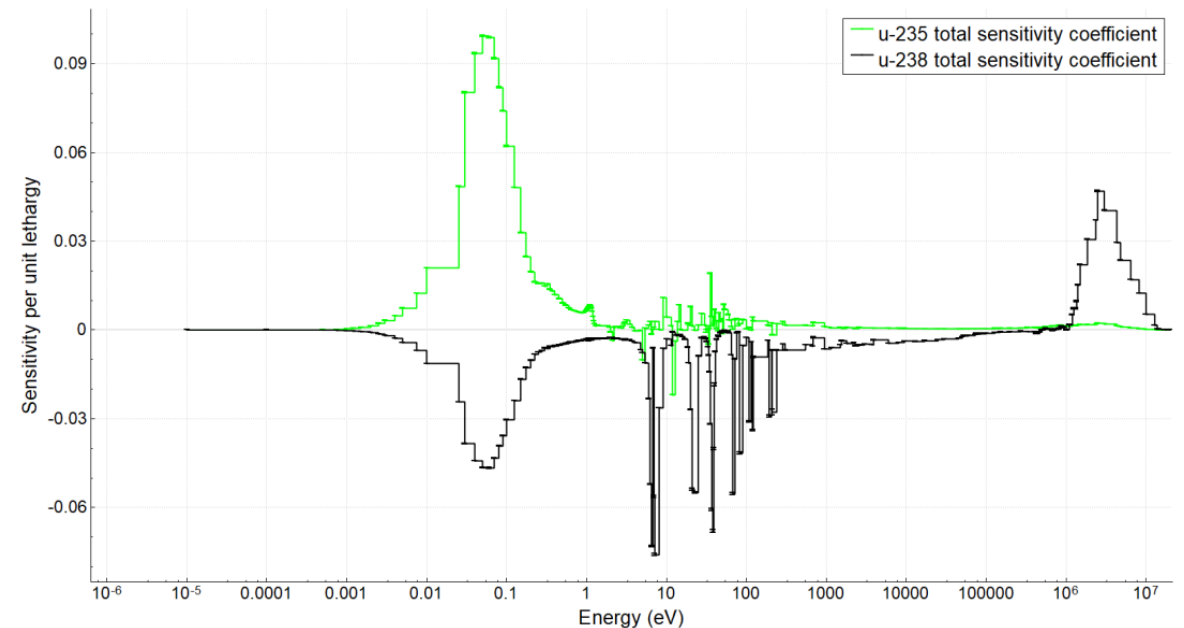
- These responses can be k_{eff} (or ratios of reaction rates)
- The input parameters are typically nuclear data
 - Cross sections, multiplicity (nubar: $\bar{\nu}$), fission spectrum (chi: χ)
- The sensitivity coefficients are dimensionless ratios
 - What would happen to the system k_{eff} if some piece of data were changed by some amount?
 - The sensitivity coefficient is calculated **without** making the change

$$S = \frac{\frac{\delta k}{k}}{\frac{\delta \Sigma}{\Sigma}}$$

Sensitivity coefficients

Sensitivities can be positive or negative and may change signs at different energies

- The sign of the sensitivity coefficients determine if k_{eff} increases (+) or decreases (-)
- Sensitivity coefficients can be summed over reactions for a specific nuclide and over multiple nuclides for a mixture



LEU-COMP-THERM-042-004

Adjoint perturbation theory

- TSUNAMI uses adjoint perturbation theory to compute sensitivity coefficients
 - One of the definitions of the adjoint is that it can be used as an importance function that tells us the contribution of each region to the response we are trying to calculate, in our case k_{eff}
 - In radiation transport, this means that the forward flux (ψ) is where the particles are and the adjoint flux ($\psi^\dagger$) is representative of their importance
- Predict the expected change in a response (k) due to a change in some input parameter (Σ)
 - k_{eff} responses are almost the only ones we consider
 - Input parameters are nuclear data
- Depending on the problem complexity we can perform these calculations using several SCALE sequences (TSUNAMI-1D, -2D, or -3D)

$$S_{k, \Sigma(\vec{r})} = \frac{\Sigma(\vec{r})}{k} \frac{\delta k}{\delta \Sigma(\vec{r})}$$



$$= \frac{\Sigma(\vec{r})}{k} \frac{\left\langle \phi^\dagger(\vec{\xi}) \left(\frac{\delta A[\Sigma(\vec{\xi})]}{\delta \Sigma(\vec{r})} - \frac{1}{k} \frac{\delta B[\Sigma(\vec{\xi})]}{\delta \Sigma(\vec{r})} \right) \phi(\vec{\xi}) \right\rangle}{\left\langle \phi^\dagger(\vec{\xi}) \frac{1}{k^2} B[\Sigma(\vec{\xi})] \phi(\vec{\xi}) \right\rangle}$$



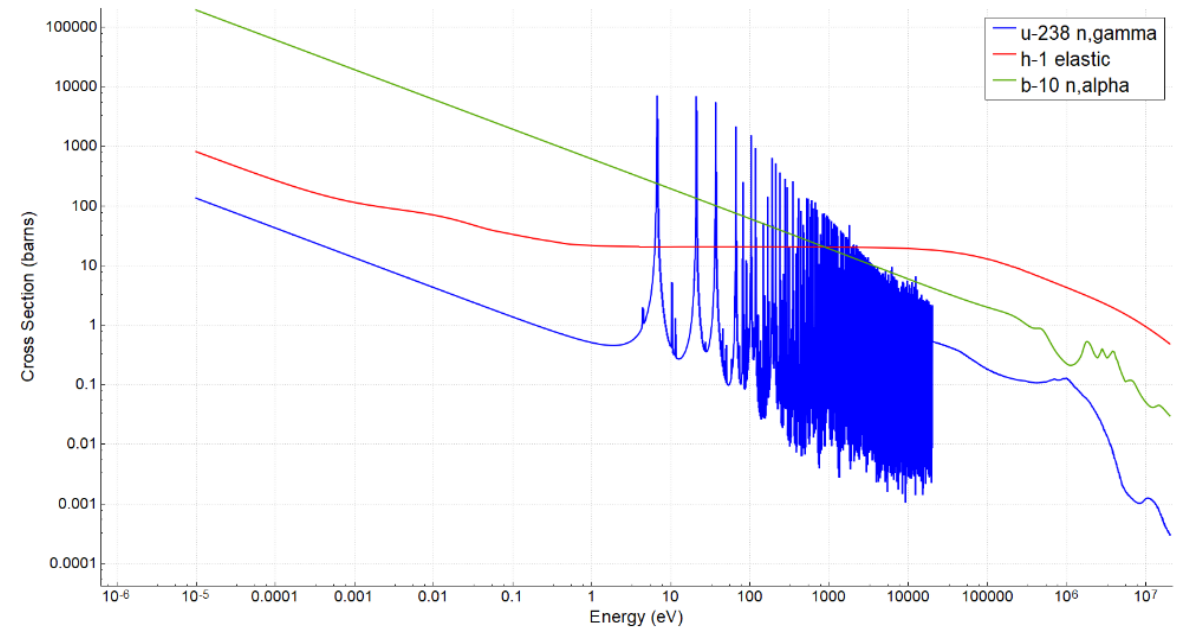
$$S = \frac{\delta k}{\frac{k}{\frac{\delta \Sigma}{\Sigma}}}$$

Nuclear data

Three types of nuclear data relevant to S/U analysis

1. Reaction cross sections
2. Neutron multiplicity ($\bar{\nu}$)
3. Fission neutron energy spectrum (χ)

Only sensitivities to reaction cross sections can be confirmed with direct perturbation calculations (DP)



TSUNAMI implementation of k_{eff} sensitivity methods

1. TSUNAMI-1D
Deterministic, Multigroup
2. TSUNAMI-2D
Deterministic, Multigroup
3. TSUNAMI-3D
 - Multigroup TSUNAMI-3D
Monte Carlo, Multigroup
 - Iterated Fission Probability (IFP) Method
Monte Carlo, Continuous-Energy
 - CLUTCH Method
Monte Carlo, Continuous-Energy

- TSUNAMI offers several options for sensitivity calculations based on the desired level of accuracy and runtime.

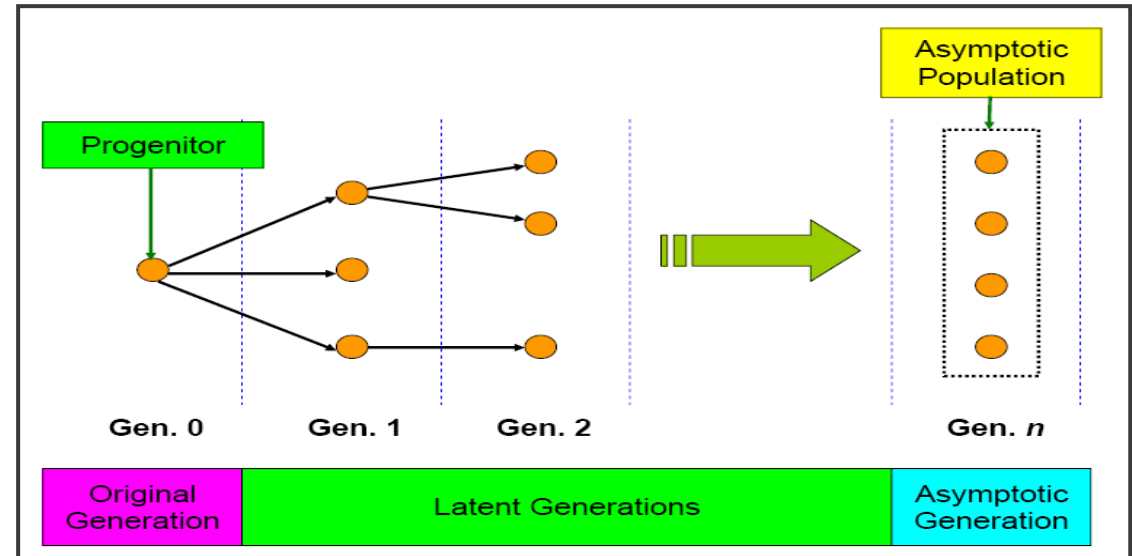
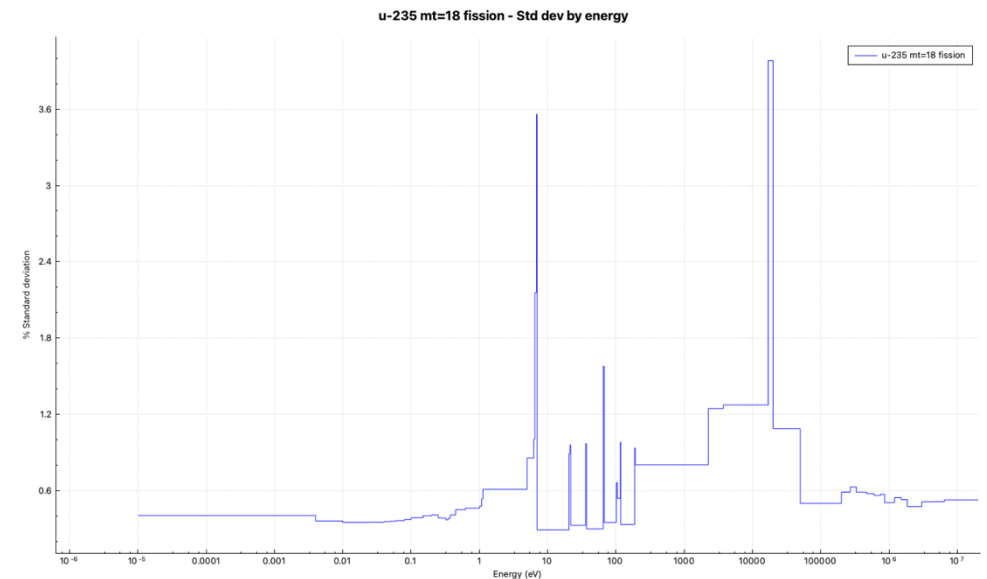
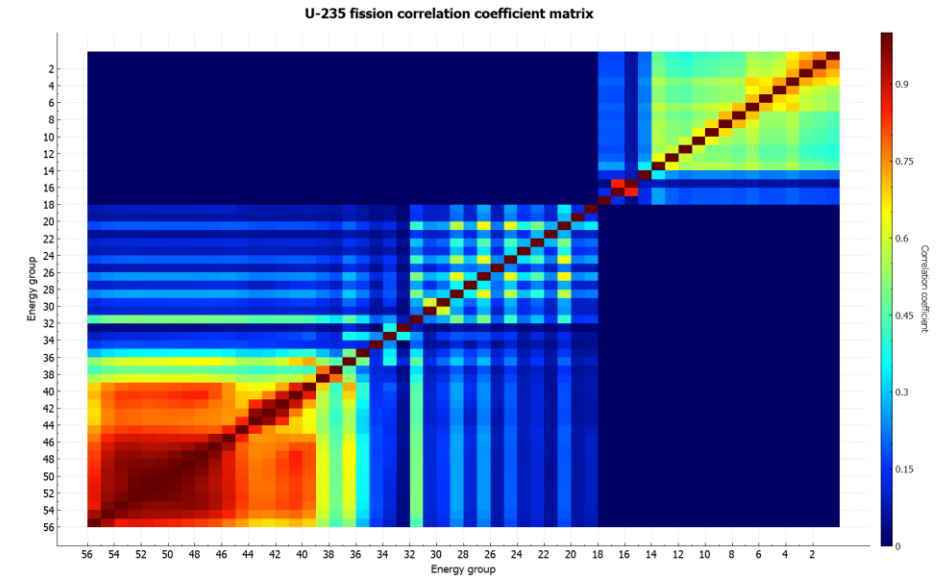


Illustration of the IFP process. Image courtesy of Brian Kiedrowski.

Nuclear covariance data

- Covariance data correspond to relative uncertainties assembled from a variety of sources, including evaluations from ENDF/B-VIII.0, ENDF/B-VII.1, ENDF/B-VI, and approximated uncertainties from a collaborative project performed by Brookhaven National Laboratory (BNL), Los Alamos National Laboratory (LANL), and Oak Ridge National Laboratory (ORNL)
- No inherently “true” uncertainty can be defined for nuclear data
- Differences in nuclear data evaluations directly impact calculations that can be affirmed by comparisons with benchmark experiments; but there is no established procedure to quantify the reliability of uncertainty estimates
- In general, the SCALE covariance library should be viewed as a best-estimate assessment of data uncertainties



Uncertainty analysis

- Referred to as “data-induced uncertainty,” the focus is on propagating the nuclear data covariance with sensitivity coefficients to examine the uncertainty in k_{eff} resulting from the uncertainty in nuclear data
- The chain rule allows for propagation of cross section uncertainties to quantify the data-induced uncertainty in k_{eff} (σ_k^2)

$$\sigma_k^2 = \mathbf{S} \mathbf{C}_{\alpha\alpha} \mathbf{S}^T$$

- where $\mathbf{S}$ is a matrix of all energy-dependent sensitivity coefficient data for all systems considered ($\mathbf{S}^T$ is the transpose)
- $\mathbf{C}_{\alpha\alpha}$ is a matrix containing energy-dependent covariance information evaluated for all nuclear data



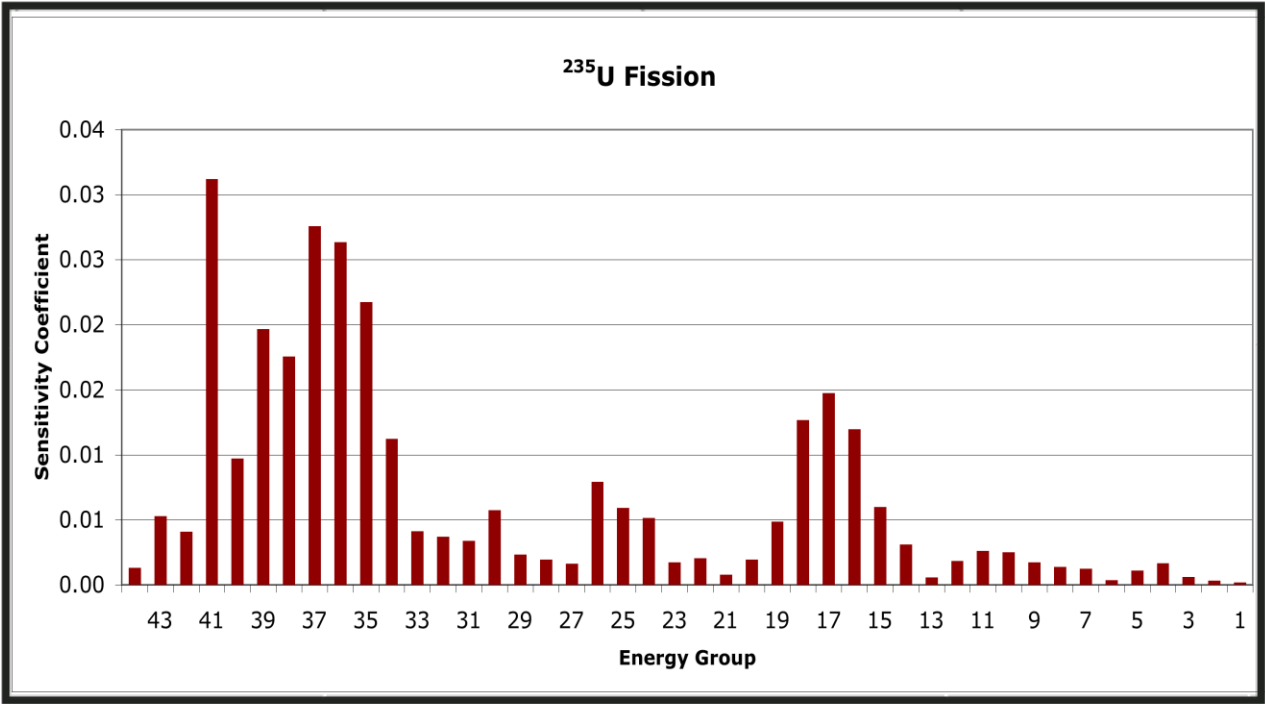
Propagation of cross section uncertainties

Matrix of sensitivity coefficients

- For each nuclide in the problem, the sensitivity to each reaction is stored in energy-dependent bins. For example:

List of
nuclide
reactions

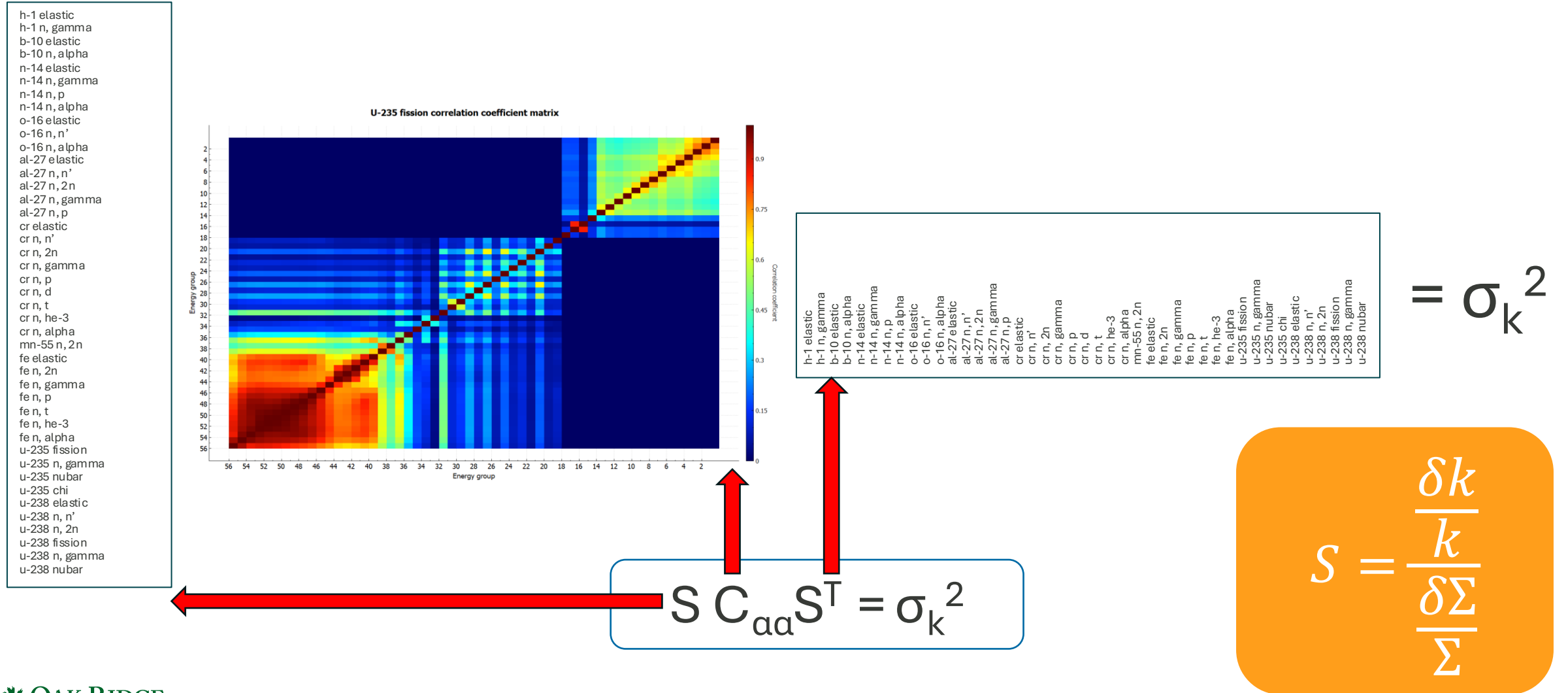
Energy-
dependent
bins



- h-1 elastic
- h-1 n, gamma
- b-10 elastic
- b-10 n, alpha
- n-14 elastic
- n-14 n, gamma
- n-14 n, p
- n-14 n, alpha
- o-16 elastic
- o-16 n, n'
- o-16 n, alpha
- al-27 elastic
- al-27 n, n'
- al-27 n, 2n
- al-27 n, gamma
- al-27 n, p
- cr elastic
- cr n, n'
- cr n, 2n
- cr n, gamma
- cr n, p
- cr n, d
- cr n, t
- cr n, he-3
- cr n, alpha
- mn-55 n, 2n
- fe elastic
- fe n, 2n
- fe n, gamma
- fe n, p
- fe n, t
- fe n, he-3
- fe n, alpha
- u-235 fission
- u-235 n, gamma
- u-235 nubar
- u-235 chi
- u-238 elastic
- u-238 n, n'
- u-238 n, 2n
- u-238 fission
- u-238 n, gamma
- u-238 nubar

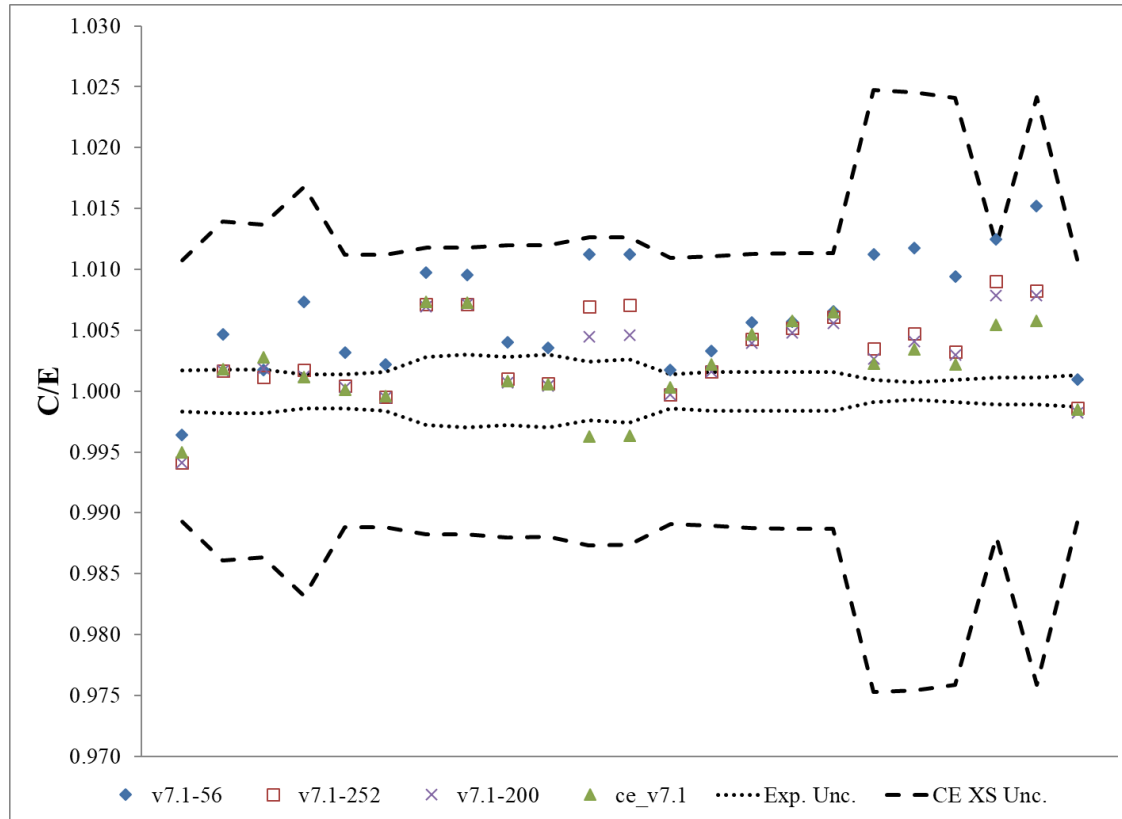
Propagation of cross section uncertainties

- Uncertainty in k_{eff} of a single system: combine the pieces via the “sandwich formula”

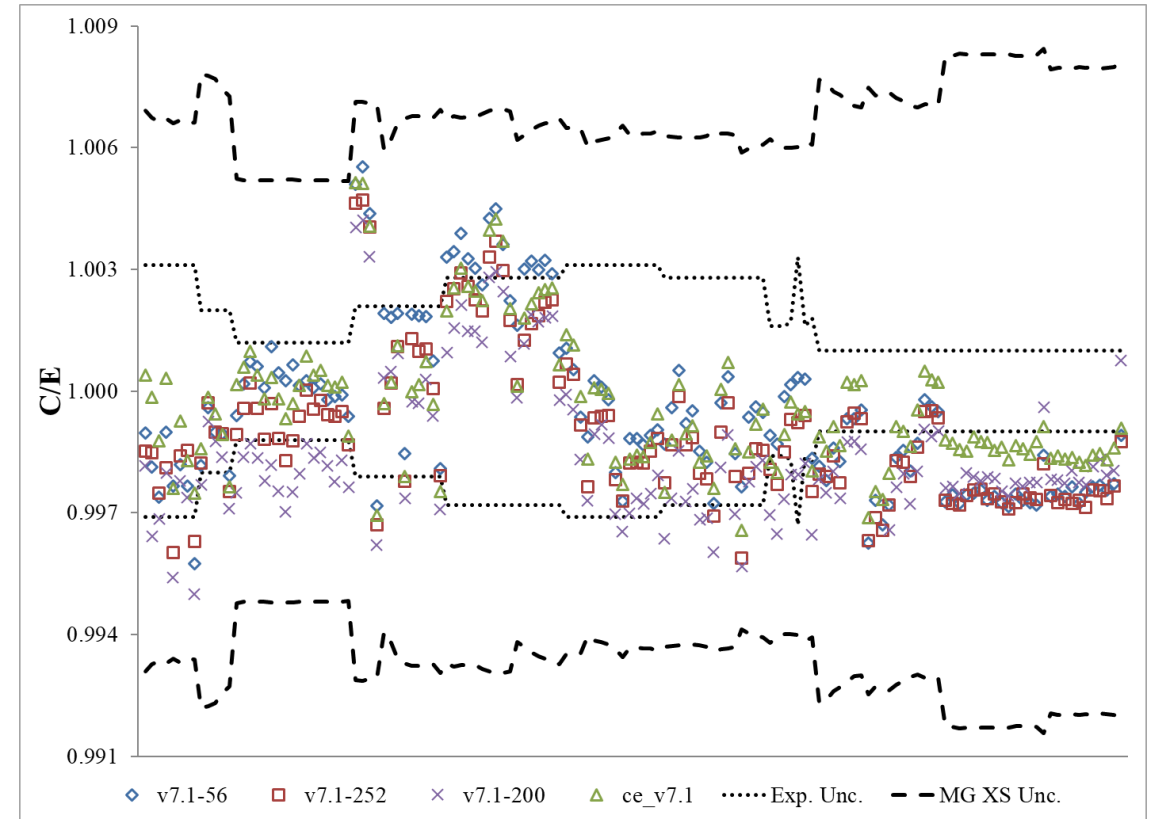


Cross section uncertainty bands

HEU-MET-FAST



LEU-COMP-THERM



Similar plots show largely similar trends for every category of experiments that has been examined.

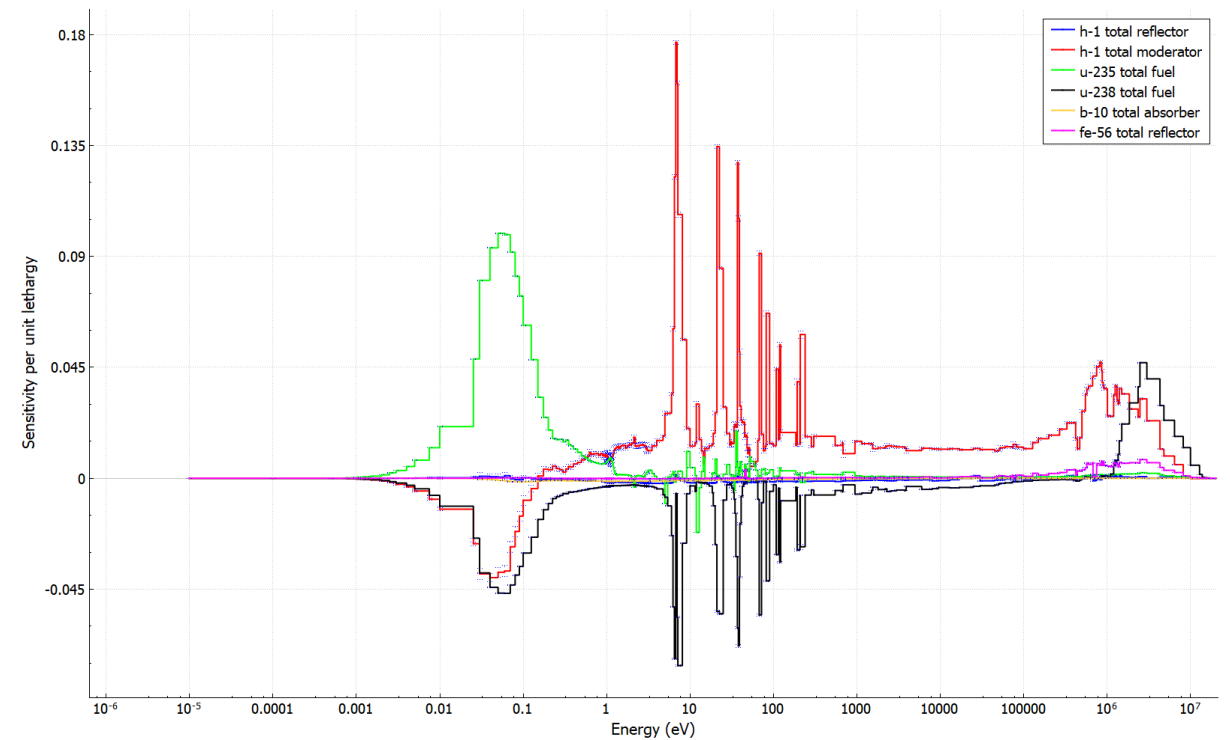
Comparison of bias and data-induced uncertainty for multiple systems

Category	Number of cases	Avg. C/E (CE_V8.1)	Avg. exp. unc. (pcm)	St. dev. of C/Es (pcm)	Avg. 1 σ XS unc. (pcm)
HMF	91	1.00019	222	403	961
HST	61	0.99935	526	689	709
IMF	13	1.00155	269	325	1007
LCT	144	0.99967	202	203	590
LST	19	0.99870	318	273	812
MCT	49	0.99504	400	327	551
MST	10	0.99494	452	213	744
PMF	25	1.00000	214	324	729
PST	92	1.00160	484	470	607

Similarity assessment

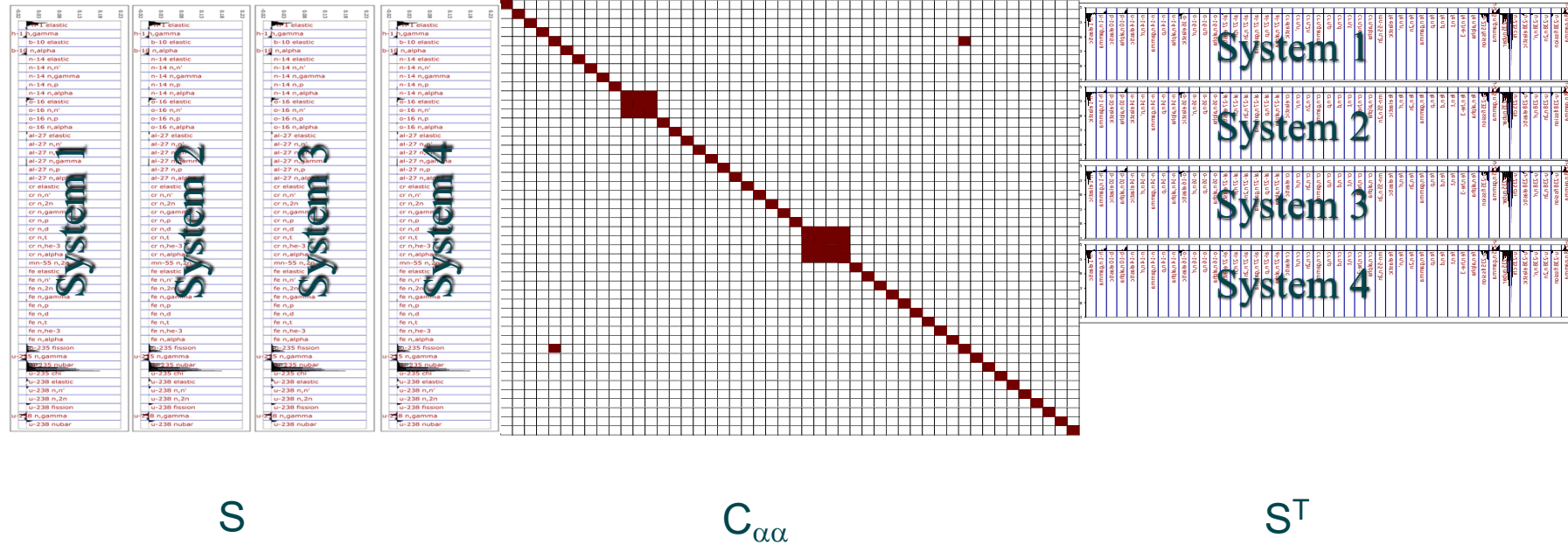
Fundamental theorem of TSUNAMI validation

- The majority of the code bias comes from nuclear data errors
- The nuclear data errors are bounded by their covariance data
- Benchmarks that use the same nuclear data in the same energy-dependent way will manifest the same bias – uncertainties act as weighting functions
- These are the systems that are most representative of the application and should be used in validation
- Comparisons must examine nuclide-, reaction-, and energy-dependent data



Uncertainty propagation

Suppose we have sensitivity information for multiple systems:



Diagonal elements are variance in each system

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

Off-diagonal elements are covariance between two systems

Correlation coefficient c_k for system 1 and system 4

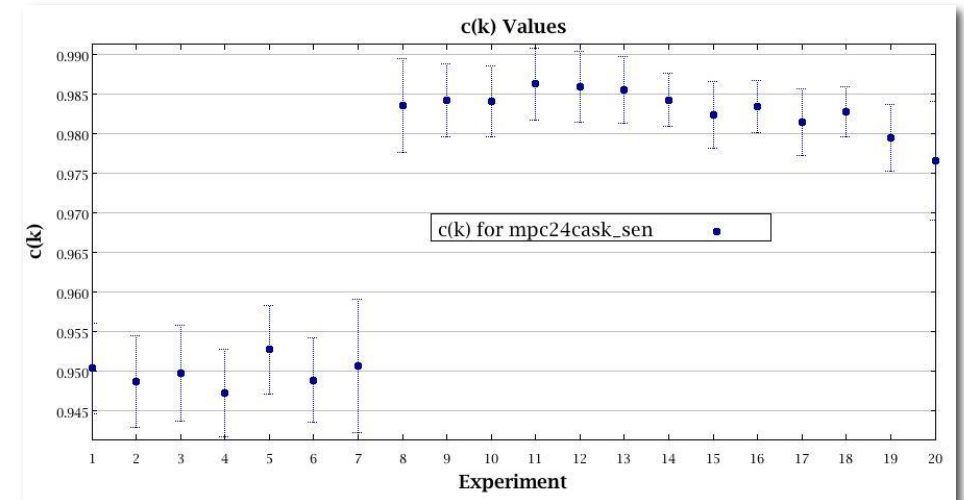
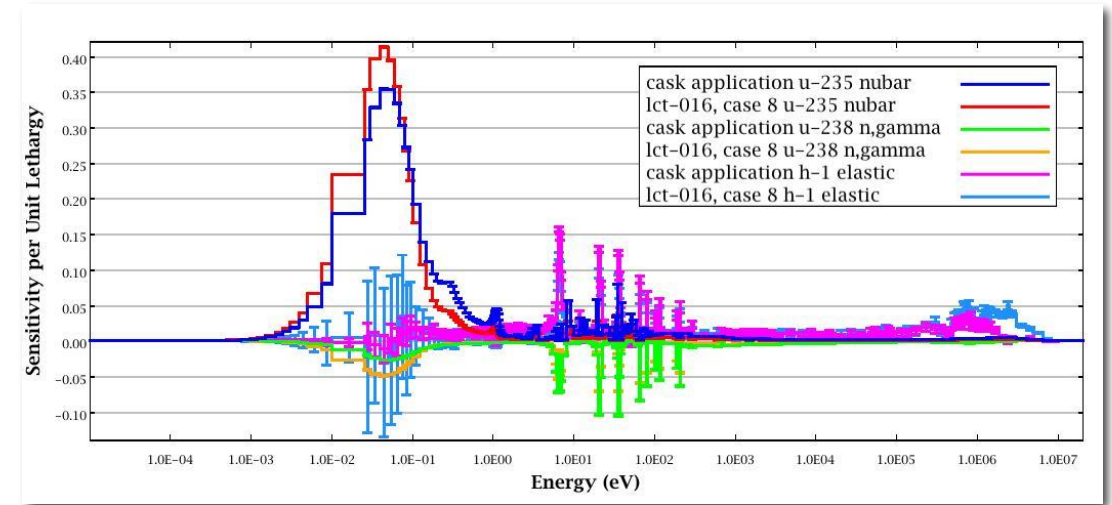
$$\sigma_k^2 = \begin{bmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \sigma_{13}^2 & \sigma_{14}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & \sigma_{23}^2 & \sigma_{24}^2 \\ \sigma_{31}^2 & \sigma_{32}^2 & \sigma_{33}^2 & \sigma_{34}^2 \\ \sigma_{41}^2 & \sigma_{42}^2 & \sigma_{43}^2 & \sigma_{44}^2 \end{bmatrix}$$

$$c_k = \frac{\sigma_{R_1, R_2}^2}{\sigma_{R_1} \sigma_{R_2}} \longrightarrow c_k = \frac{\sigma_{14}^2}{\sqrt{\sigma_{11}^2 \sigma_{44}^2}}$$

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 -1.0 to $+1.0$
 - $+1.0$ is exactly the same system
 - 0 is completely uncorrelated
 - -1.0 is exactly the opposite system



Benchmark applicability

- Current guidance for applicability of critical experiments for bias and bias uncertainty determination:

$c_k \geq 0.9$ → applicable

$0.9 > c_k \geq 0.8$ → marginally applicable

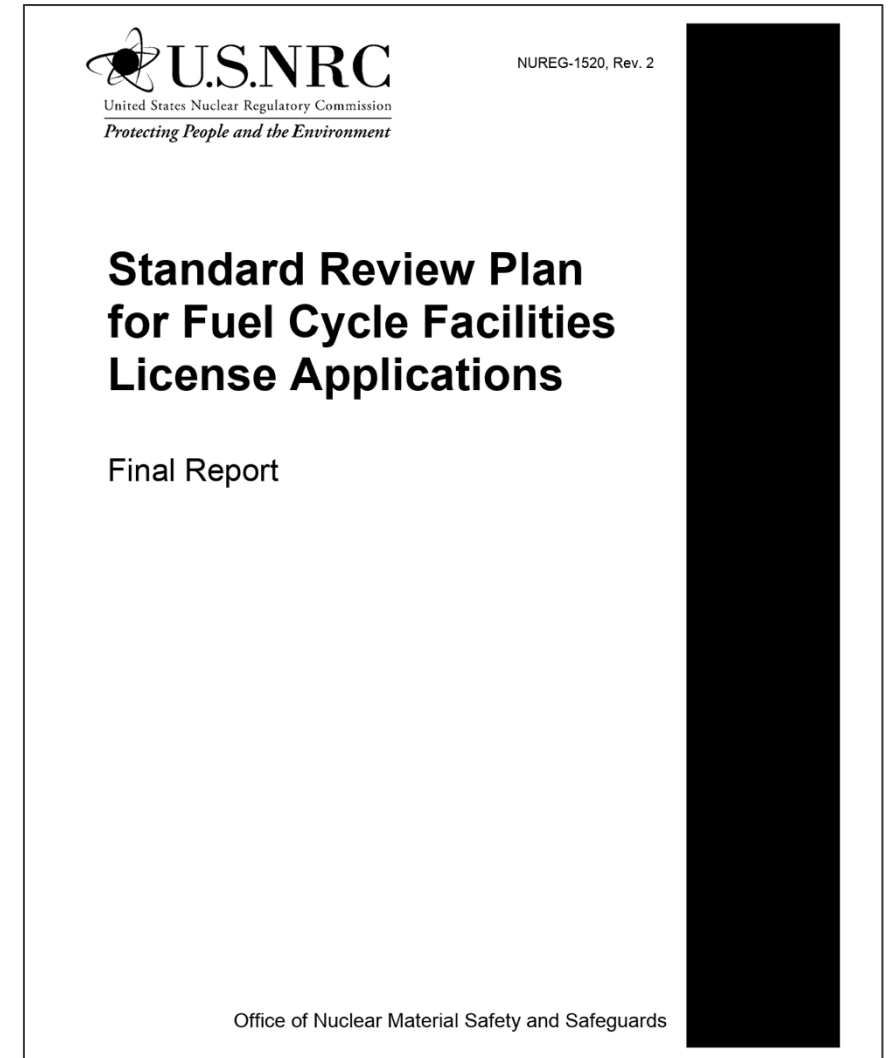
$c_k < 0.8$ → not applicable

- From NUREG-1520, Rev. 2, Appendix 5B:

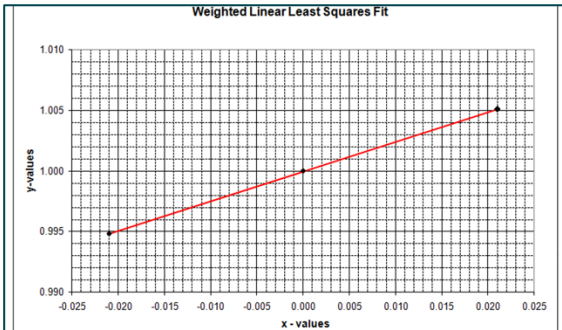
$c_k \geq 0.95$ → very high degree of similarity

$0.9 > c_k \geq 0.95$ → high degree of similarity*

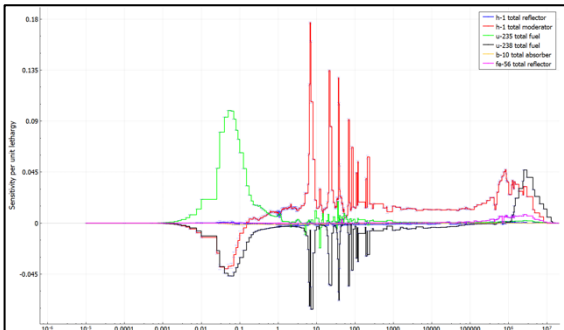
*Similarity determination should be supplemented with other methods



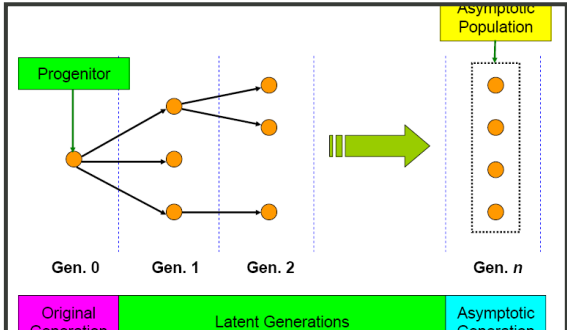
Application recommendations for S/U methods in NCS validation



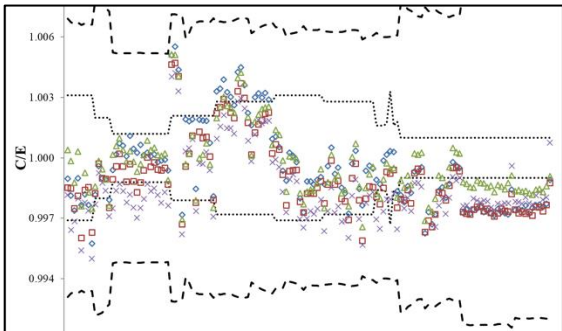
Direct perturbation calculations



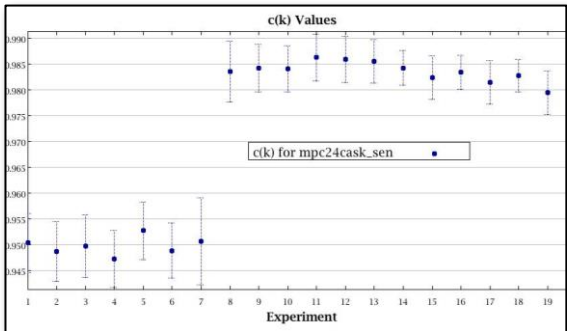
SCALE multigroup methods



SCALE continuous-energy methods



Uncertainty analysis



Similarity assessment

Direct perturbation calculations

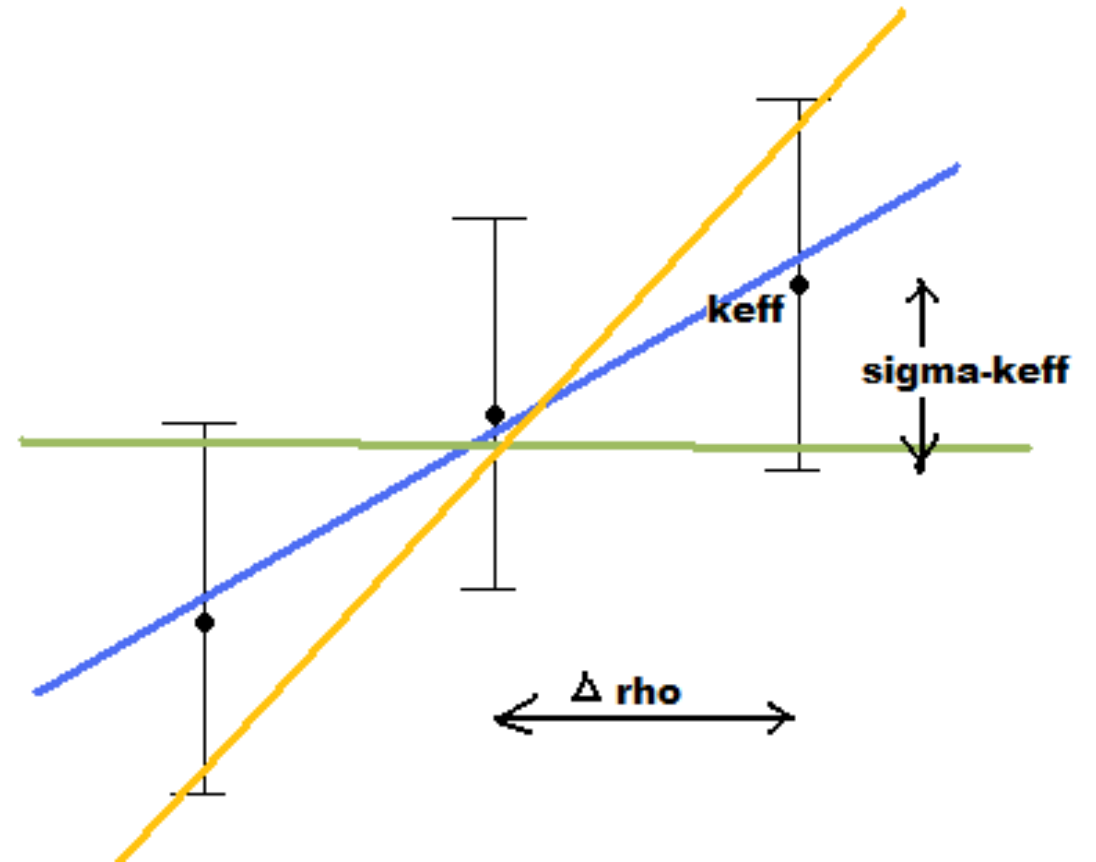
- Direct Perturbation (DP) calculations involve recalculating k_{eff} while varying the density of a nuclide, element, mixture or region
- k_{eff} results and density perturbations are used to manually calculate **energy-integrated total sensitivity**
- $S_{\text{DP}} = (\Delta k / k) / (\Delta \rho / \rho)$
- Equivalent to perturbing all “macroscopic” or density dependent cross sections
- S_{DP} equals TSUNAMI “total” sensitivity

Pick candidates:

- Main fissile and, if present, moderating species
- In various regions to verify that forward and adjoint Monte Carlo solutions in TSUNAMI calculations are locally converged.
- From “special features” of the model such as:
 - A soluble fission product in a fission product critical experiment
 - Important features of a safety basis model like the neutron absorber in poison plates

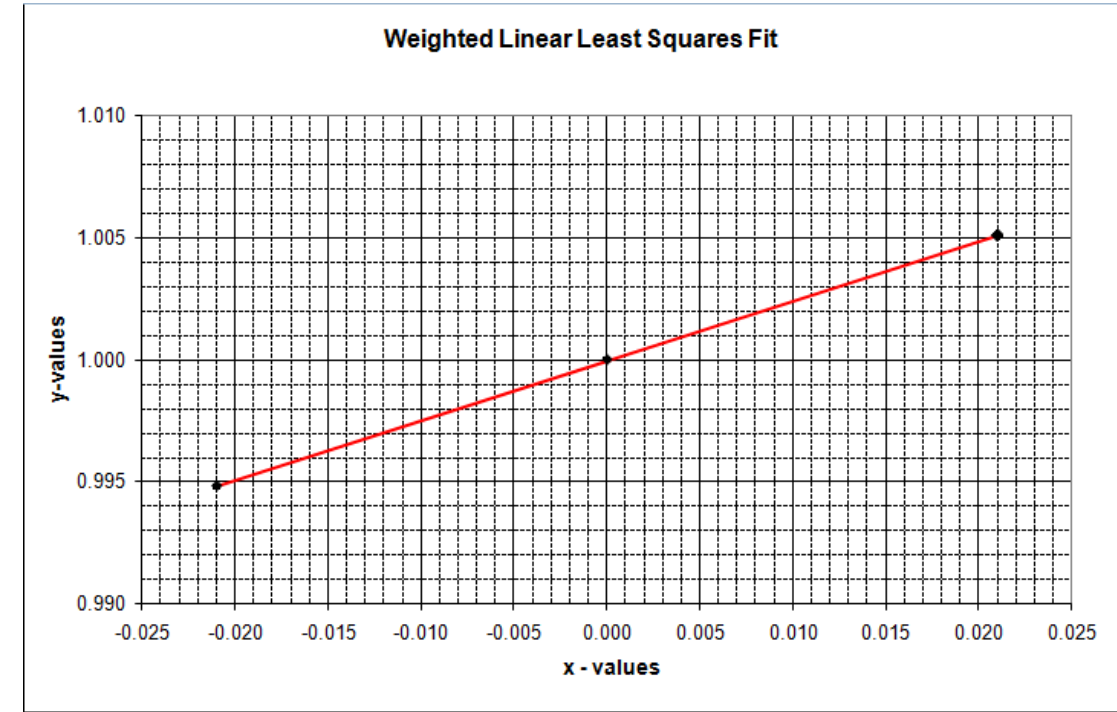
Direct perturbation calculations

- Use TSUNAMI sensitivities to identify good candidates - Focus on sensitivities greater than 0.02 $(\Delta k/k)/(\Delta \sigma/\sigma)$
- Vary density of target nuclide or mixture $\pm$ a few percent
 - ρ_+ , k_+ , ρ_{nom} , k_{nom} , ρ_- , k_-
- Variation should target a 0.5% change in k_{eff} ($0.005 \Delta k_{\text{eff}}$)
- The $\Delta \rho$ needs to be:
 - Large enough to yield a useful σ_{SDP}
 - Small enough to be a linear perturbation



Direct perturbation calculations

- Use TSUNAMI Sensitivity to estimate $\Delta\rho = \frac{\left(\frac{0.005}{k_{eff}}\right)}{S_{Total}}$
- Example $S=0.25$ and $k_{eff}=1$: $\Delta\rho = 0.02$
 - The impact of k_{eff} on $\Delta\rho$ is pronounced for deeply subcritical application systems, but negligible for critical experiments
- For total sensitivities of 0.02 or higher, $\Delta\rho$ will be 25% or less
- Larger perturbations may depart from linear behavior



S	σ	% σ	n	R ²
0.2446	0.0023	0.92%	3	1.0000

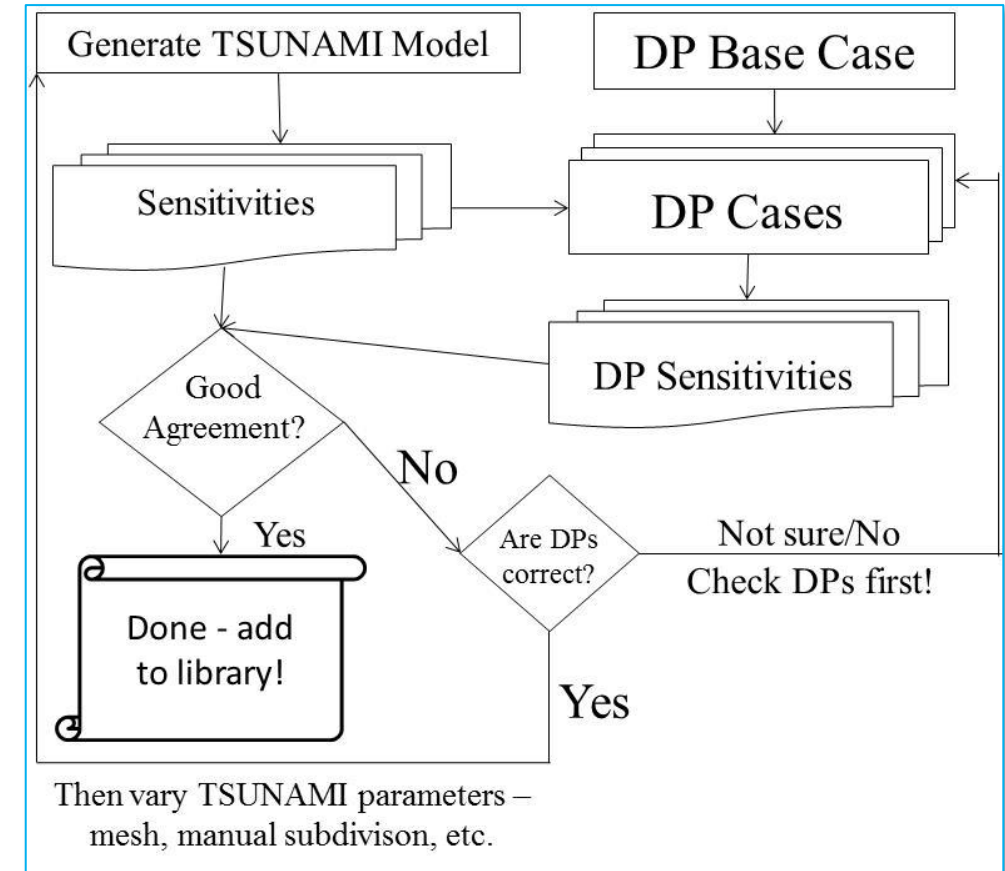
n = number of points used for the linear fit
 R² = goodness of fit parameter, R² = unity means a perfect fit
 S = slope of the line, = direct perturbation sensitivity estimate based on the linear fit
 σ = the uncertainty of the slope, = uncertainty of the DP estimate
 % σ = the uncertainty of the slope as a percentage of the slope

S_{DP}

σ_{SDP}

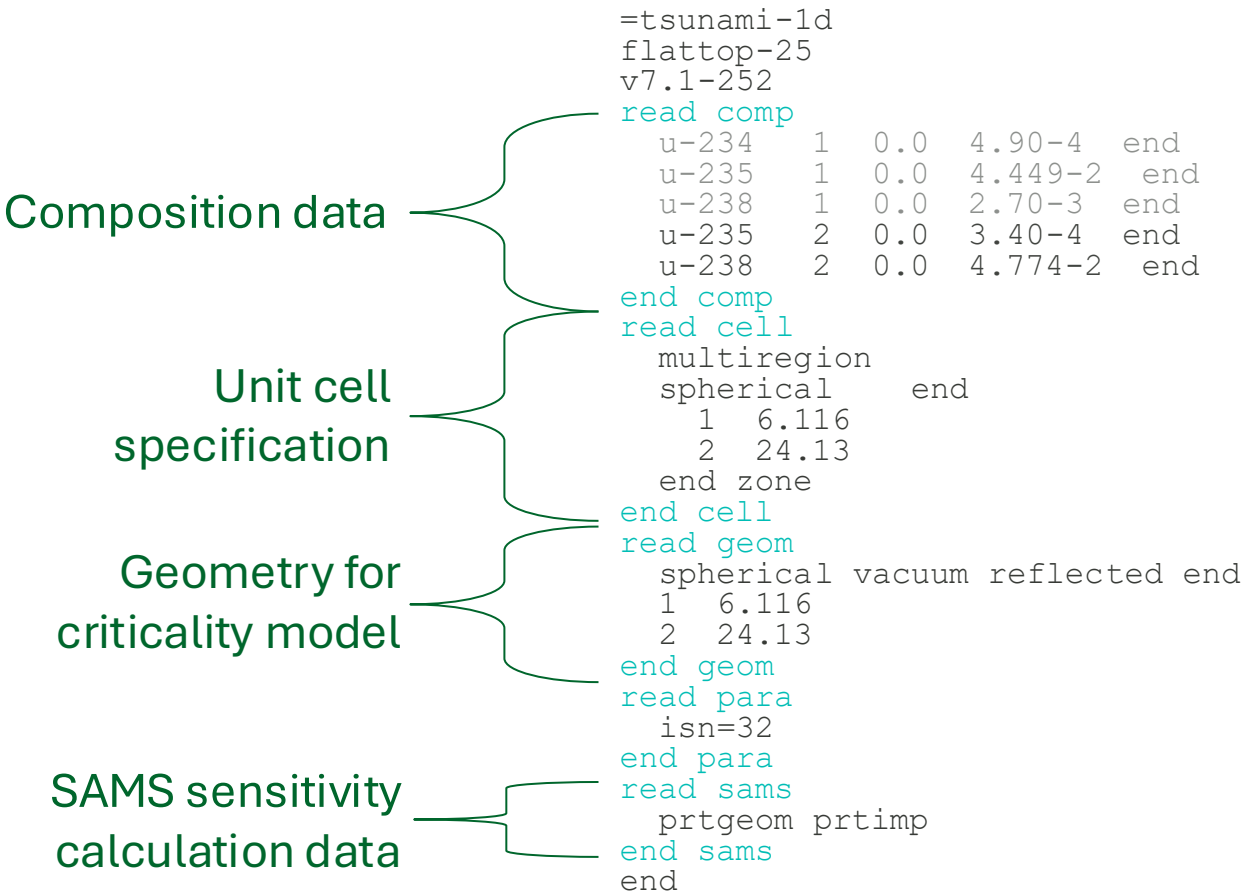
Direct perturbation calculations

- DP sensitivity coefficient is the **reference result** for comparison with TSUNAMI results
- If TSUNAMI and DP disagree:
 1. Convince yourself that the DP is correctly calculated
 2. Examine your TSUNAMI analysis approach
- Heuristic criteria for TSUNAMI accuracy with DP
 - Less than 0.01 difference in absolute calculations
 - Less than 5% difference in relative calculations
 - Less than 2σ between calculations



SCALE multigroup methods

- TSUNAMI uses linear adjoint perturbation theory to compute sensitivity coefficients
 - MG methods use both implicit and explicit components
- TSUNAMI calculations can be performed using SCALE's 1D (XSDRN), 2D (NEWT), or 3D (KENO V.a/VI) transport codes

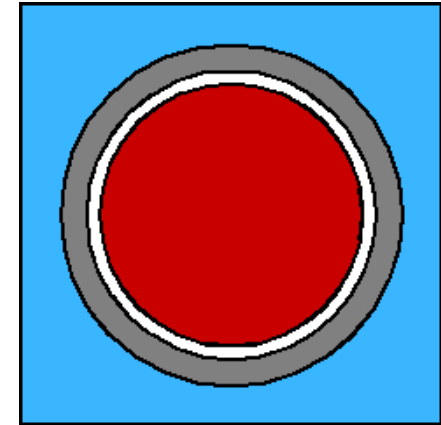


TSUNAMI-1D Input

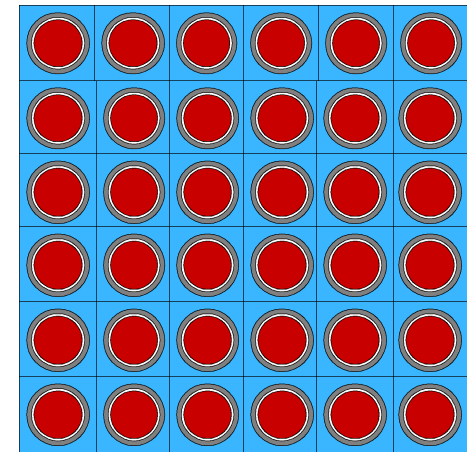
SCALE multigroup methods

TSUNAMI-3D calculations

- Forward and adjoint flux moments are accumulated, multiplied together, and summed over a region
- Region sensitivities are computed based on these fluxes
- Nuclide/mixture sensitivities calculated by summing sensitivities over all regions in which the nuclide occurs in each mixture
- Total nuclide sensitivities calculated by summing all instances of a nuclide
- Total mixture sensitivities calculated by summing all nuclides in each mixture
- Sensitivity coefficient generation happens in SAMS



4 flux regions
fuel, gap, clad, mod.

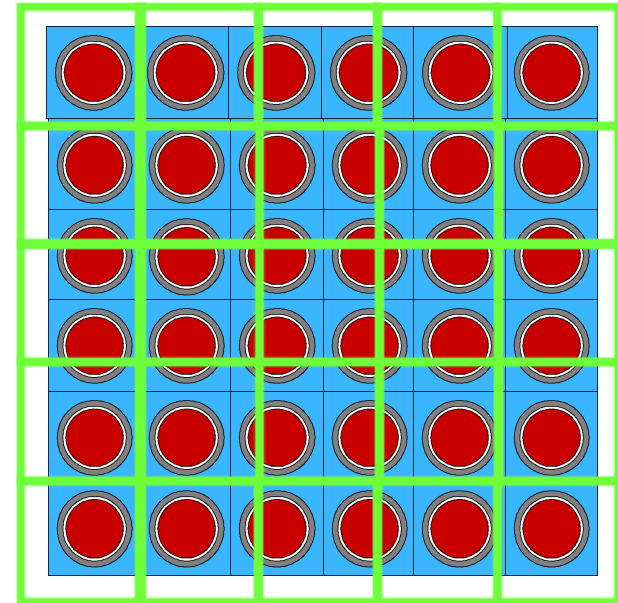


6×6 Array of 4-region cell
for 144 regions

SCALE multigroup methods

TSUNAMI-3D calculations

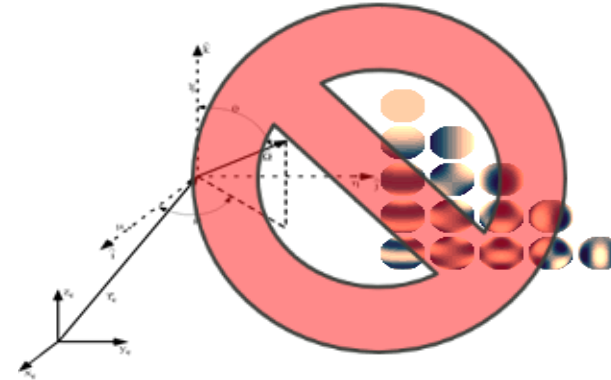
- Use mesh to refine flux solution
- Automated spatial mesh generates uniform mesh over entire model
- Alternatively, the user can define the mesh
- Tracking is the same with or without the mesh, but flux solutions are refined within the mesh



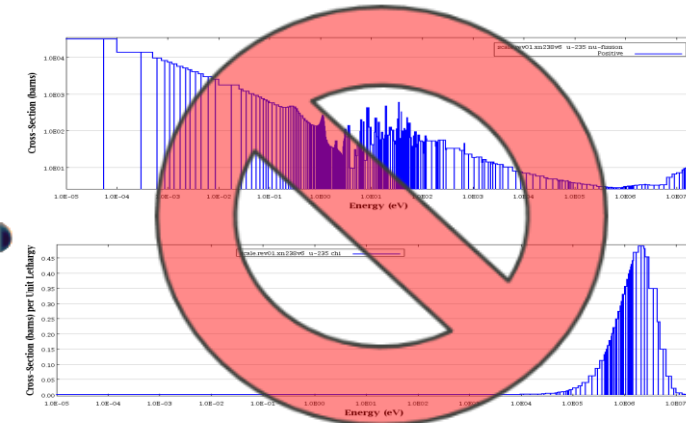
SCALE continuous-energy methods

- Use of CE physics more accurately models the physics of neutron interactions
- CE TSUNAMI-3D can avoid the large memory footprints that can be required by MG TSUNAMI-3D
- CE TSUNAMI-3D calculates sensitivity coefficients without:
 - Flux moment calculations
 - Volume calculations
 - Problem-dependent cross section self-shielding or implicit sensitivity effects
 - Adjoint transport simulation
 - One method does not require a spatial mesh
- Sensitivity coefficients are calculated in the Monte Carlo code
 - SAMS used for editing, not for calculation

Flux Moments



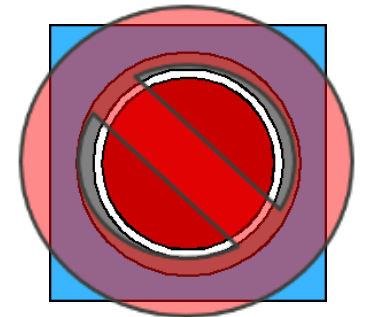
Separate Adjoint Transport Solution



Volume Calculations

$$points = \frac{volume}{\ln(volume/5000)}$$

Cross Section Self-Shielding



Iterated fission probability method (IFP)

- The Iterated Fission Probability (IFP) method estimates the adjoint function with the population of neutrons present in the system during a future generation subsequent to an event
 - IFP requires storing reaction rate tallies for multiple 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
 - **Generally, the most reliable method**

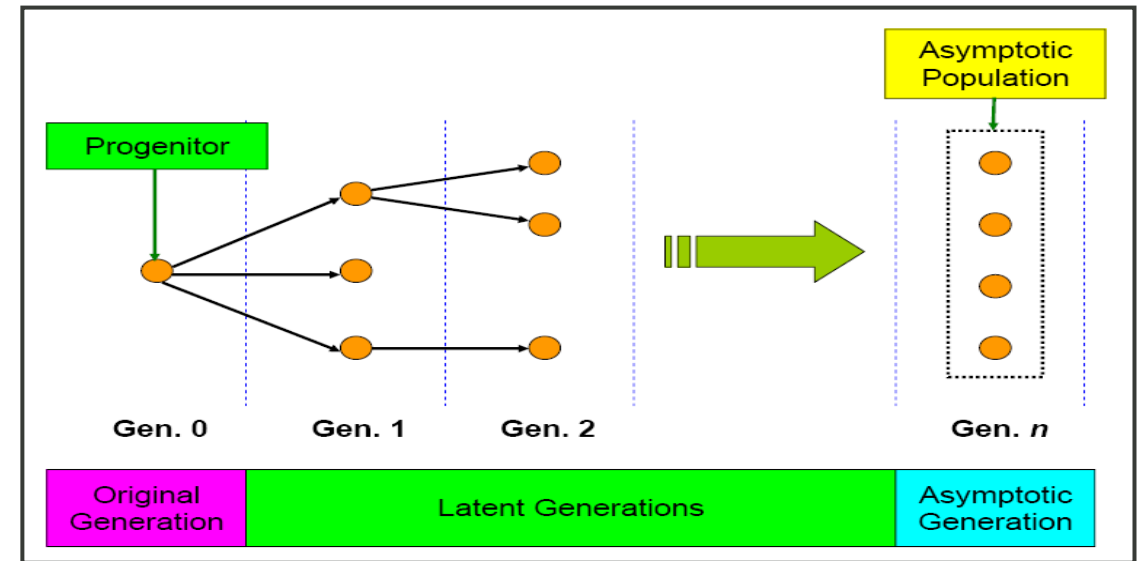


Illustration of the IFP process. Image courtesy of Brian Kiedrowski.

- MCNP KSEN uses IFP
- BLOCKSIZE parameter = latent generations + original + asymptotic = CFP+2

CLUTCH/Contributon methodology

- The CLUTCH method calculates the importance of collisions by tallying how many fission neutrons are created by a particle after it leaves the collision:

$$\boxed{\phi^*(\tau_S)} = \int_V G(\tau_S \rightarrow r) F^*(r) dr,$$

Neutron
importance

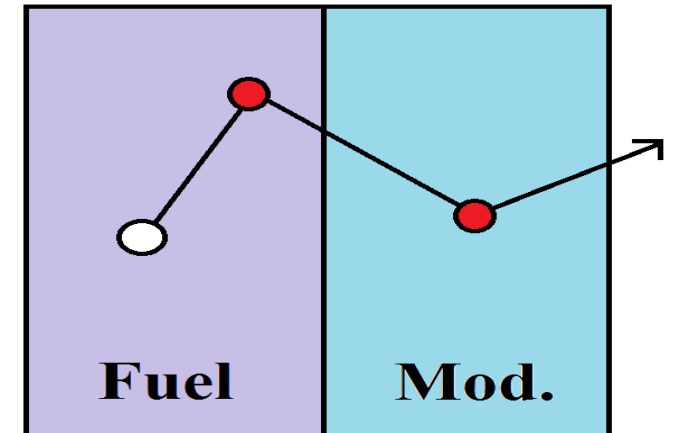
where:

$G(\tau_S \rightarrow r)$ = The number of fission neutrons created at r by the neutron originating in the phase space τ_S .

$F^*(r)$ = The average importance of fission neutrons born at r , or:

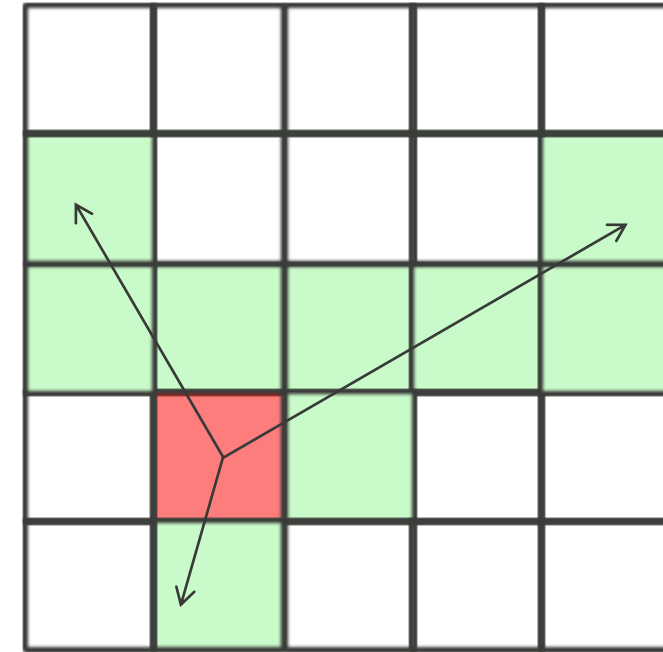
$$F^*(r) = \int_E \int_{\Omega} \frac{\chi(r, E)}{4\pi} \boxed{\phi^*(r, E, \Omega)} d\Omega E.$$

Adjoint flux



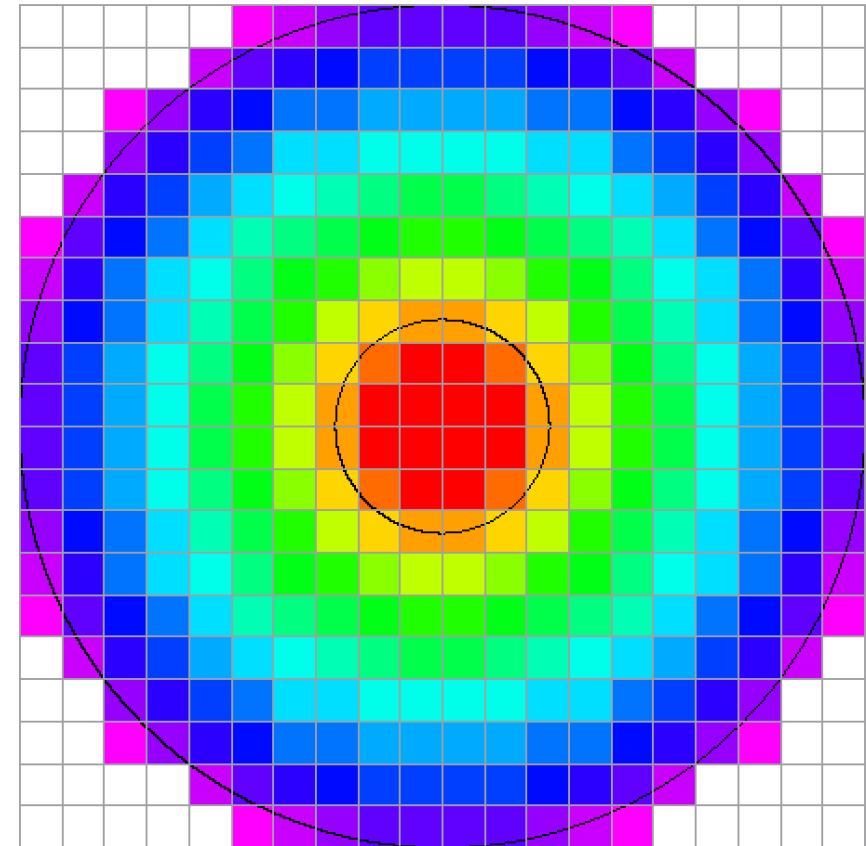
The $F^*(r)$ Function

- The CLUTCH Method uses an importance weighting function, $F^*(r)$, to compute multi-generational sensitivity effects
- The $F^*(r)$ function describes the average importance generated by fission neutrons born at location r
- The $F^*(r)$ function can be calculated using the IFP method during inactive generations with no significant loss of accuracy and with significant memory savings
 - This requires a significant increase in the number of inactive generations: up to hundreds or more



Best Practices for $F^*(r)$ Mesh Generation

- Experience has shown that an $F^*(r)$ mesh with 1–2 cm intervals often yields accurate sensitivity coefficients
 - Much larger mesh have been used successfully in some applications
- The $F^*(r)$ mesh must cover all regions in a problem containing **fissionable** material
- The $F^*(r)$ function is tallied during skipped generations, so NSK must be adjusted to allow for $F^*(r)$ convergence
 - Simulating between 1 and 100 inactive particle histories per $F^*(r)$ mesh interval may produce an accurate $F^*(r)$ tally
 - Lady Godiva with a 1 cm cubic mesh has 5,832 intervals ($18 \times 18 \times 18$)
 - 5,832 mesh intervals $\times$ 100 histories per interval / 10,000 particles per gen. = ~58 skipped generations



Uncertainty analysis

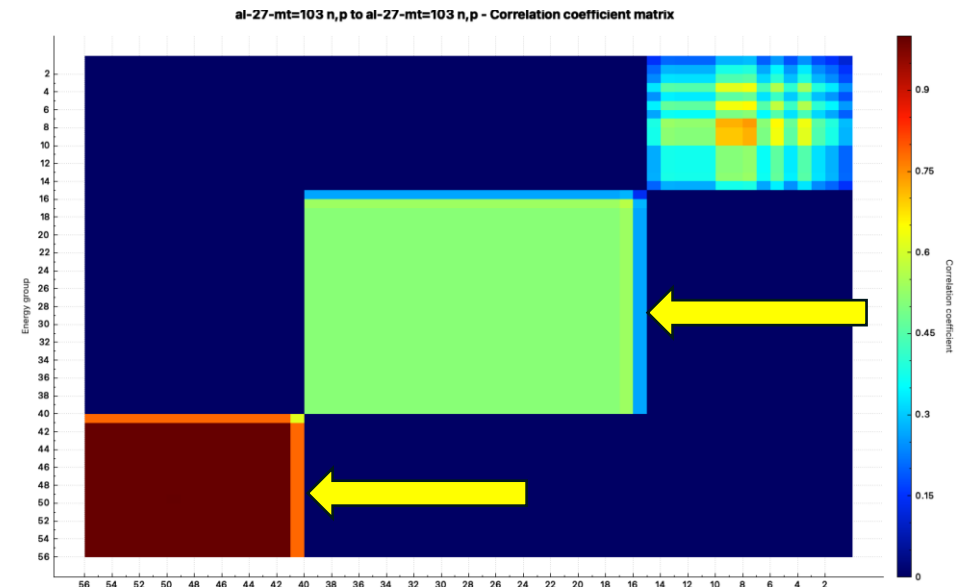
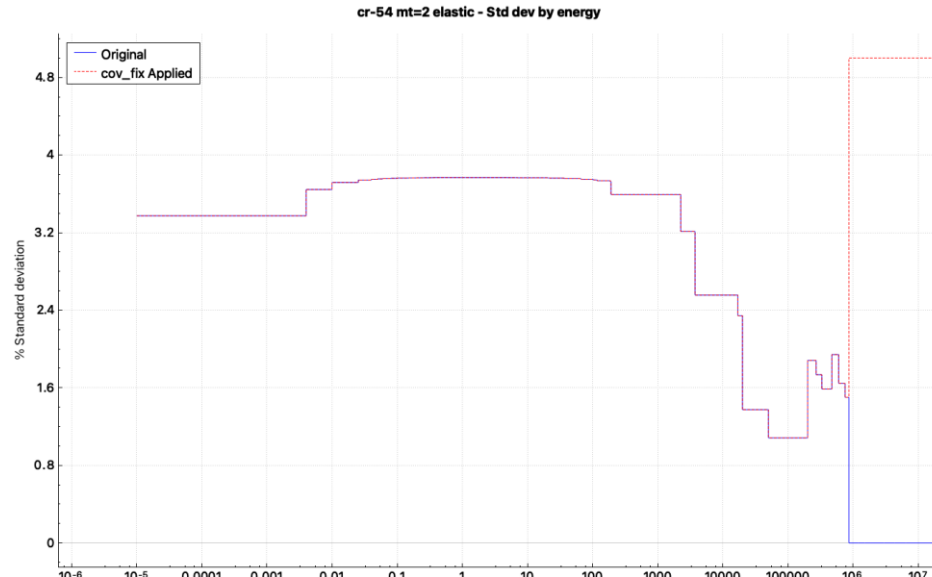
- Uncertainty is estimated uncertainty in system k_{eff} caused by cross section uncertainty
 - Unit is $\% \Delta k/k$
 - Estimated based on measurements, correlations, etc.
- Uncertainty in the system k_{eff} is propagated from the cross section uncertainty using the sensitivity coefficient:

$$\sigma_{k_{\text{eff}}} \left(\frac{\% \Delta k}{k} \right) = \sigma_{\sigma} \left(\frac{\% \Delta \sigma}{\sigma} \right) \times S \left(\frac{\frac{\Delta k}{k}}{\frac{\Delta \sigma}{\sigma}} \right)$$

- “Fundamental theorem of TSUNAMI”: biases are caused by nuclear data errors which are bounded by the nuclear data uncertainties
- Uncertainty therefore gives an upper bound for the magnitude of the bias

Patching covariance data

- The covariance library is not exhaustive—some reactions in some energy groups for some nuclides have no data
- TSUNAMI-IP allows these data to be patched
 - *cov_fix*: Replace zero and large (standard deviation > 1000%) values on diagonal of cross section covariance data with user input values and default values (default is off)
 - *use_dcov*: Use user-defined default covariance data for nuclide-reaction pairs not included on the covariance data file (default is off)



Patching covariance data

- Parameters **udcov_fast**, **udcov_inter**, and **udcov_therm** specify default standard deviation in respective energy ranges when finer control is needed
 - Fully correlated within respective energy ranges
 - Historically, values of 40%, 10% or 20%, and 5% have been used
- Any values calculated in an extended c_k or uncertainty edit are flagged if patched data are used

al-27 n,p

al-27 n,p

1.0381E-04 +/- 8.0750E-11 *

cr-54 elastic

cr-54 elastic

9.1691E-05 +/- 1.3890E-10 ***

- Straightforward to turn on and off and gauge impact

```
cov_fix
use_dcov
udcov_therm=0.05
udcov_inter=0.10
udcov_fast=0.40
```

Mechanics of Bias Estimation

- Extended uncertainty edit needed
 - *uncert_long* in TSUNAMI-IP
- Collect uncertainties for all reactions for nuclide of interest
 - Include chi and nubar for fissile species
- RSS uncertainties for all reactions together to get total uncertainty:

$$\sqrt{\Sigma(\textit{positive_values})^2 - \Sigma(\textit{negative_values})^2}$$

- Uncertainty addresses size of bias, but not direction

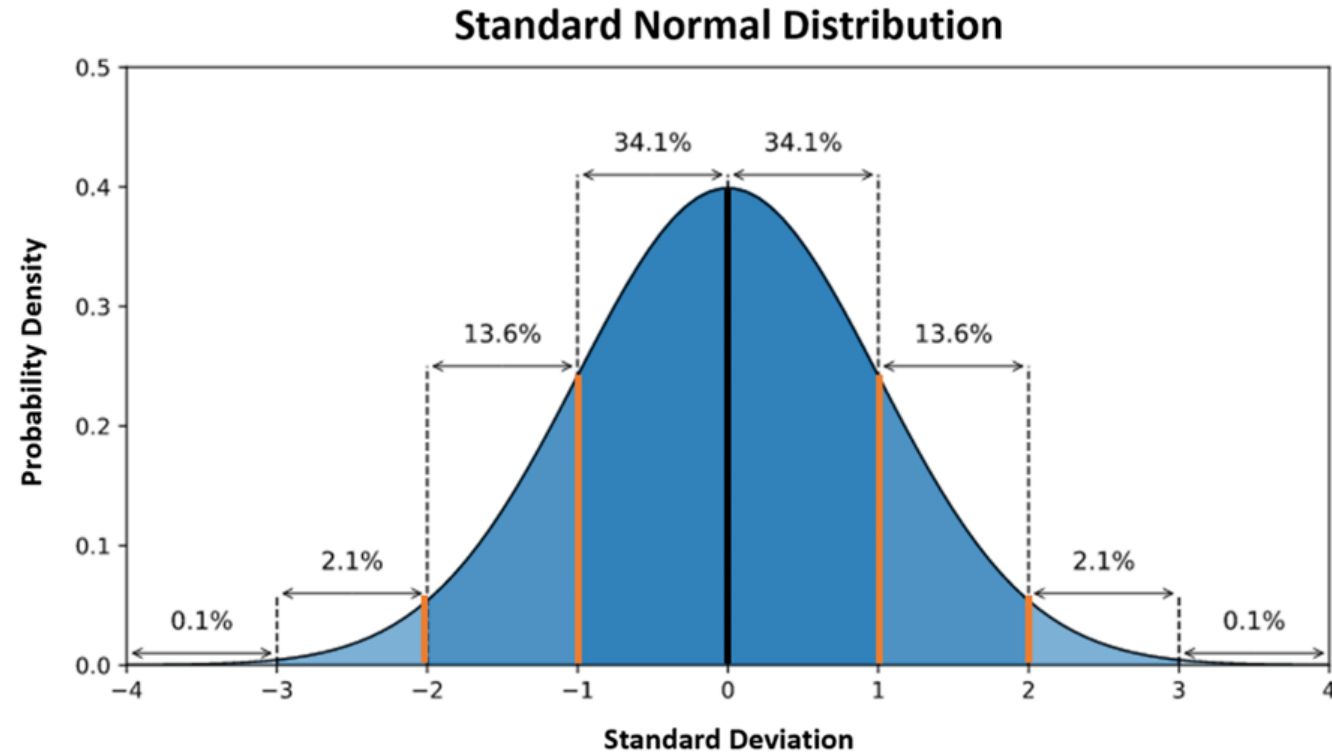
UF₆ package example: ¹⁹F uncertainties

Covariance Matrix Nuclide/Reaction with Nuclide/Reaction		Uncertainty Resulting from This Matrix (%Δk/k)
elastic	elastic	7.7453E-2 ± 1.1507E-4
(n, n')	elastic	-5.4268E-2 ± 9.2636E-5
(n, n')	(n, n')	4.9825E-2 ± 1.0833E-4
(n, α)	(n, α)	3.3215E-2 ± 1.1823E-6
(n, α)	elastic	1.0290E-2 ± 1.9386E-6
(n, p)	(n, p)	3.3352E-3 ± 3.1509E-8
(n, γ)	(n, γ)	2.1309E-3 ± 1.1539E-9
(n, p)	elastic	1.9835E-3 ± 5.3537E-8
(n, d)	elastic	4.4065E-4 ± 3.1825E-9
(n, γ)	elastic	-3.9572E-4 ± 1.6918E-9
(n, d)	(n, d)	3.5893E-4 ± 1.0069E-9
(n, 2n)	elastic	-1.9932E-4 ± 1.9929E-9
(n, t)	elastic	1.2846E-4 ± 2.9849E-10
(n, t)	(n, t)	5.6156E-5 ± 5.4188E-11
(n, n')	(n, 2n)	-1.8009E-5 ± 7.4920E-11
(n, 2n)	(n, 2n)	1.0539E-5 ± 1.0567E-11

- $k_{\text{eff}} = 0.93592 \pm 0.00019$
- 16 nuclide/reaction uncertainty contributions listed, 12 positive and 4 negative values
- Sum of the squares of the positive terms is 0.00971 (%Δk/k)², and the sum of the squares of the negative terms is 0.00295 (%Δk/k)²
- The difference between these two numbers is 0.00677 (%Δk/k)² and the square root of the difference is 0.082 %Δk/k

UF₆ package example

- This value should be multiplied by the system k_{eff} of 0.93592 to determine the reactivity margin as 0.077 % Δk or 77 pcm
- This nominally provides a 1σ estimate of the uncertainty, so it could be increased to a 95% confidence interval by multiplying by 1.96, assuming a normally distributed uncertainty and two-sided statistics
- The final result of this calculation is 151 pcm



Benchmark applicability

- Current guidance for applicability of critical experiments for bias and bias uncertainty determination:

$c_k \geq 0.9$ → applicable

$0.9 > c_k \geq 0.8$ → marginally applicable

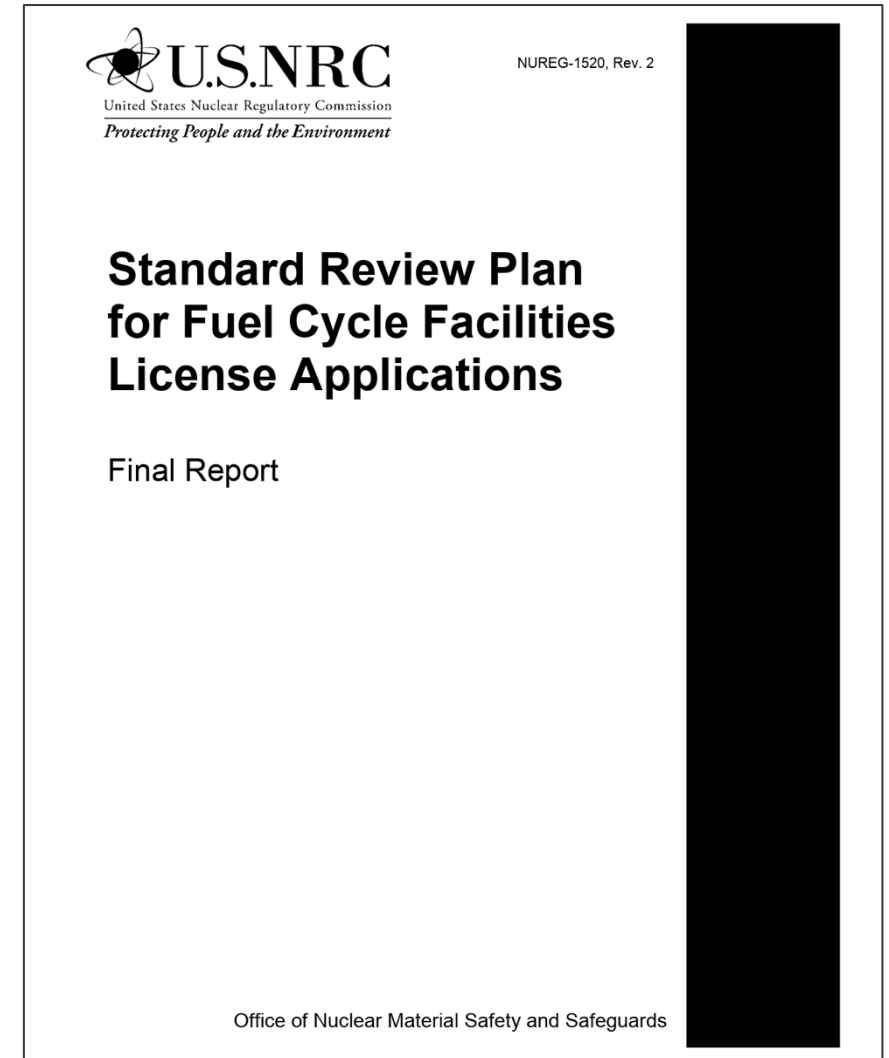
$c_k < 0.8$ → not applicable

- From NUREG-1520, Rev. 2, Appendix 5B:

$c_k \geq 0.95$ → very high degree of similarity

$0.9 > c_k \geq 0.95$ → high degree of similarity*

*Similarity determination should be supplemented with other methods



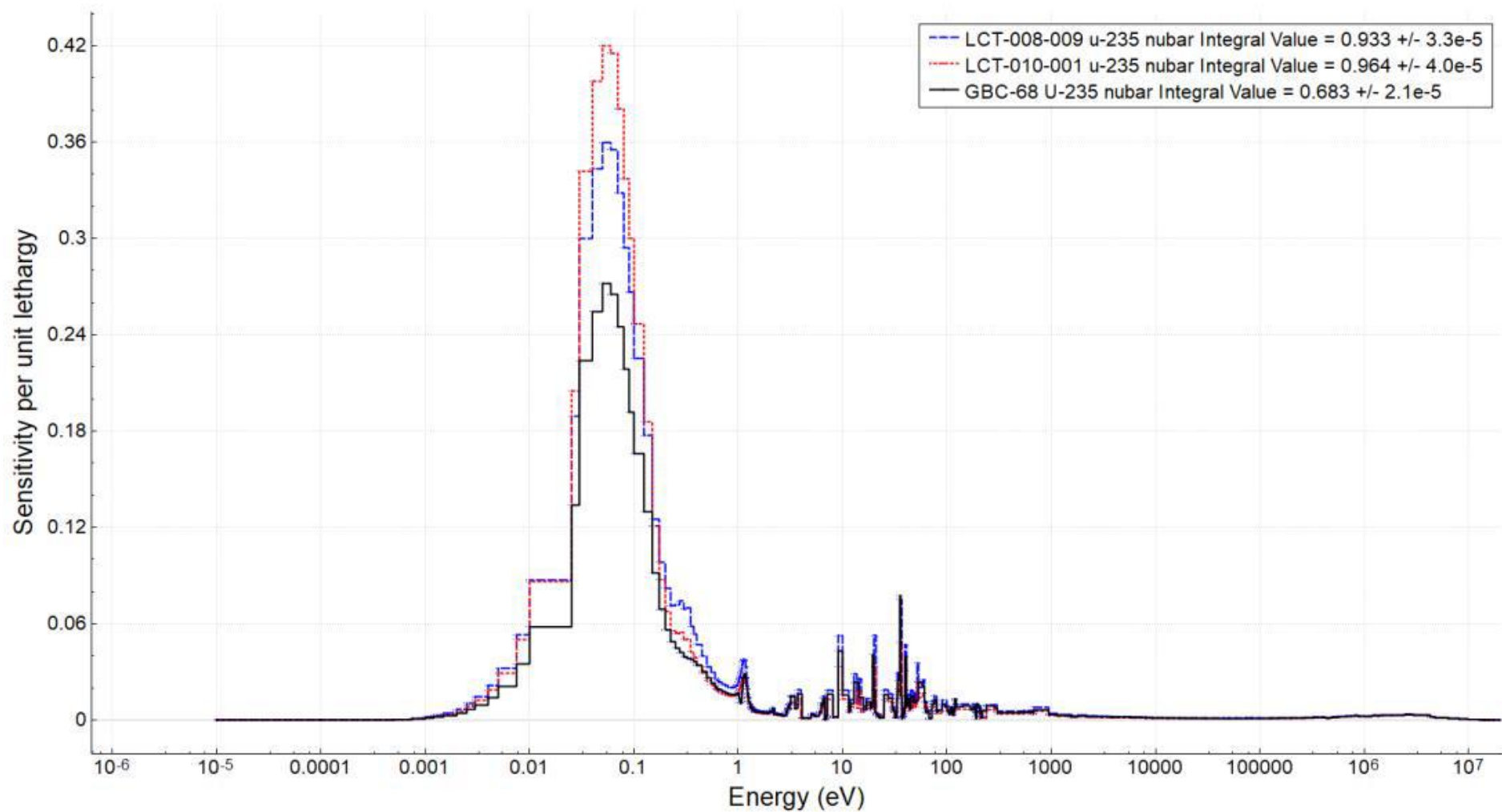
BWR BUC example with GBC-68 cask

The top five contributing nuclide-reaction pairs for two benchmarks with GBC-68 cask

LEU-COMP-THERM-008-009		c_k
nuclide-reaction	nuclide-reaction	contribution
$^{235}\text{U } \bar{\nu}$	$^{235}\text{U } \bar{\nu}$	0.40558
$^{238}\text{U } (n, \gamma)$	$^{238}\text{U } (n, \gamma)$	0.21637
$^{235}\text{U } (n, \gamma)$	$^{235}\text{U } (n, \gamma)$	0.06966
$^{235}\text{U } (n, \text{fission})$	$^{235}\text{U } (n, \text{fission})$	0.05445
$^1\text{H } (n, \gamma)$	$^1\text{H } (n, \gamma)$	0.03701
$c_k = 0.8850$		

LEU-COMP-THERM-010-001		c_k
nuclide-reaction	nuclide-reaction	contribution
$^{235}\text{U } \bar{\nu}$	$^{235}\text{U } \bar{\nu}$	0.30959
$^{238}\text{U } (n, \gamma)$	$^{238}\text{U } (n, \gamma)$	0.09580
$^{235}\text{U } (n, \gamma)$	$^{235}\text{U } (n, \gamma)$	0.06303
$^1\text{H } (n, \gamma)$	$^1\text{H } (n, \gamma)$	0.05884
$^{235}\text{U } (n, \text{fission})$	$^{235}\text{U } (n, \text{fission})$	0.03157
$c_k = 0.6438$		

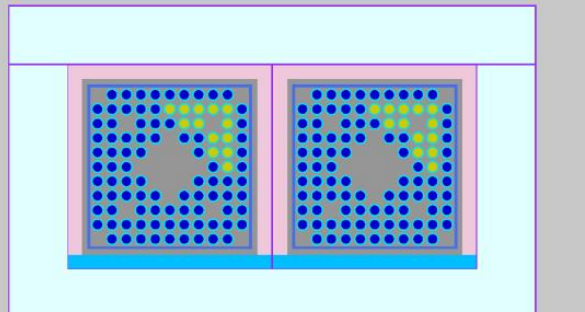
BWR BUC example with GBC-68 cask



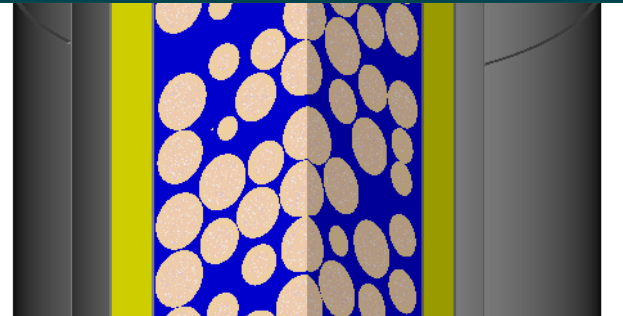
²³⁵U Sensitivities for GBC-68 and Two ICSBEP Benchmarks

Case studies

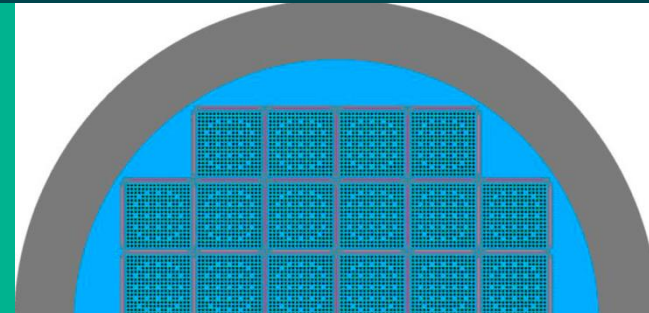
**BWR Fresh
Fuel Shipping
Package**



**Drum-Type
Package
Containing
TRISO Fuel**

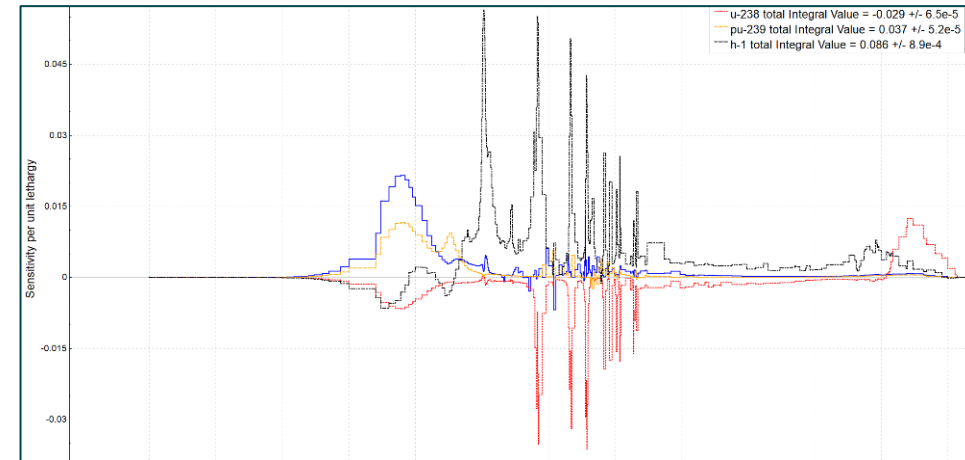
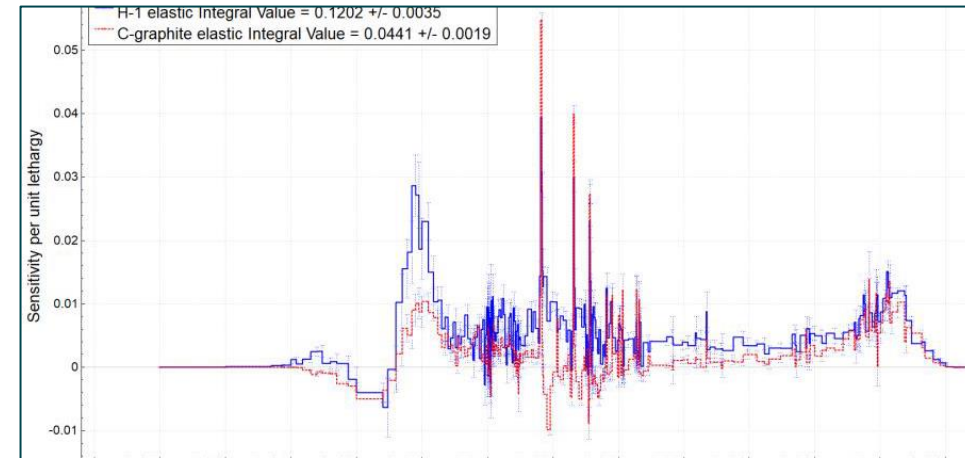
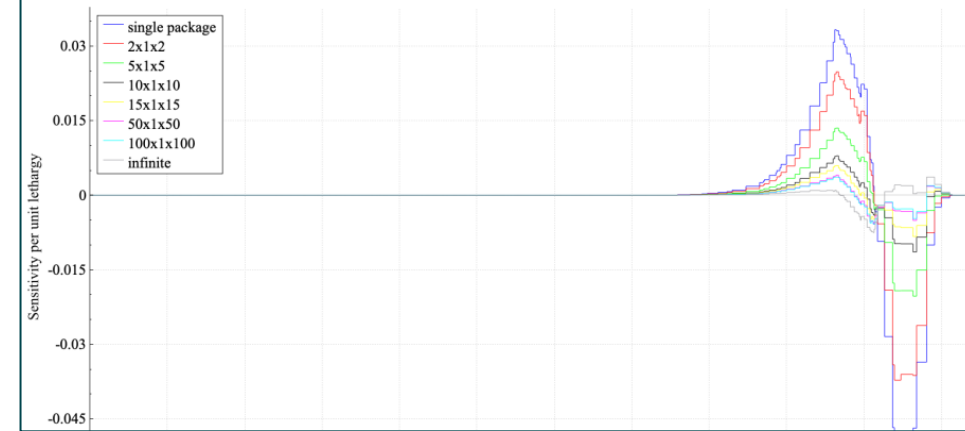


**Generic
Storage Cask
for PWR SNF**



Case studies

- Demonstrates the S/U methods presented in the NUREG with application-specific recommendations
 - Case studies provide clarification and demonstration of the SCALE TSUNAMI S/U tools in NCS validation
- Three case studies are presented:
 1. A fresh fuel package containing two BWR fuel assemblies
 2. A drum-type package containing TRISO fuel
 3. A generic SNF storage canister containing irradiated PWR assemblies
- Each case study presents different challenges and highlights different aspects of using S/U tools in NCS validation

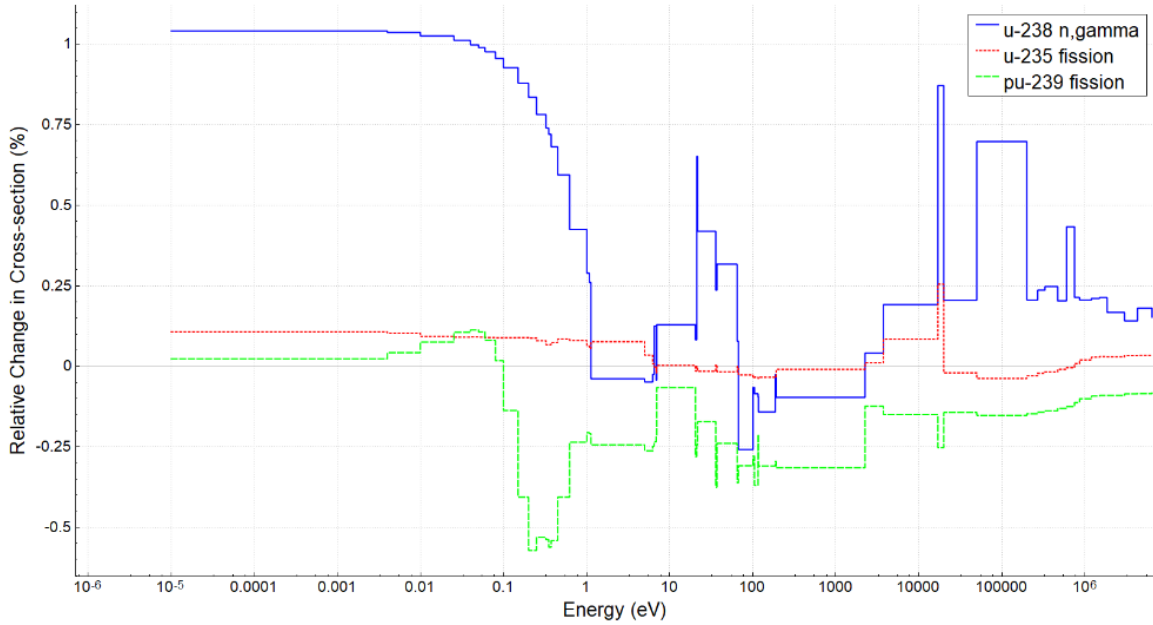


Demo: BWR package

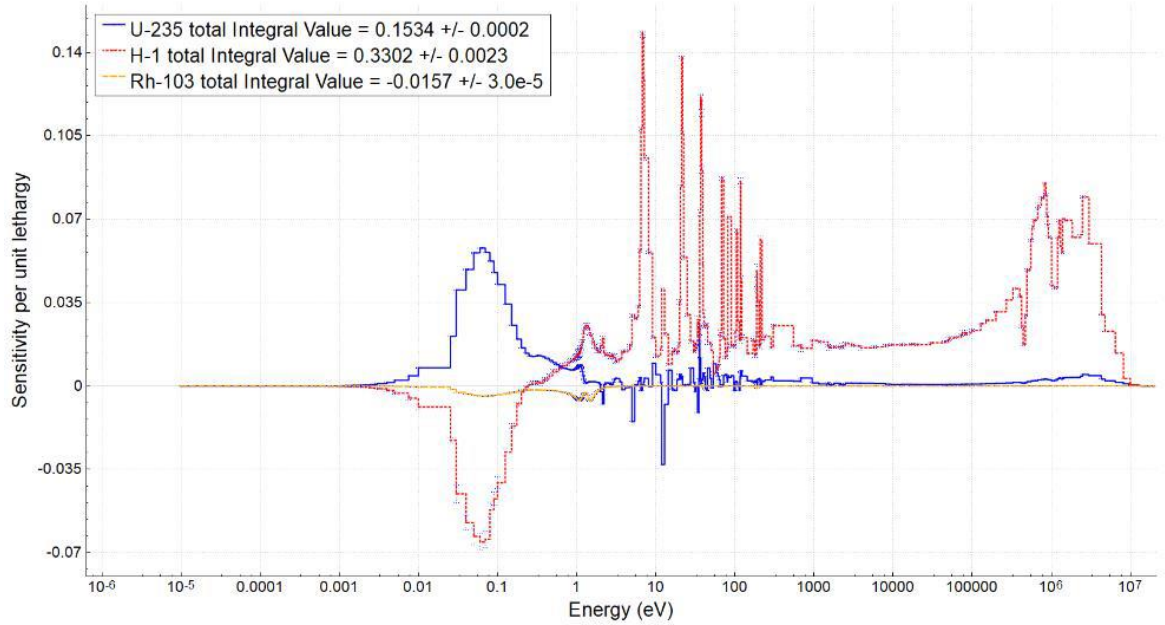
- TSUNAMI-3D
 - Visualize model with Fulcrum
 - Plot SDF
- TSUNAMI-IP
 - Run application with benchmark set for c_k values with both libraries
 - Examine largest contributors to c_k
 - Examine largest contributors to nuclear data-induced uncertainty

Advanced methods

TSURFER



TSAR



TSURFER



Tool for S/U analysis of Response Functionals using Experimental Results

- Biases are differences between measured and calculated values
- Measured systems have potentially correlated uncertainties
- Calculated values have uncertainties, primarily due to uncertainties in the nuclear data, that are correlated between systems that use the same data
- A consistent set of data adjustments can be determined that eliminates biases for the benchmarks, accounting for the uncertainties and correlations, within a known uncertainty
- The adjustments can be used to project biases from the benchmarks to a bias and bias uncertainty for targeted application systems

Consistency assessment

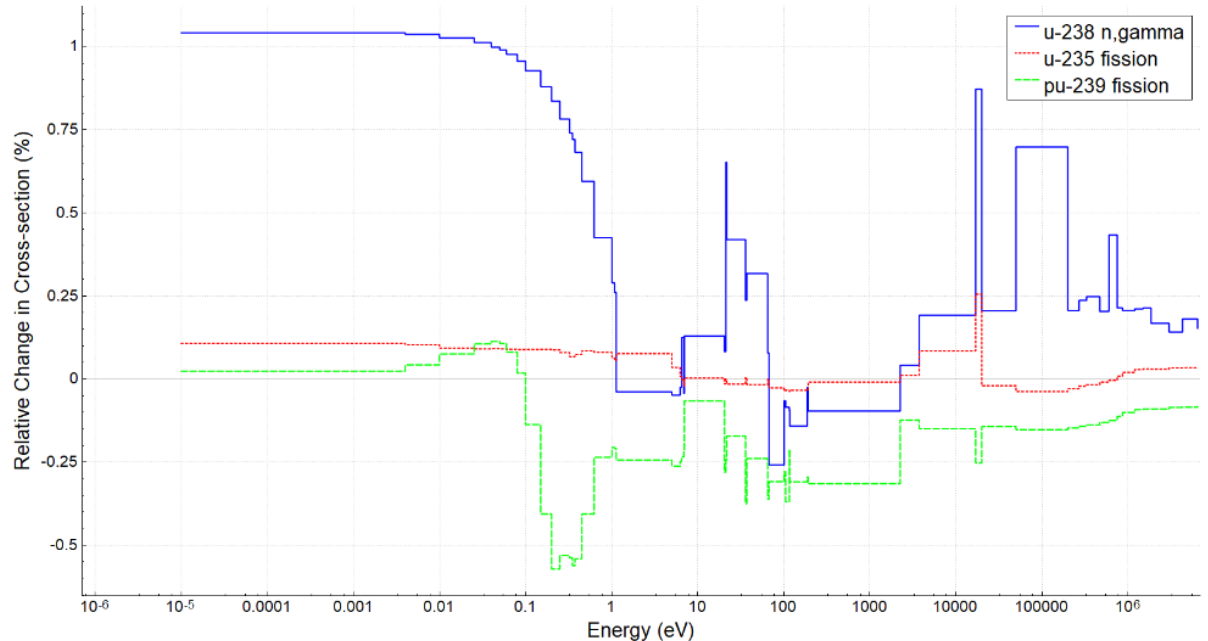
- TSURFER minimizes experimental and calculated differences by adjusting:
 - Measured data within their uncertainties
 - Nuclear data within their uncertainties
 - Identified correlations (data and experiment) are considered
- Nuclear data adjustments impact computed values as predicted by sensitivity coefficients
- χ^2 – number of standard deviations a data point moves.
 - Typical target is not to move any data point by more than $1.2 \chi^2$
- Nuclear data adjustments are constrained by all experiments that use the same cross section in the same spectrum
- Experiment adjustments are constrained by correlations among experiments

Impact of an Adjustment on your Application

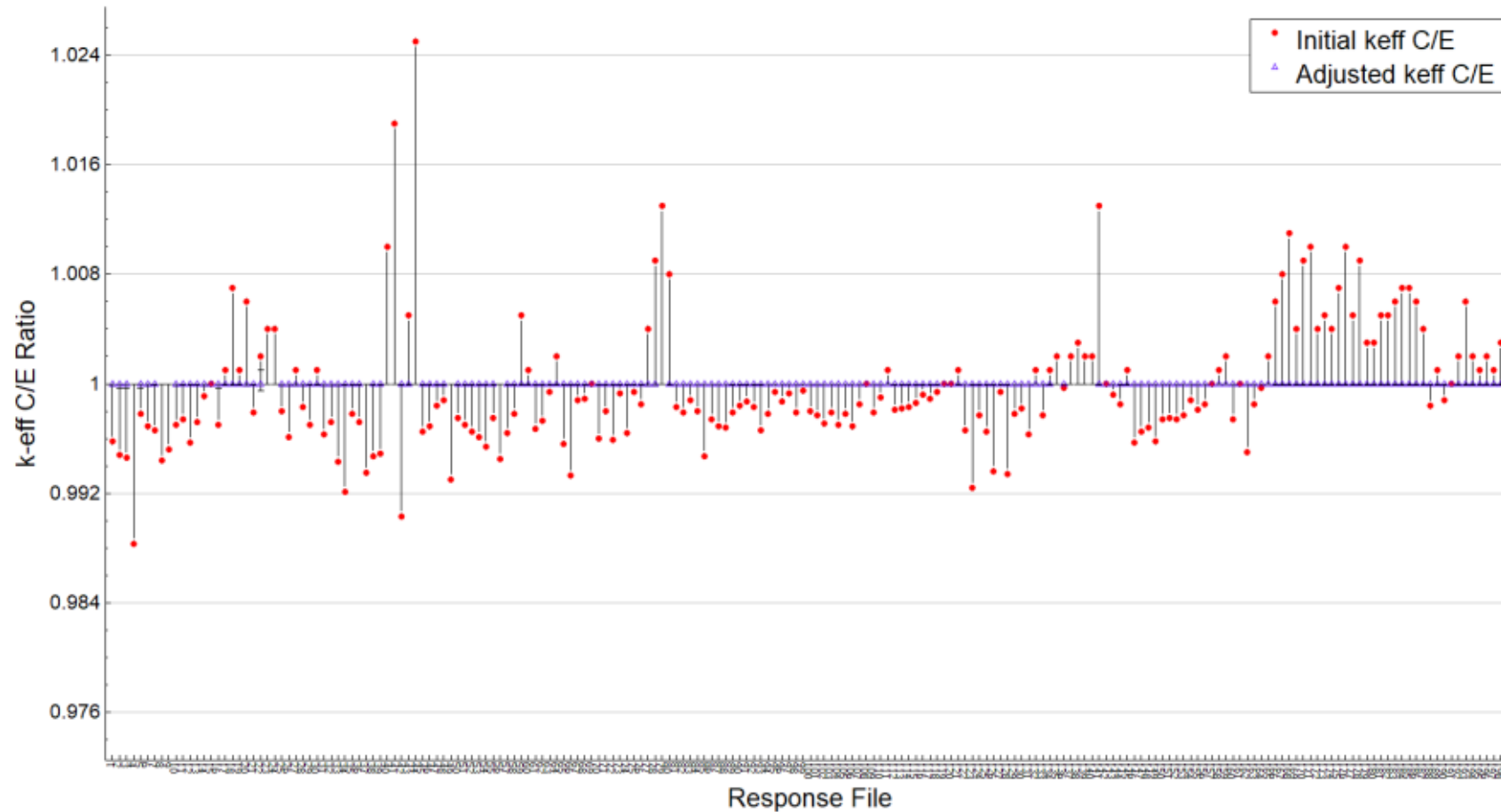
- GLLS data-adjustments are determined by matching calculated and measured responses for experiments
- There are no measured results for applications
 - Application shares common nuclear data with the experiments
- Data adjustments also impact application:

$$k_{eff}^{adj} = k_{eff}^{nom} + S(a' - a),$$

- where: $a' - a$ is the adjustments determined by TSURFER and S are the calculated sensitivities for the application

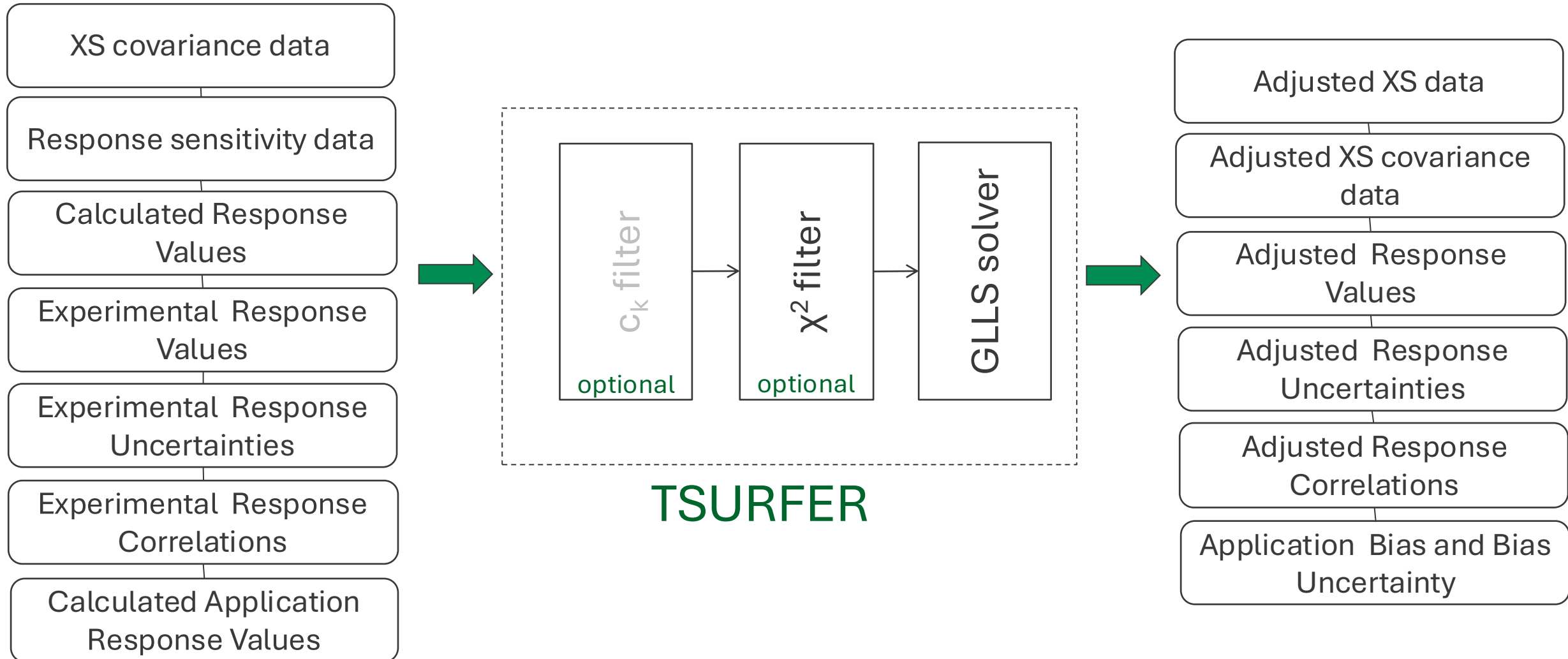


Data Adjustment Techniques for Bias Assessment



After adjustment $C' = E' (k_{calc}^{adj} = k_{meas}^{adj})$ and $\sigma_{e'} = \sigma_{c'} (C_{kk'} = C_{mm'})$

TSURFER Computation



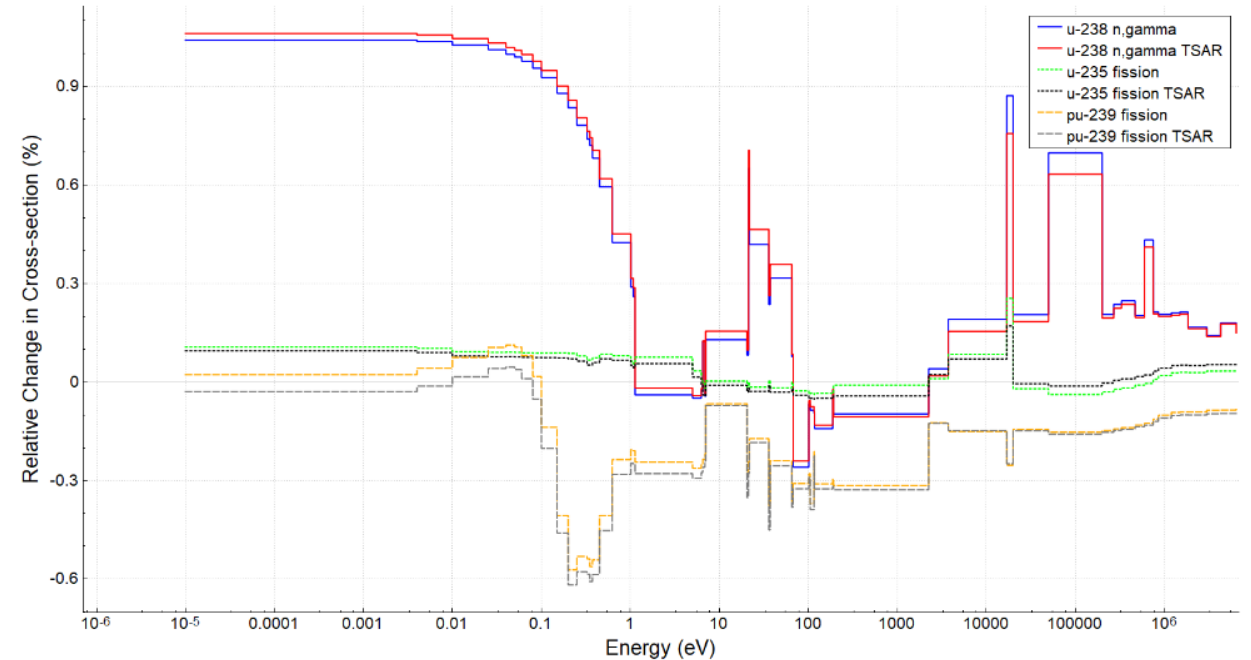
TSAR

- TSAR –Tool for Sensitivity AnalYsis of Reactivity - is a tool that computes reactivity sensitivities from k_{eff} sensitivity data computed from TSUNAMI-1D and -3D
 - Uses covariance data to compute reactivity uncertainty
 - Magnifies important processes that can lead to k_{eff} biases
 - Example: When using replacement experiments, the difference in k_{eff} of the experiment with and without the test material is due primarily to any bias introduced by the test material
 - TSAR will give the sensitivity of the change in k_{eff} due to this test material.



TSAR

- Reactivity, in this case, is the difference between states and is not necessarily one state measured relative to the critical state
- The reactivity sensitivity isolates the impact of factors that change between the two configurations in a way that k_{eff} sensitivities do not
- TSAR calculates these reactivity sensitivities given the k_{eff} sensitivities from both state points, making the TSAR calculation an additional step after two TSUNAMI-1D or -3D calculations
- The reactivity sensitivities can be provided to TSURFER as additional measurements with which to adjust nuclear data
 - This pair of tools is particularly useful for extracting additional information from substitution experiments
 - TSAR also propagates nuclear data covariances with the reactivity sensitivities to determine the data-induced uncertainty in the reactivity response.



Summary

Goal: To provide an up-to-date document on best practices for S/U methods and how the tools should be used by NRC staff and applicants for nuclear criticality safety (NCS) validation

NCS validation: to ensure that modeling used in evaluations are validated against benchmark experiments that are neutronically similar to the application systems

S/U methods allow for quantifying similarity between systems and estimating bias and bias uncertainties in k_{eff} , as well as estimations of gap penalties for insufficient validations

Discussion focus on SCALE TSUNAMI tools/methods; however, general S/U methods are consistent across code packages

Sensitivity/Uncertainty Methods for Nuclear Criticality Safety Validation

Manuscript Completed: December 2024
Date Published: April 2025

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Online Platform for Benchmark Experiment Selection

Improving criticality safety predictions through information-theoretic experiment evaluation

Why It Matters

- Accurate criticality safety predictions depend on relevant benchmark experiments
- Benchmarks reduce uncertainty in eigenvalue bias calculations
- Current methods use sensitivity profiles and prior covariance matrices
- Key challenge: selecting new experiments that maximize uncertainty reduction

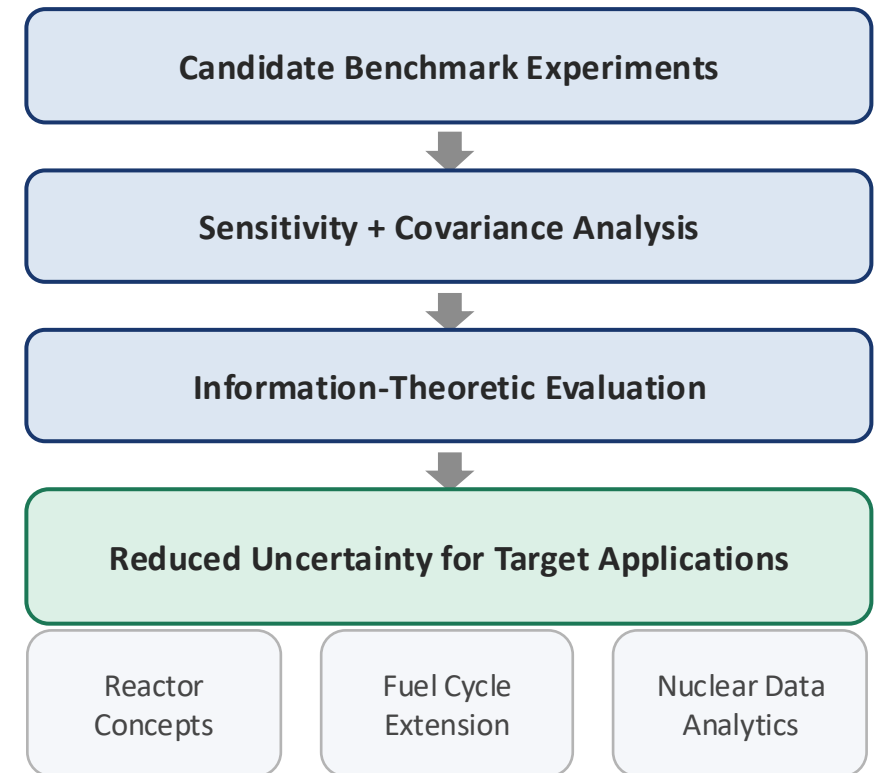
What Is Being Developed

- An open-source Python toolkit with a web-based interface
- Quantitative evaluation of proposed benchmark experiments
- Built around an information-theoretic metric developed in earlier work
- Identifies experiments that reduce uncertainties not covered by existing benchmarks

Impact

- New fuel and reactor concepts
- Extended fuel life cycles
- Nuclear data pipeline enhancements

Workflow



Questions?



ORNL

