



February 12, 2025

Sensitivity Uncertainty Methods for Criticality Safety Validation

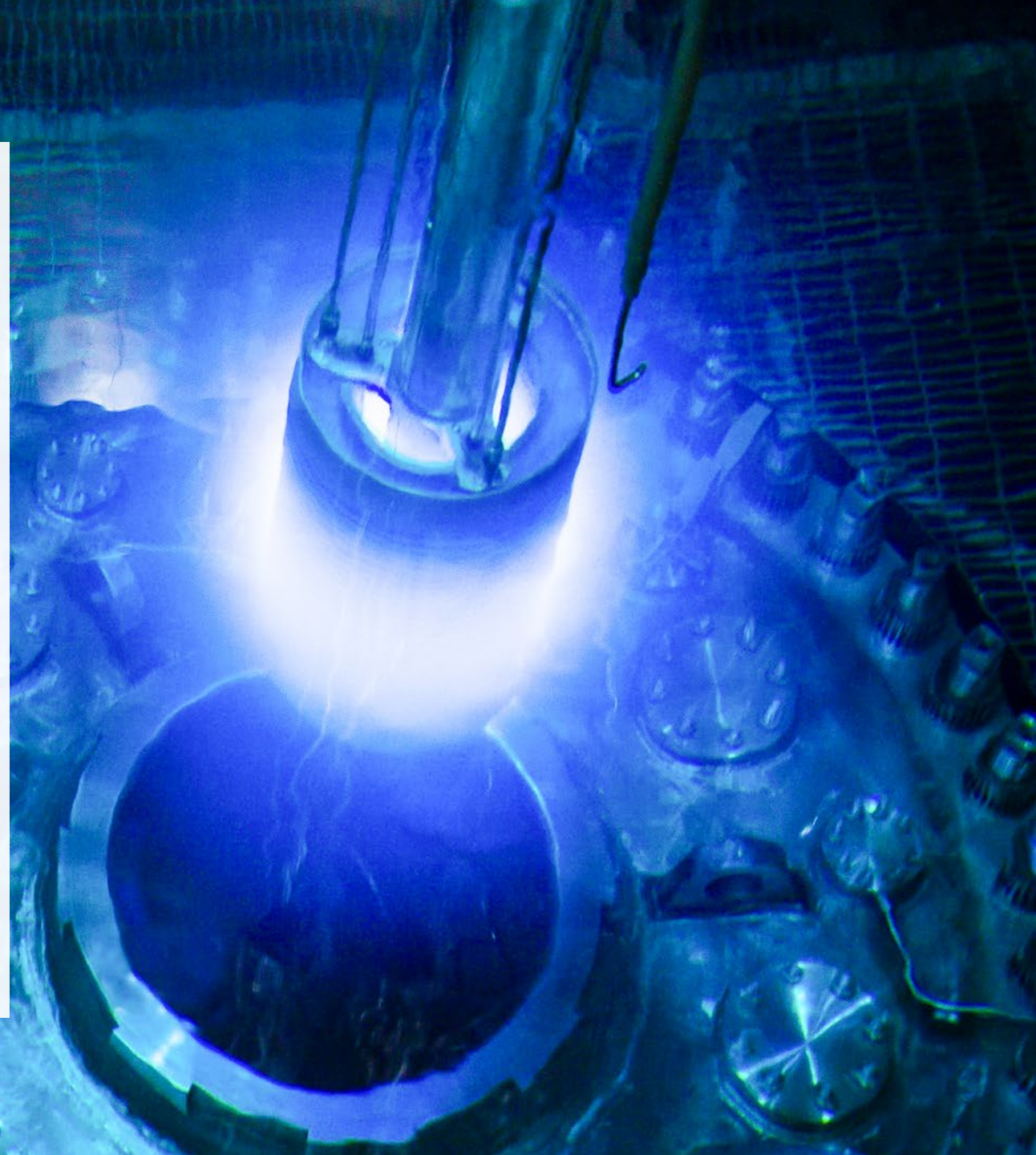
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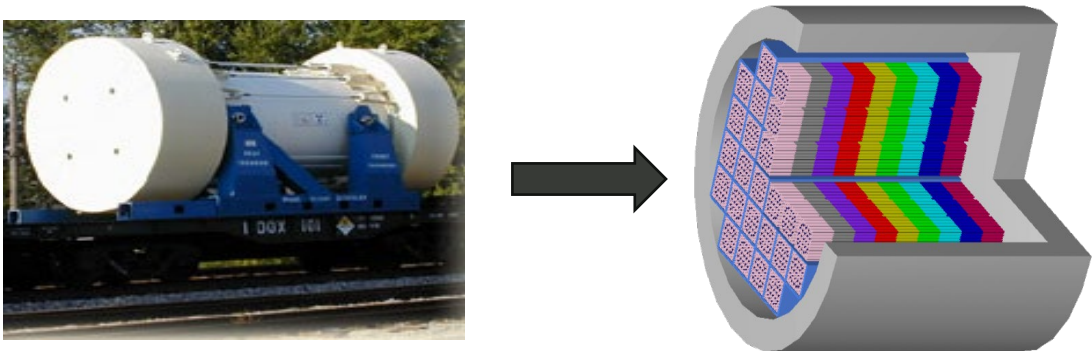


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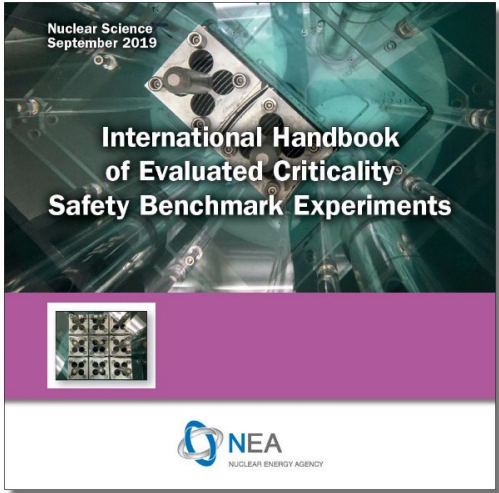
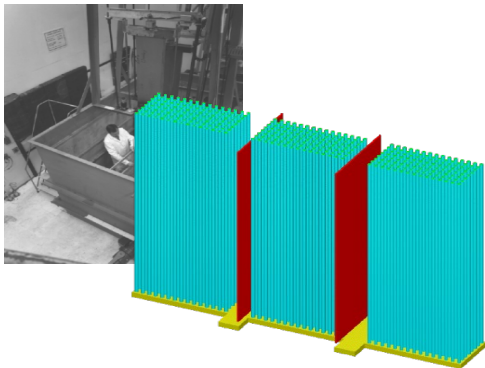
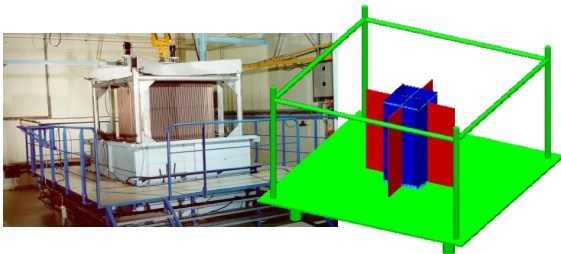
ORNL offers several Sensitivity Uncertainty (SU) tools to help validation efforts



Can I predict the error in my computational model?
How much confidence do I have in my error prediction?



I know the computational error in these experiments. Can I somehow use that knowledge ?

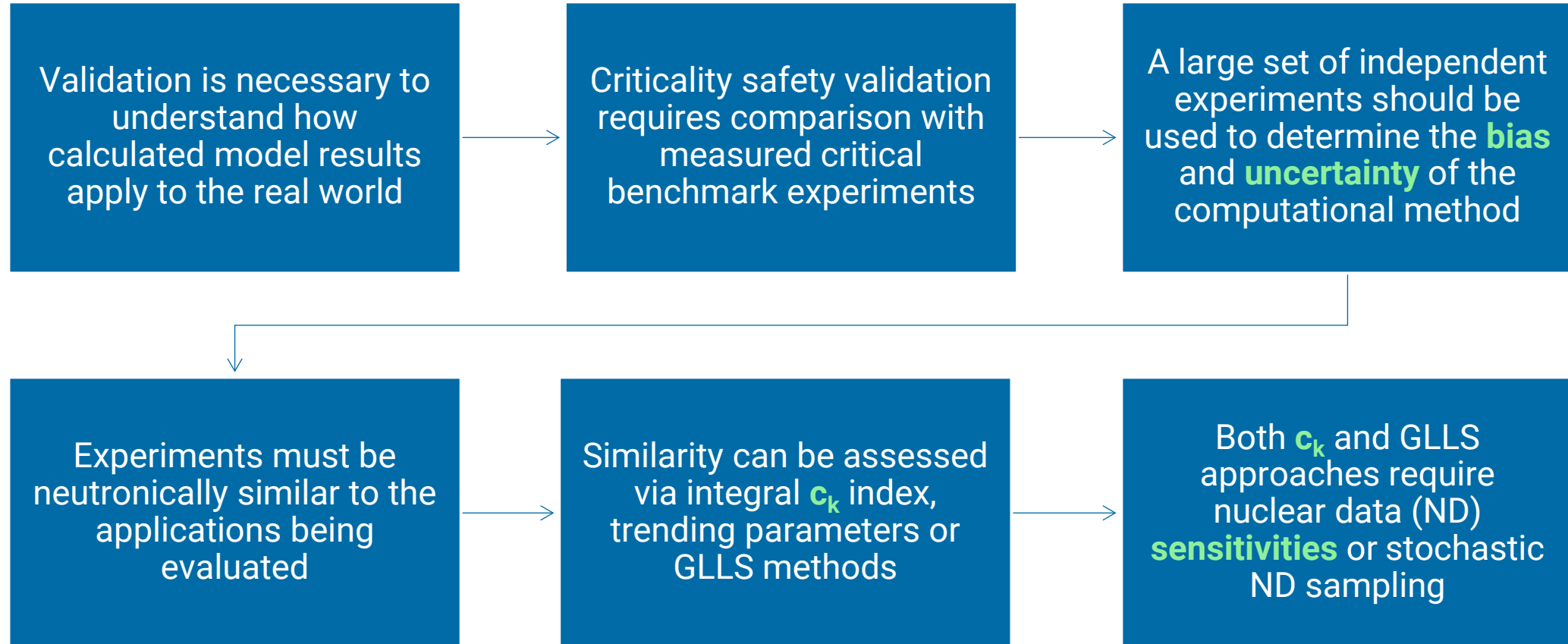


VADER

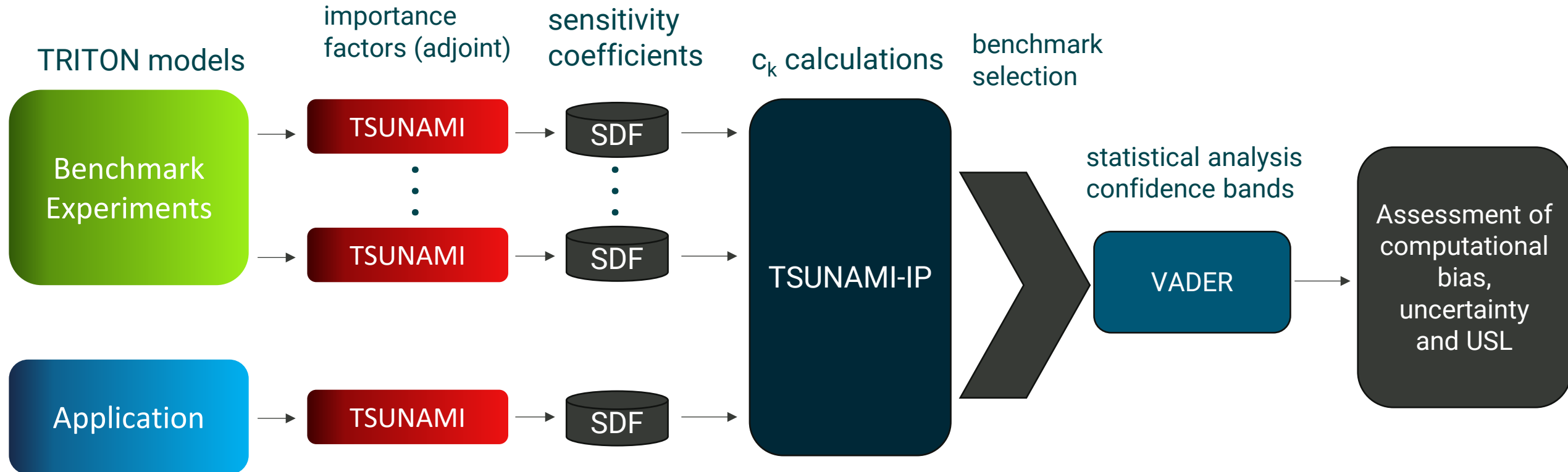
Qc



We need SU methods for identification of benchmarks that are similar to our application



The current validation process at ORNL is based on c_k methodology



The main assumption in similarity-based methods : Bias is caused by errors in nuclear data

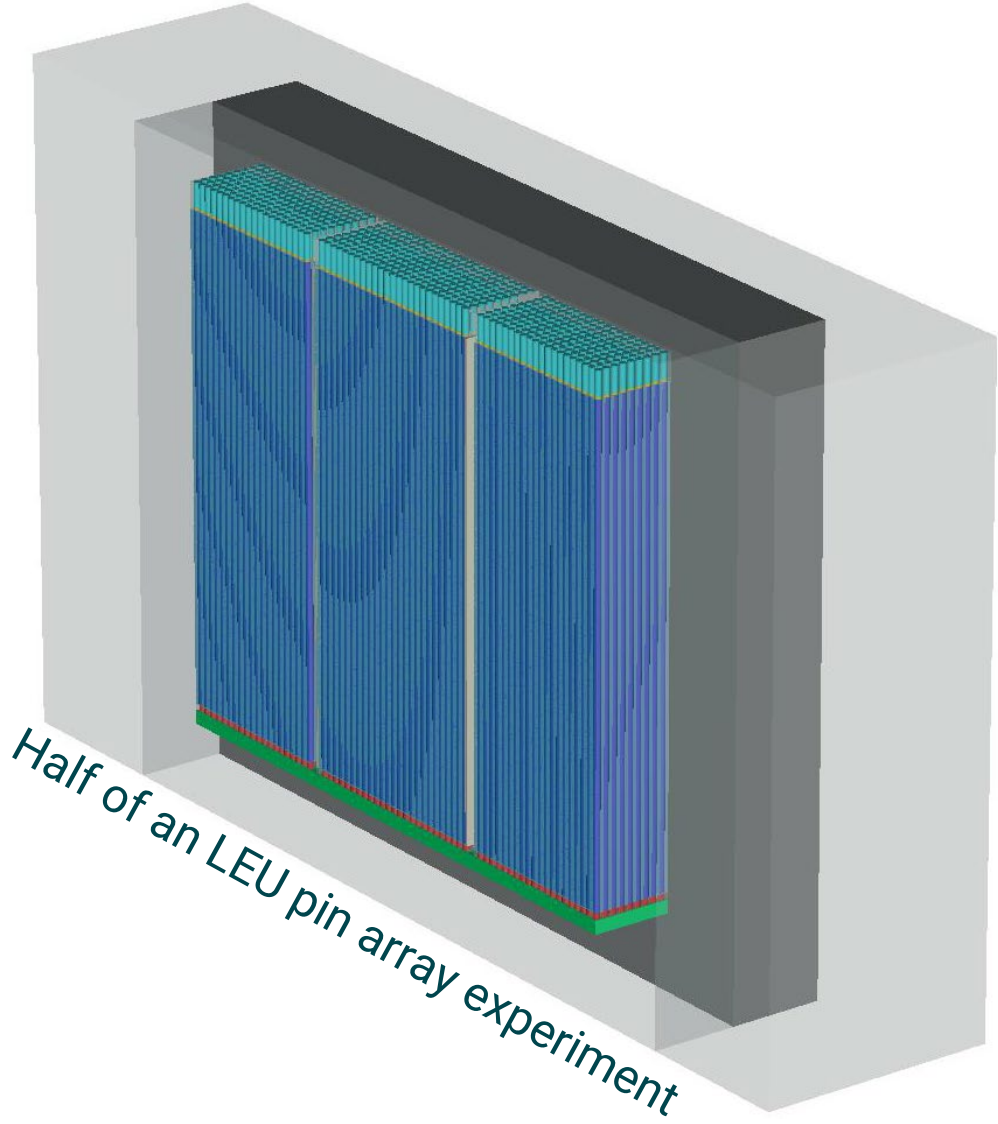
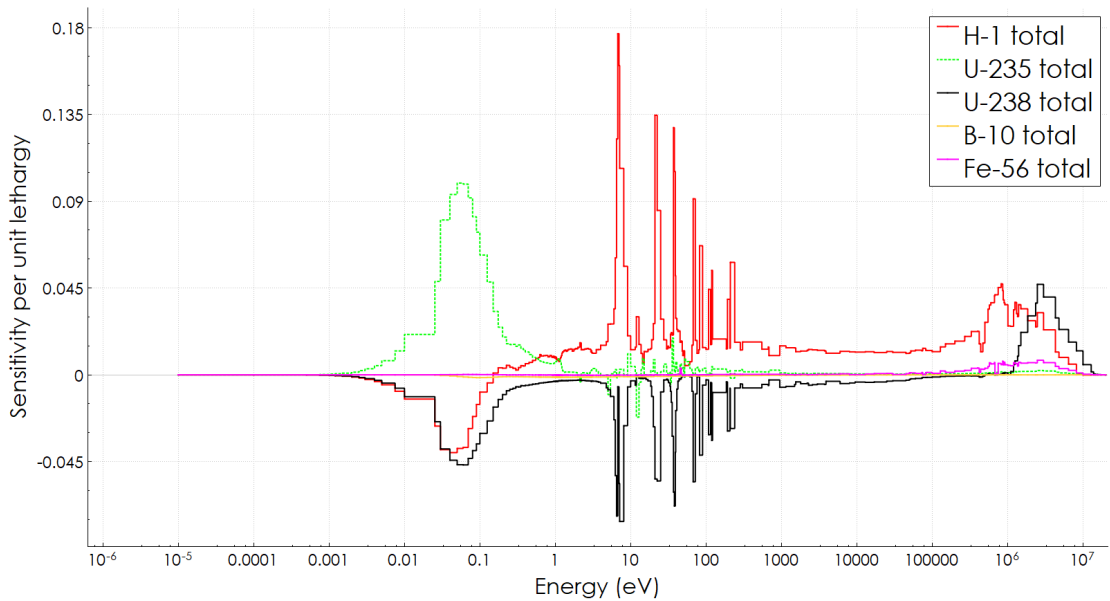
- **Assumption/Principle:** Bias is caused by errors in nuclear data, which are bounded by their uncertainties (covariances)
- Systems will have **similar computational biases** if they have **similar sensitivities** to the same **nuclear data** errors
- System sensitivity combined with nuclear data uncertainties estimate potential for bias in each system

$$s = \frac{\partial k}{\partial \Sigma} \longleftrightarrow \Delta k_{eff} = s \Delta \Sigma$$

- Comparison examines nuclide-, reaction-, and energy-dependent data

An example of k_{eff} sensitivity coefficients for a critical experiment

Nuclide	Material	Sensitivity
H-1	Moderator	0.240
U-235	Fuel	0.242
U-238	Fuel	-0.140
B-10	Absorber	-0.010
Fe-56	Reflector	0.020



Sensitivity coefficients help us to propagate ND uncertainties

- Our methods employ dimensionless sensitivity coefficients
- Sensitivity coefficients represent the relative expected change in k_{eff} due to a relative change in nuclear data
- What would happen to the system k_{eff} if some piece of data were changed by some amount

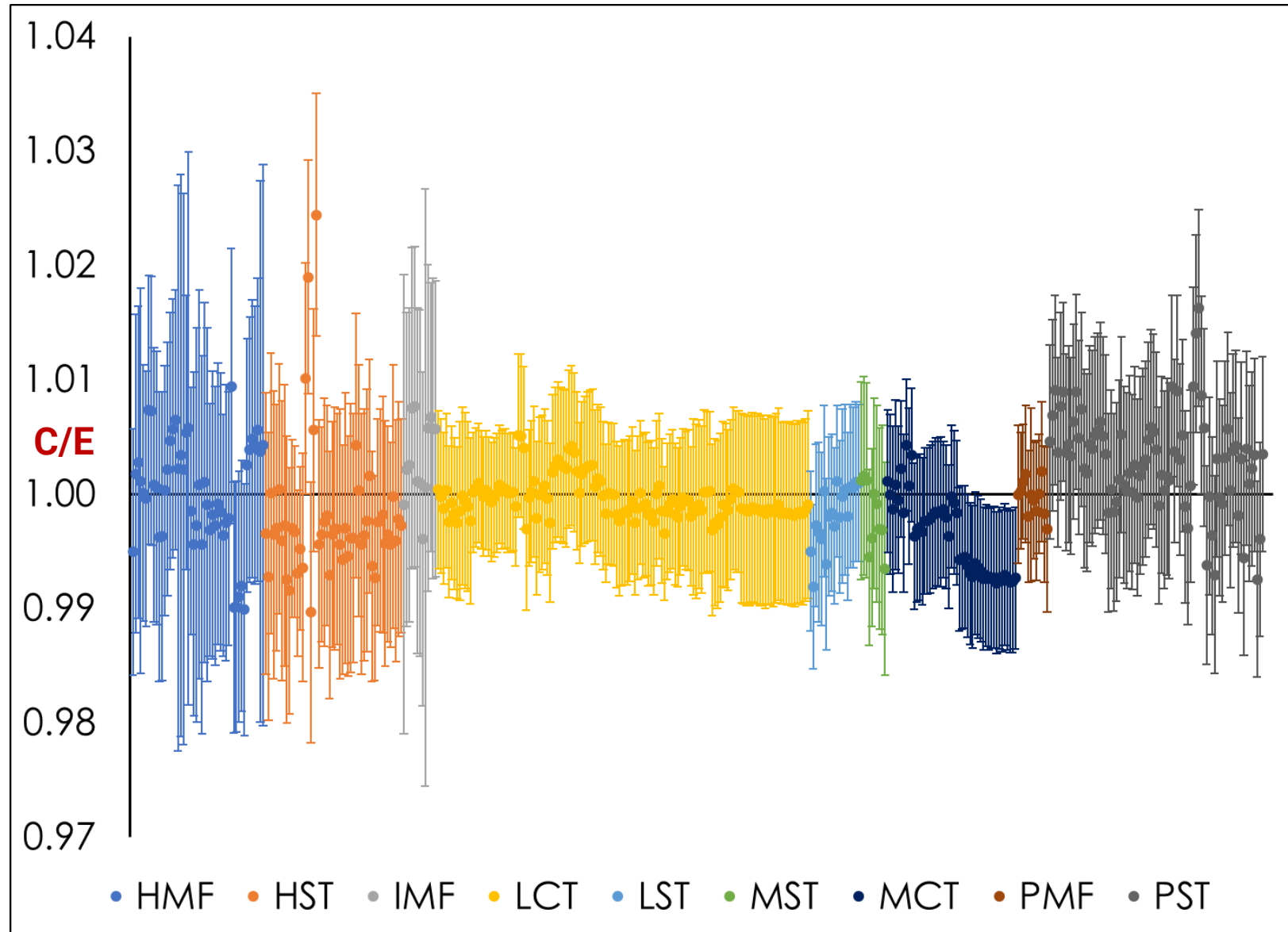
$$s_{k,\Sigma} = \frac{\frac{\partial k}{\partial \Sigma}}{\frac{k}{\Sigma}} \quad \longleftrightarrow \quad \Delta k_{\text{eff}} = (s_{k,\Sigma}) \left(\frac{\Delta \Sigma}{\Sigma} \right) \xrightarrow{\text{Matrix Form}} \mathbf{C}_{kk} = \mathbf{S} \mathbf{C}_{aa} \mathbf{S}^T$$

energy-dependent nuclear data uncertainties (covariance matrix) energy-dependent sensitivity coefficients

Propagates uncertainties from nuclear data ($\mathbf{C}_{aa}$) to uncertainties in k_{eff} ($\mathbf{C}_{kk}$)

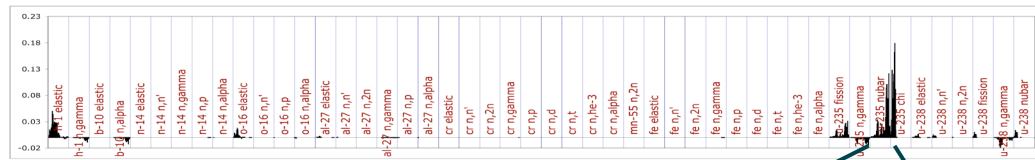
Uncertainties for critical benchmarks experiments

- Results from SCALE 6.2.2 Validation Report (ORNL/TM-2018/884)
- ~96.5% of C/E values within 1σ of unity
- **Uncertainty bounds bias!**

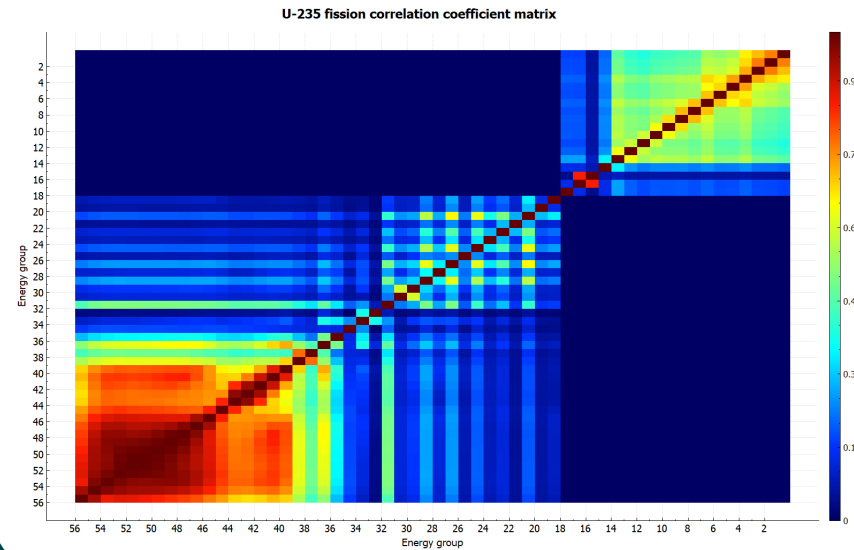
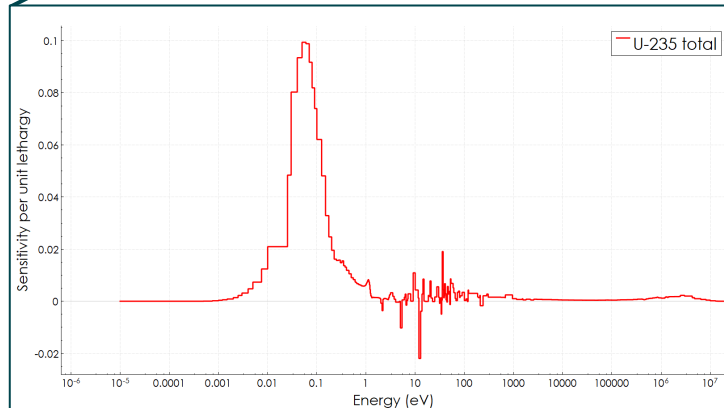


Uncertainty propagation: single system uncertainty

- Uncertainty in k_{eff} of a single system



$$S \left(\frac{\partial k}{\partial \Sigma} \right) \frac{k}{\Sigma}$$



$$C_{\alpha\alpha} \left(\frac{d\Sigma}{\Sigma} \right)^2$$

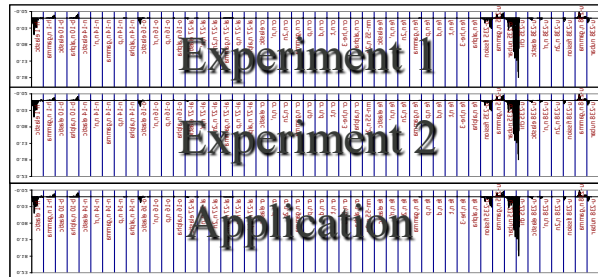
h-1 elastic
h-1 gamma
b-10 elastic
b-10 alpha
n-14 elastic
n-14 n, n'
n-14 n, gamma
n-14 n, p
n-14 n, alpha
o-16 elastic
o-16 n, n'
o-16 n, p
o-16 n, alpha
al-27 elastic
al-27 n, n'
al-27 n, 2n
al-27 n, gamma
al-27 n, p
al-27 n, alpha
cr elastic
cr n, n'
cr n, 2n
cr n, gamma
cr n, p
cr n, d
cr n, t
cr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

$$S^T \left(\frac{\partial k}{\partial \Sigma} \right) \frac{k}{\Sigma}$$

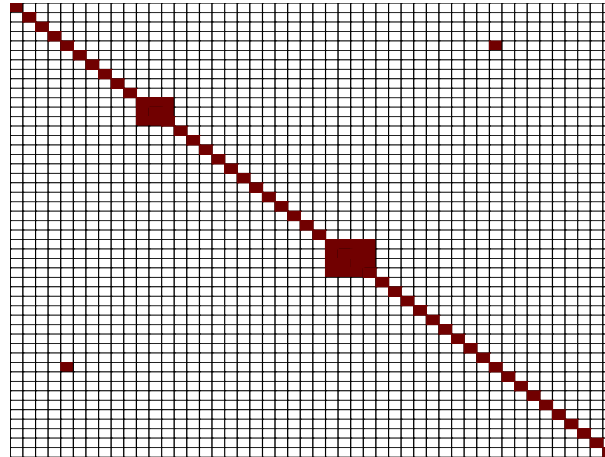
$$= \left(\frac{dk}{k} \right)^2 C_{KK}$$

Uncertainty propagation: multiple system uncertainties

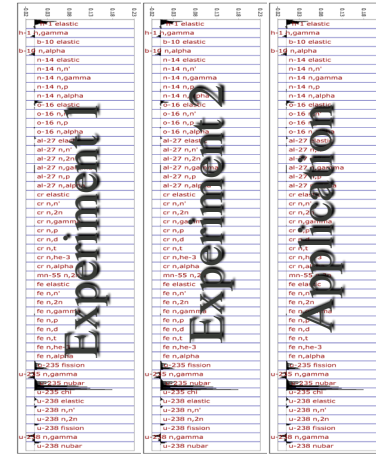
- Suppose we have sensitivity information for multiple systems:



S



$C_{\alpha\alpha}$



S^T

Diagonal elements are variance in each system

$$= \begin{bmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \sigma_{13}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & \sigma_{23}^2 \\ \sigma_{a1}^2 & \sigma_{a2}^2 & \sigma_{aa}^2 \end{bmatrix}$$

Off-diagonal elements are covariance between two systems

Covariance shows common variation(co-variance) in two systems due to ND uncertainties.
Does it sound familiar?

Correlation (or similarity) coefficient (c_k) is normalized covariance between two systems

- Integral index c_k between two systems is normalized covariance or Pearson correlation coefficient.
 - Example: c_k between Experiment 1 and the Application

$$C_{kk} = \begin{bmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \sigma_{13}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & \sigma_{23}^2 \\ \sigma_{a1}^2 & \sigma_{a2}^2 & \sigma_{aa}^2 \end{bmatrix} \quad c_k^{app-exp1} = \frac{\sigma_{a1}^2}{\sigma_{11}\sigma_{aa}} \longrightarrow -1.0 \leq c_k \leq 1.0$$

- Uncertainty weighted comparison of sensitivity profiles between an application and a critical benchmark experiment
- Measure of data-induced uncertainty shared by systems and thus a measure of the shared bias
- So, what c_k should an experiment have to be included in bias calculations??

How do we use c_k in benchmark selection ?

- S/U-based parameters are useful in identifying similar benchmark systems
 - Basis for similarity is both sensitivity information and nuclear data uncertainties
 - c_k can be used to filter benchmarks used in any validation approach
 - c_k values can be used in trending analyses to determine subcritical limits

$$\begin{array}{ll} 0.9 \leq c_k & : \text{highly similar} \\ 0.8 \leq c_k < 0.9 & : \text{marginally similar} \end{array}$$

- ORNL recommends c_k values greater than 0.8 for inclusion in validation (more on that later)
- Are we done?
 - Considering number of nuclides, energy groups and reaction types, calculation of all sensitivity coefficients (a derivative) is not a trivial task using direct perturbations
 - We haven't talked about bias calculation once we select our benchmarks

SU Calculations with TSUNAMI

TSUNAMI uses Generalized Perturbation Theory (GPT) to provide a cost effective way to calculate sensitivities

the relative change in k_{eff}

$$\frac{\delta k}{k} = \frac{\left\langle \phi^* \left(\frac{1}{k} \frac{\partial P}{\partial \Sigma} - \frac{\partial L}{\partial \Sigma} \right) \phi \delta \Sigma \right\rangle}{\left\langle \phi^* \frac{P}{k} \phi \right\rangle}$$

relative change in neutron balance equation

Old Flux no need to solve for the new flux

Rearranging

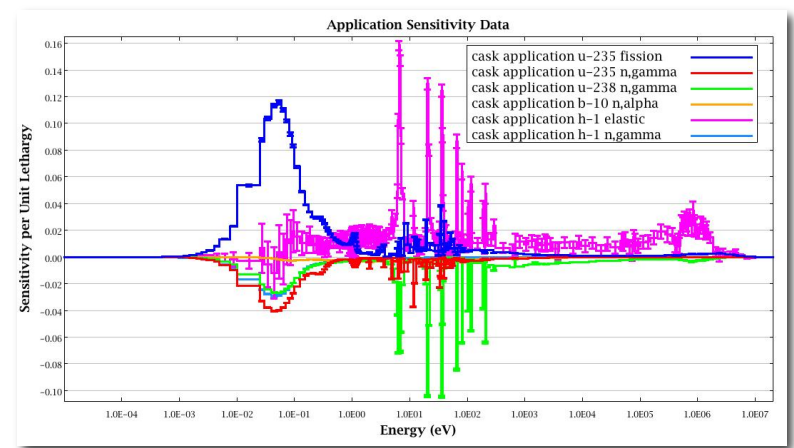
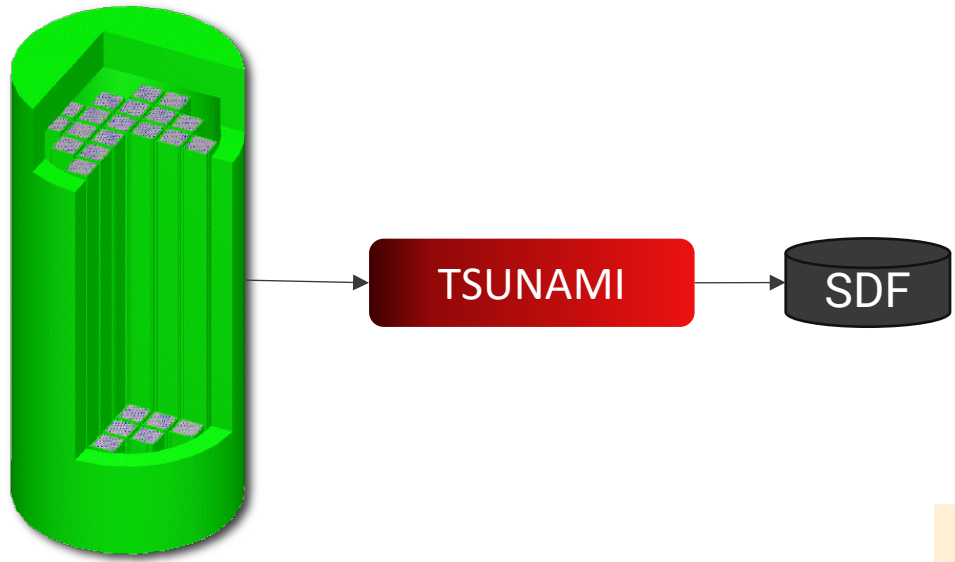
$$\frac{\partial k}{k} = \frac{\Sigma \left\langle \phi^* \left(\frac{1}{k} \frac{\partial P}{\partial \Sigma} - \frac{\partial L}{\partial \Sigma} \right) \phi \right\rangle}{\left\langle \phi^* \frac{P}{k} \phi \right\rangle} \frac{\partial \Sigma}{\Sigma}$$

Looks awfully close to our uncertainty propagation equation

$$\frac{\partial k}{k} = S_{k,\Sigma} \frac{\partial \Sigma}{\Sigma}$$

Importance function that gives higher weight to spatial locations, energies, directions that are important for k_{eff}

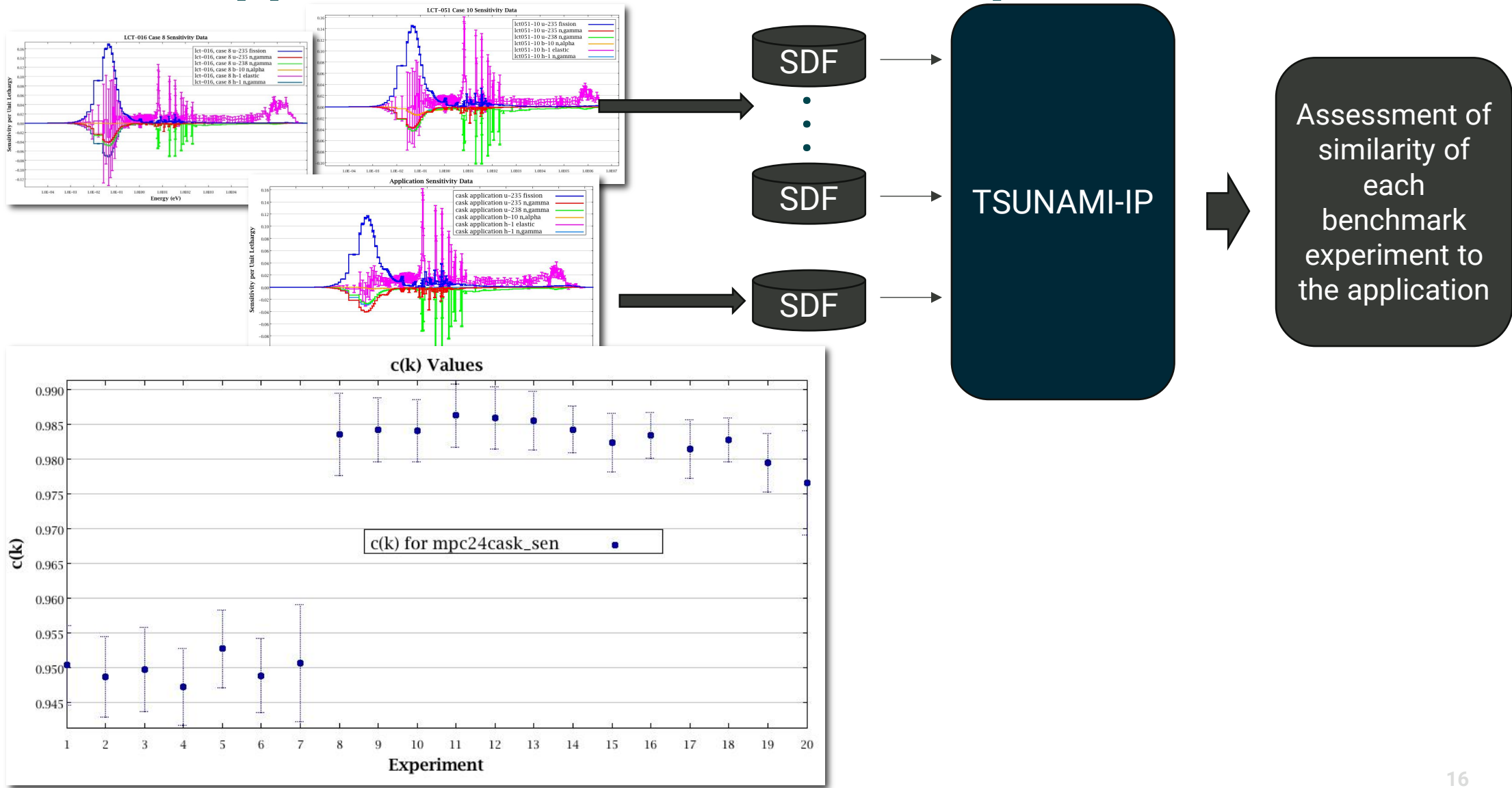
Sensitivity coefficients allow us to calculate the uncertainty in reactivity caused by nuclear data uncertainty



Extended uncertainty edit from TSUNAMI or TSUNAMI-IP identifies most important nuclides and reactions for validation based on their contribution to the change in reactivity

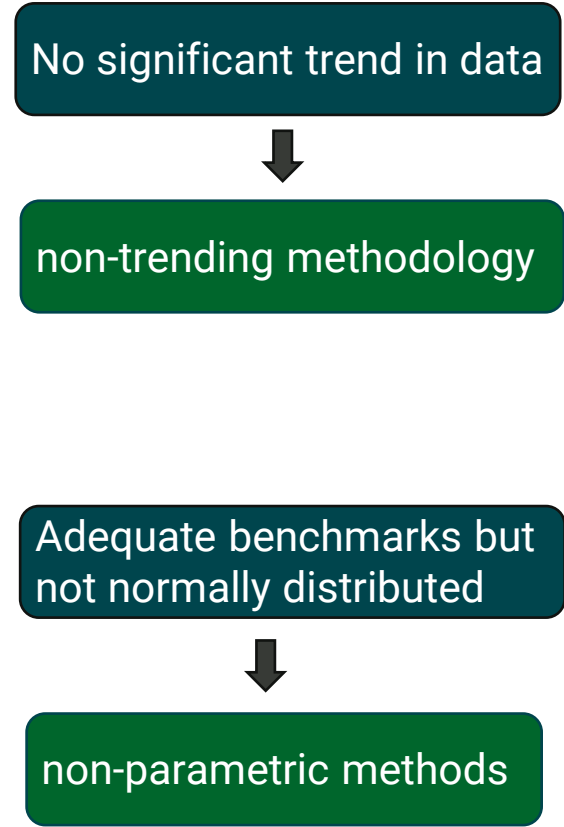
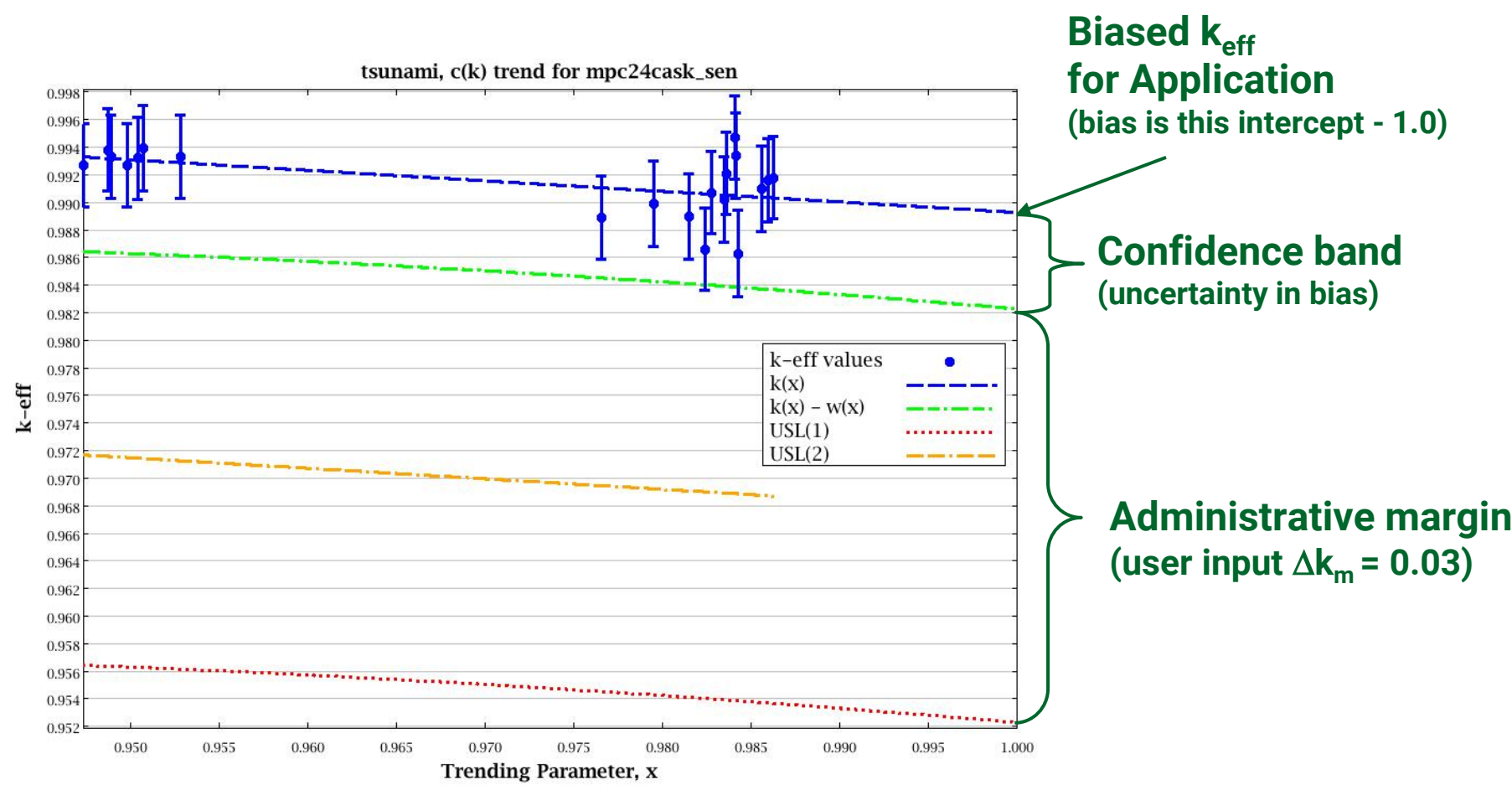
Covariance Matrix		% $\Delta k/k$
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{235}U nubar	^{235}U nubar	$6.3617\text{E-}01 \pm 8.2485\text{E-}05$
^{238}U n,gamma	^{238}U n,gamma	$3.0432\text{E-}01 \pm 1.9298\text{E-}04$
^{235}U n,gamma	^{235}U n,gamma	$2.7772\text{E-}01 \pm 1.7979\text{E-}04$
^1H elastic	^1H elastic	$1.6750\text{E-}01 \pm 6.3447\text{E-}03$
^{235}U fission	^{235}U fission	$1.5340\text{E-}01 \pm 1.2479\text{E-}04$
^{235}U chi	^{235}U chi	$8.2659\text{E-}02 \pm 2.2448\text{E-}03$
^{238}U fission	^{238}U fission	$6.6381\text{E-}02 \pm 5.5139\text{E-}05$
^1H n,gamma	^1H n,gamma	$4.6581\text{E-}02 \pm 3.6404\text{E-}05$
^{238}U n,n'	^{238}U n,n'	$4.5916\text{E-}02 \pm 1.6625\text{E-}03$

TSUNAMI-IP calculates c_k using sensitivity coefficients calculated for application and benchmark experiments



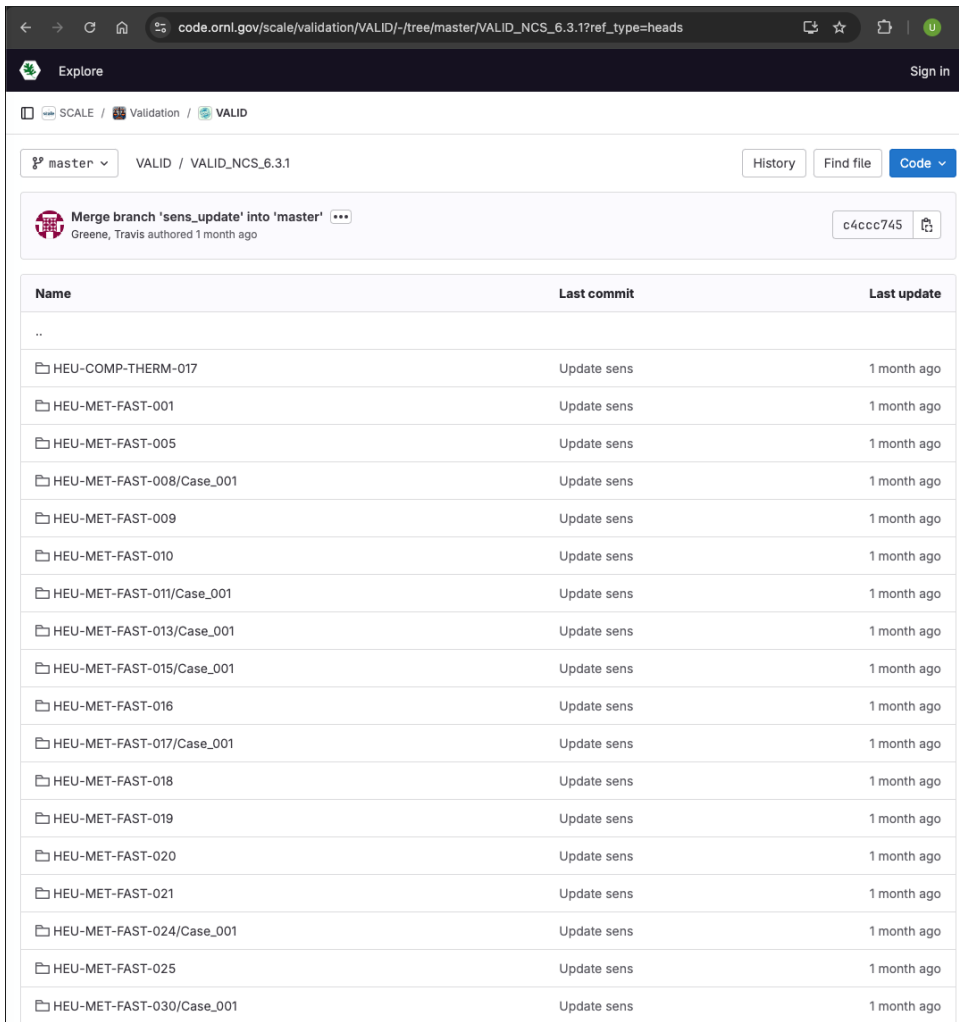
Bias and bias uncertainty are calculated with administrative margins using statistical packages in VADER (new USL)

VADER Upper Subcriticality Limit (USL) determination



You can download high-quality Sensitivity Files (SDFs) for 620 critical experiments to support your validation needs from our public repository

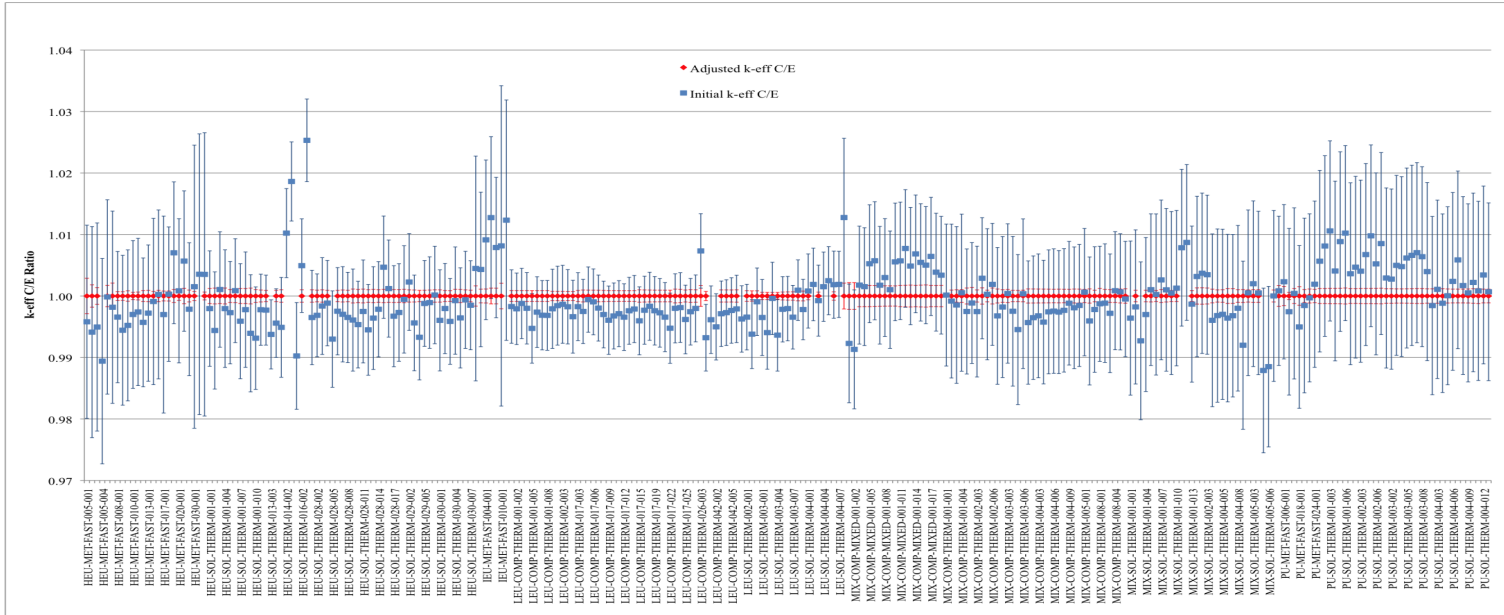
<https://code.ornl.gov/scale/validation/VALID>



Evaluation	Cases	Fissile material	Moderator	Experiment description
HEU-COMP-THERM-017	9	80% enriched U oxide	Heavy water	RB Reactor: Lattices of 80%-Enriched Uranium Elements in Heavy Water
HEU-MET-FAST-001	2	93.71% enriched U metal	None	Bare, Highly Enriched Uranium Sphere (Godiva)
HEU-MET-FAST-005	6	90% enriched U metal	None	Beryllium- and Molybdenum-Reflected Cylinders of Highly Enriched Uranium
HEU-MET-FAST-008	1	90% enriched U metal	None	Bare Sphere of Highly Enriched Uranium
HEU-MET-FAST-009	2	90% enriched U metal	None	Spheres of Highly Enriched Uranium Reflected by Beryllium or Beryllium Oxide
HEU-MET-FAST-010	2	90% enriched U metal	None	Spheres of Highly Enriched Uranium Reflected by Boron + Beryllium or Boron + Beryllium Oxide
HEU-MET-FAST-011	1	90% enriched U metal	None	Sphere of Highly Enriched Uranium Reflected by Polyethylene
HEU-MET-FAST-013	1	90% enriched U metal	None	Sphere of Highly Enriched Uranium Reflected by Steel
HEU-MET-FAST-015	1	96% enriched U metal	None	Unreflected Cylinder of Highly Enriched Uranium
HEU-MET-FAST-016	2	96% enriched U metal	None	Beryllium-Reflected and Beryllium Oxide-Reflected Cylinders of Highly Enriched Uranium
HEU-MET-FAST-017	1	96% enriched U metal	Beryllium	Beryllium-Moderated and -Reflected Cylinder of Highly Enriched Uranium
HEU-MET-FAST-018 ^a	1	90% enriched U metal	None	Bare Spherical Assembly of ²³⁵ U (90%)
HEU-MET-FAST-019 ^a	1	90% enriched U metal	None	Graphite-Reflected Spherical Assembly of ²³⁵ U (90%)
HEU-MET-FAST-020 ^a	1	90% enriched U metal	None	Polyethylene-Reflected Spherical Assembly of ²³⁵ U (90%)
HEU-MET-FAST-021 ^a	1	90% enriched U metal	None	Steel-Reflected Spherical Assembly of ²³⁵ U (90%)
HEU-MET-FAST-024	1	90% enriched U metal	None	Sphere of Highly Enriched Uranium Reflected by Steel and Polyethylene

TSURFER adjusted ND library projects the information gained by critical benchmark experiments

Experiment biases after TSURFER data adjustment



- TSURFER provides quantification of computation biases and their sources
- TSURFER bias uncertainty provides advanced means of assessing gaps in validation coverage and their potential impacts on bias

- Although very popular in Europe, experts in US have been reluctant to employ similar methods
 - Can we use the adjusted ND library for other applications?
 - Can we use information from experiments with low c_k for data adjustment?
 - Is the provided coverage guaranteed to be conservative ?

We explore answers to these questions using our NEA/WPNCS benchmark (<https://sg14.ornl.gov>)

Qc Coverage metric can automate c_k based validation and provide gap analysis

State-of-the-art validation methods

Rely on expert judgement and well-established statistical recipes to:

- judge relevance of experiments
- calculation of biases and uncertainties in predictions

Discards experiments with low c_k and don't provide any mathematical base for the selected cut-off

Can be difficult to apply and require large penalties when not enough relevant benchmarks are identified

Qc Coverage metric

Builds on c_k approach with mathematically sound grounds

Accounts for application relevant information in low c_k experiments

Can identify erroneous experiments

Incorporates measurement uncertainties, correlations

Operates on non-linear problems

Automates or provides support to experts for the process from experiment selection to bias, bias uncertainty to experimental coverage

Assists designing new experiments and gap analysis

Can be used with inference problems other than criticality

