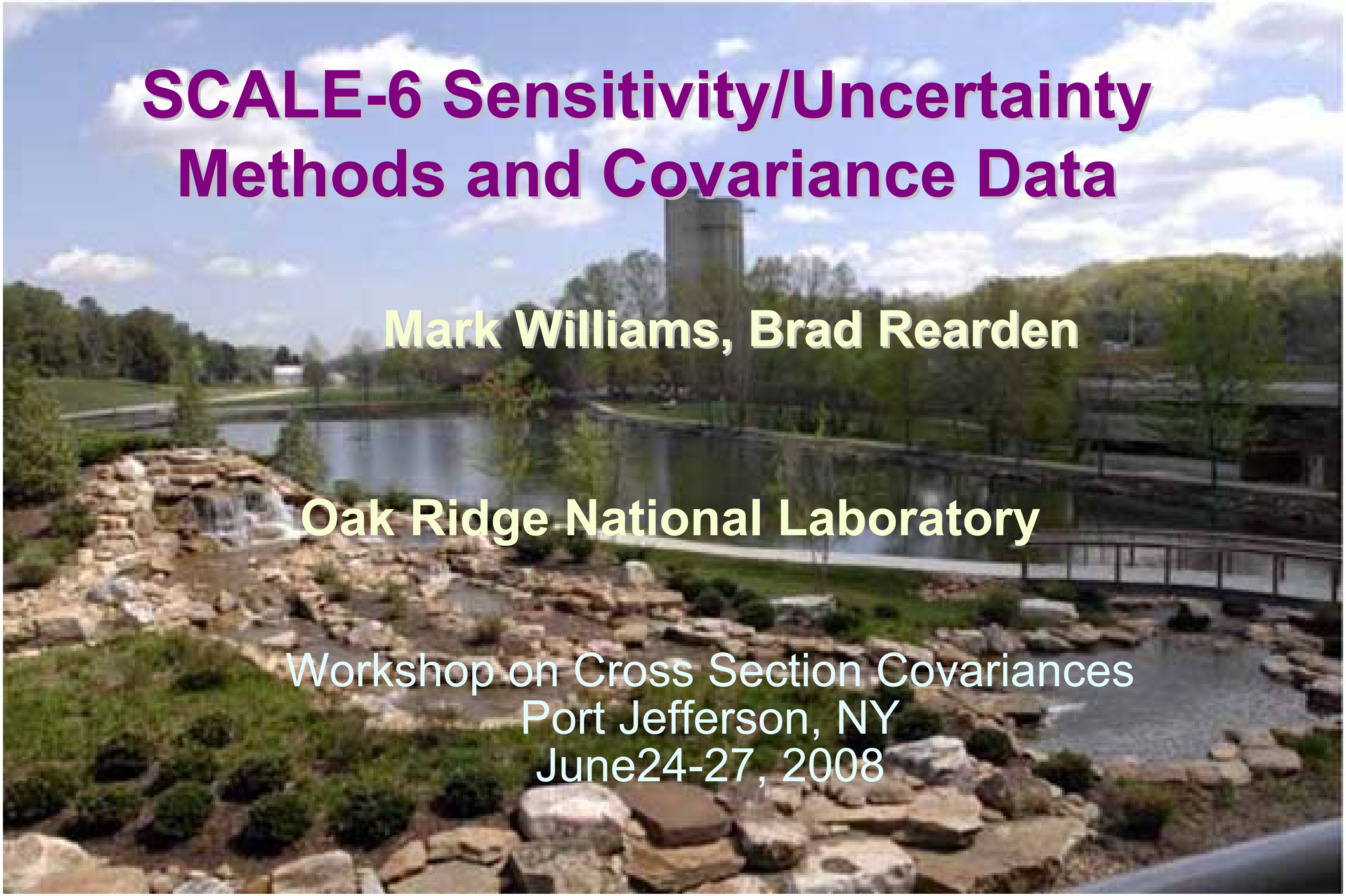

SCALE-6 Sensitivity/Uncertainty Methods and Covariance Data

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Oak Ridge National Laboratory

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T S U N A M I

Sensitivity/Uncertainty Tools in SCALE Code System

- **TSUNAMI-1D, TSUNAMI-2D, TSUNAMI-3D Sequences:**
  perform 1D, 2D or 3D forward and adjoint transport calculations;
  compute data sensitivities for response; compute response uncertainty

- **TSAR:** S/U calculations for reactivity responses (eigenvalue differences) using results from TSUNAMI-1D, 2D, 3D

- **TSUNAMI-IP:** Perform similarity analysis with S/U methods for multiple systems and responses

- **TSURFER:** Generalized linear least squares consolidation of benchmark experiments and design calculations to provide computational bias and uncertainty; adjustment in nuclear data

- **JAVAPENO**: Graphical Display of S/U Results

Impact of Evaluated Data on Multigroup Data

Evaluated data processed into *generic* multigroup

$$\left\{\Gamma^{(j)}\right\} \rightarrow x^{(j)}(E) \rightarrow \alpha_g^{(j)} \equiv \frac{\left\langle x^{(j)}(E)W(E)\right\rangle}{\left\langle W(E)\right\rangle}$$

evaluated data — processed data — generic multigroup data

$$\left\{\Delta\Gamma^{(j)}\right\} \rightarrow \Delta x^{(j)}(E) \rightarrow \Delta\alpha_g^{(j)} \Rightarrow E(\Delta\alpha_g^2) \equiv \mathbf{C}_{\alpha\alpha}$$

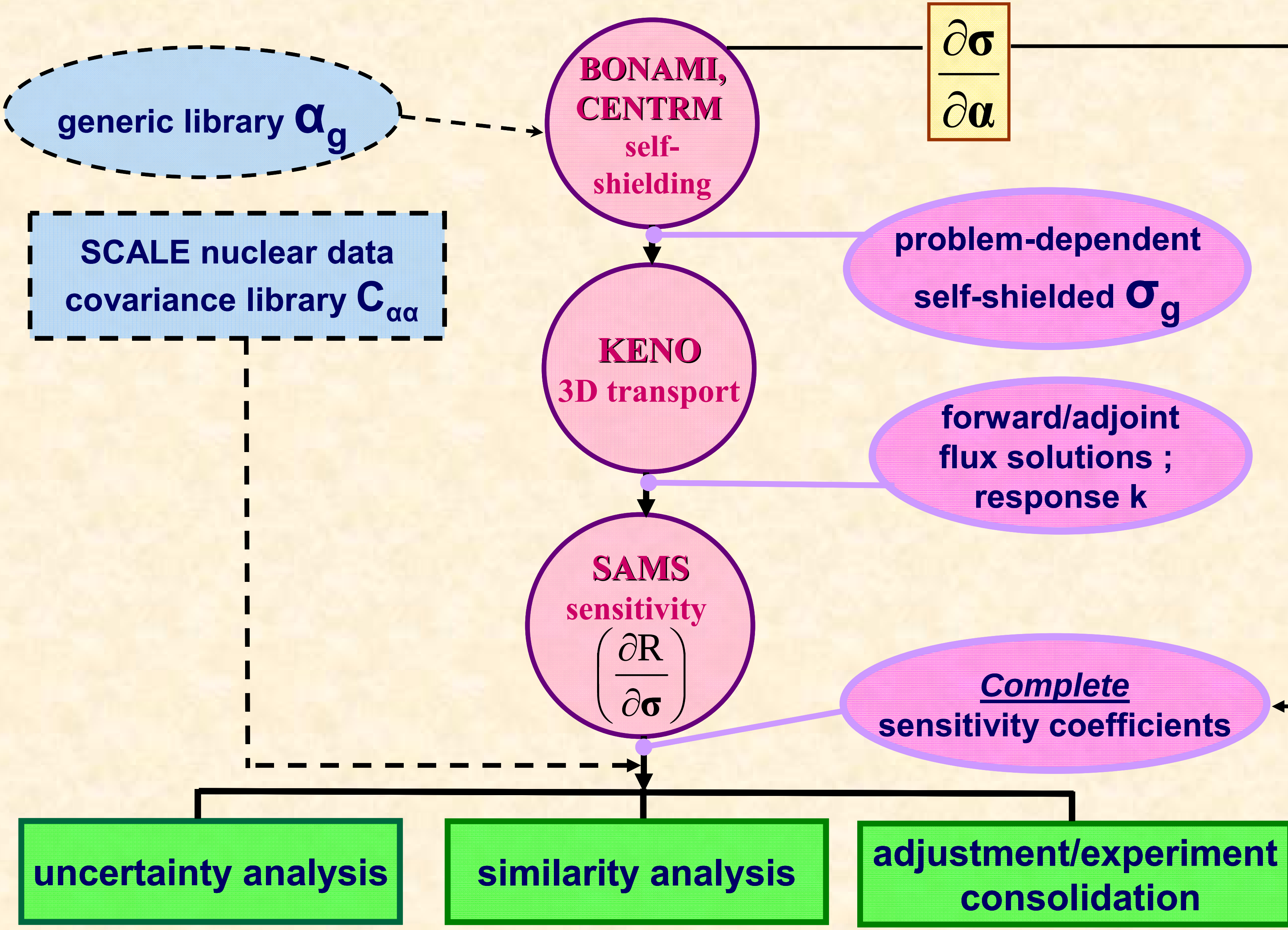
covariance data

Problem-specific **(self-shielded) multigroup data**

$$\sigma_g^{(j)} = \frac{\left\langle x^{(j)}(E)\phi_W(E)\right\rangle}{\left\langle \phi_W(E)\right\rangle} \qquad \phi_W(E) = \frac{W(E)}{\sum_i N^{(i)} x_t^{(i)}(E)}$$

NR approximation

Typical TSUNAMI Automated Computation Sequence



TSUNAMI Provides "Complete" Sensitivity Coefficient for Nuclear Data

explicit effect on response perturbation ;
implicit effect from self-shielding perturbation

$$S_{\mathrm{R},\alpha^{(x)}}^{[com]} = \frac{\alpha^{(x)}}{\mathrm{R}} \frac{d\mathrm{R}(\sigma^{(1)}(\alpha^{(x)}), \sigma^{(2)}(\alpha^{(x)}), \ldots)}{d\alpha^{(x)}}$$

$$\frac{\sigma^{(x)}}{\mathrm{R}} \frac{\partial \mathrm{R}}{\partial \sigma^{(x)}} + \sum_j \left(\frac{\sigma^{(j)}}{\mathrm{R}} \frac{\partial \mathrm{R}}{\partial \sigma^{(j)}} \right) \times \left(\frac{\alpha^{(x)}}{\sigma^{(j)}} \frac{\partial \sigma^{(j)}}{\partial \alpha^{(x)}} \right)$$

explicit **implicit**

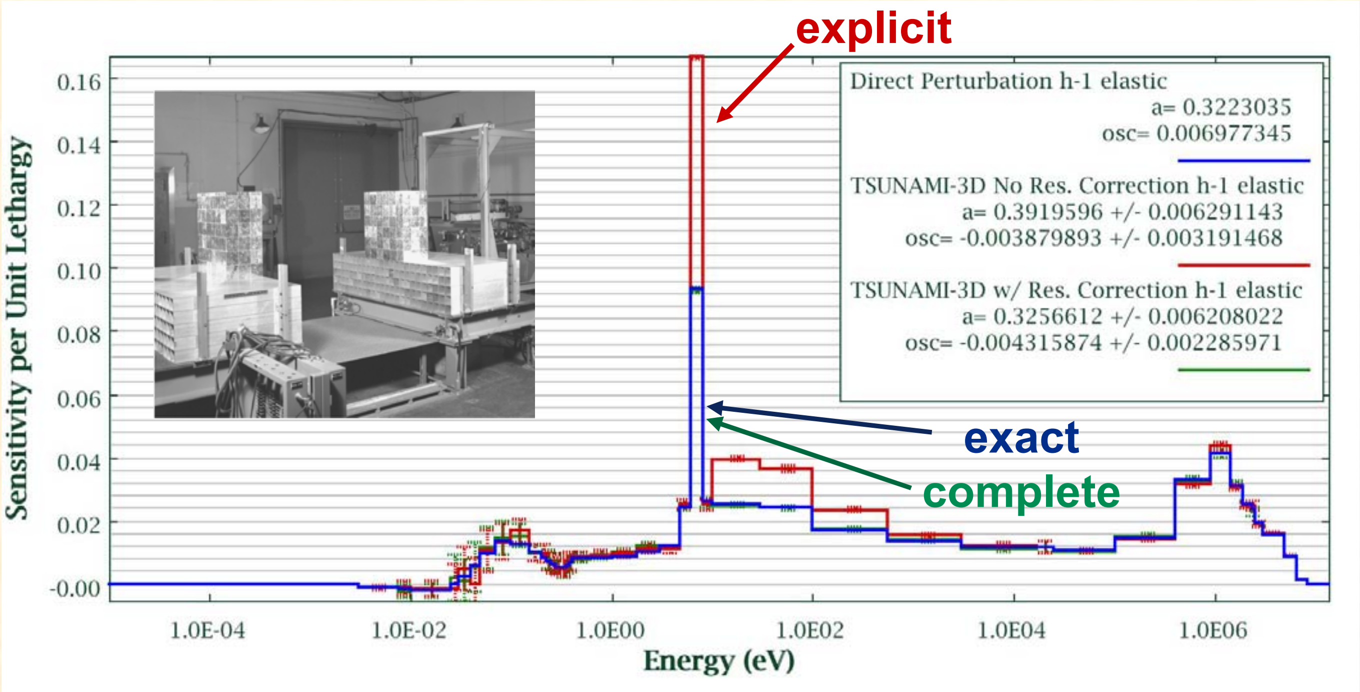
$$S_{\mathrm{R},\alpha^{(x)}}^{[com]} = S_{\mathrm{R},\sigma_x} + \sum_j S_{\mathrm{R},\sigma^{(j)}} S_{\sigma^{(j)},\alpha^{(x)}}$$

Explicit vs Implicit Sensitivity for H

- **Perturbation in $\sigma^{(H)}$ elastic will …..**

  1) change k_{eff} due to impact of H moderation

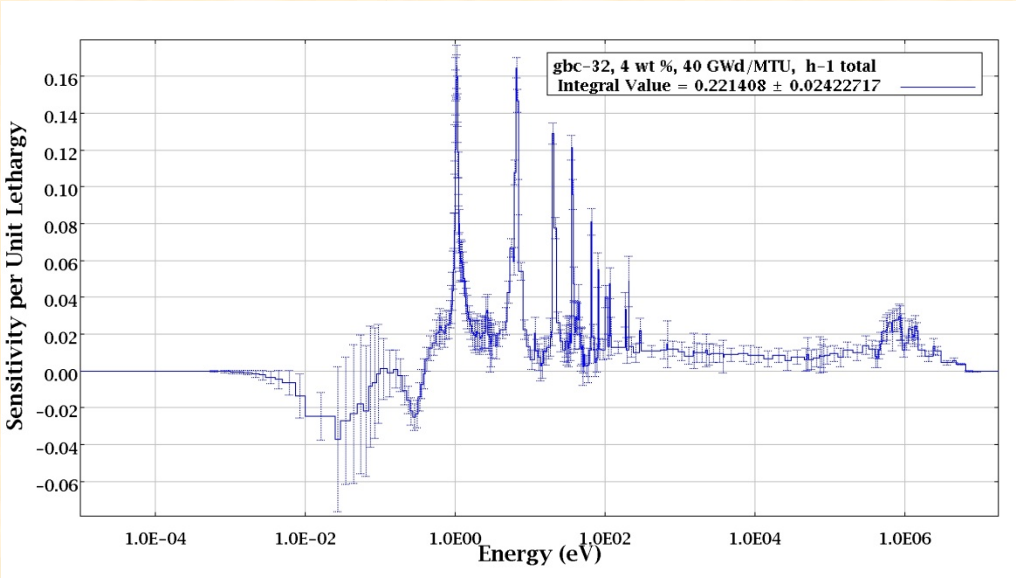
  2) change self-shielded $\sigma^{(U238)}$ → perturbation in $\sigma^{(U238)}$ causes implicit change in k_{eff}



TSUNAMI-3D Code Sequence

Monte Carlo Model for S/U Analysis of Spent-Fuel Cask

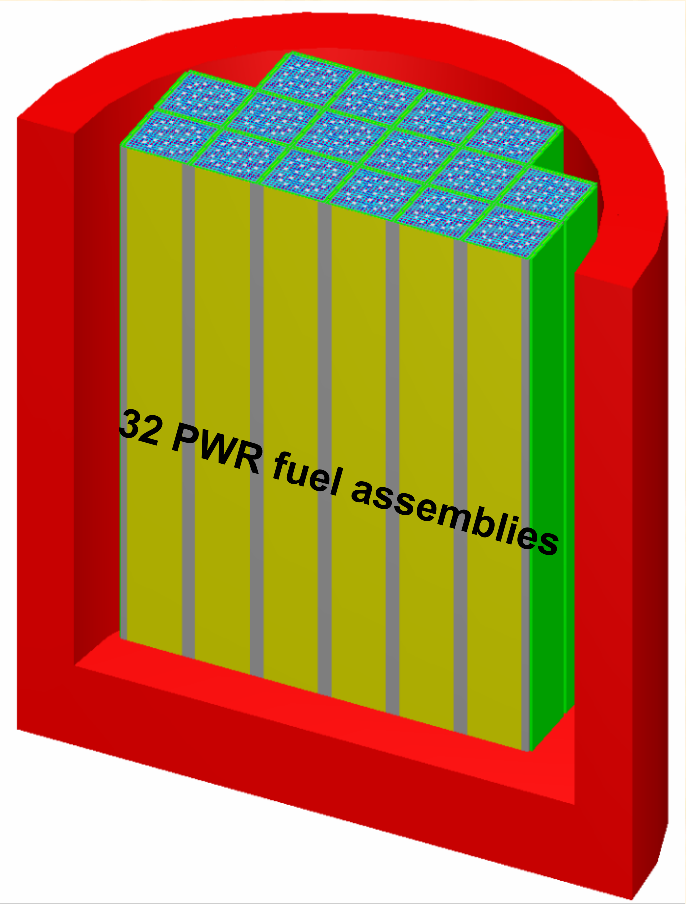
Sensitivity Coefficient for H Elastic



$$\mathrm{Var}(k) \equiv \mathbf{S}^{T}\mathbf{C}_{\alpha\alpha}\mathbf{S}$$

complete **sensitivity**

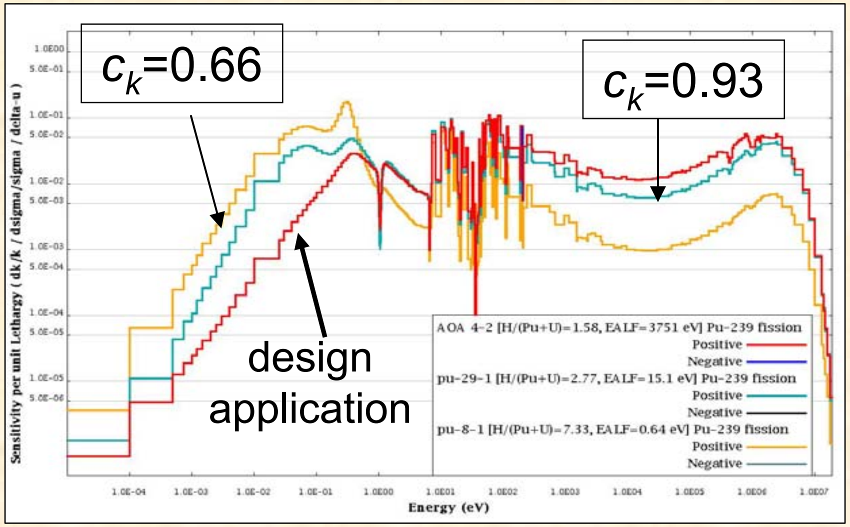
generic **covariance**



TSUNAMI-IP Code Module

Similarity Analysis to Select Benchmark Experiments for Validation

^{239}Pu Fission Sensitivity Profile



correlation coefficient for responses k_m and k_n

$$c_k^{(m,n)} = \frac{\mathbf{S}_{k_m}^{\mathrm{T}} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{k_n}}{\sqrt{Var(k_m)\,Var(k_m)}}$$

System Similarity Coefficients:

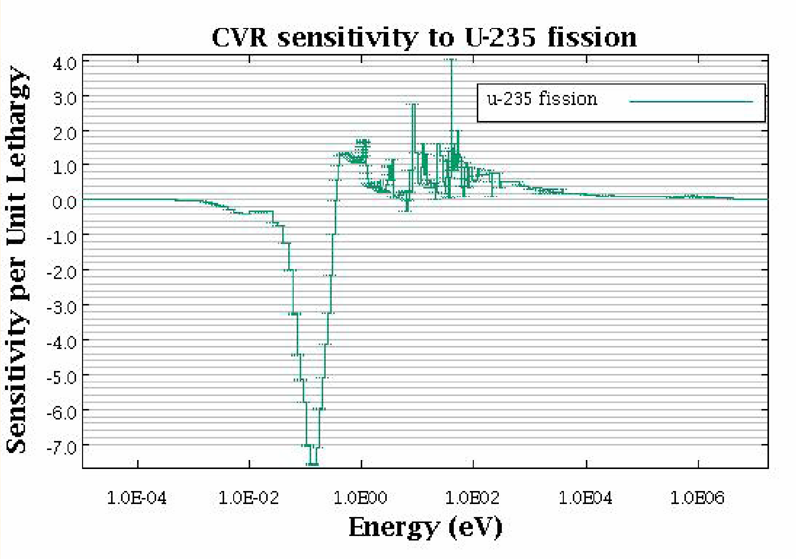
c_k = 0 no similarity between experiment and design application

c_k = 1 experiment and application have identical sensitivities

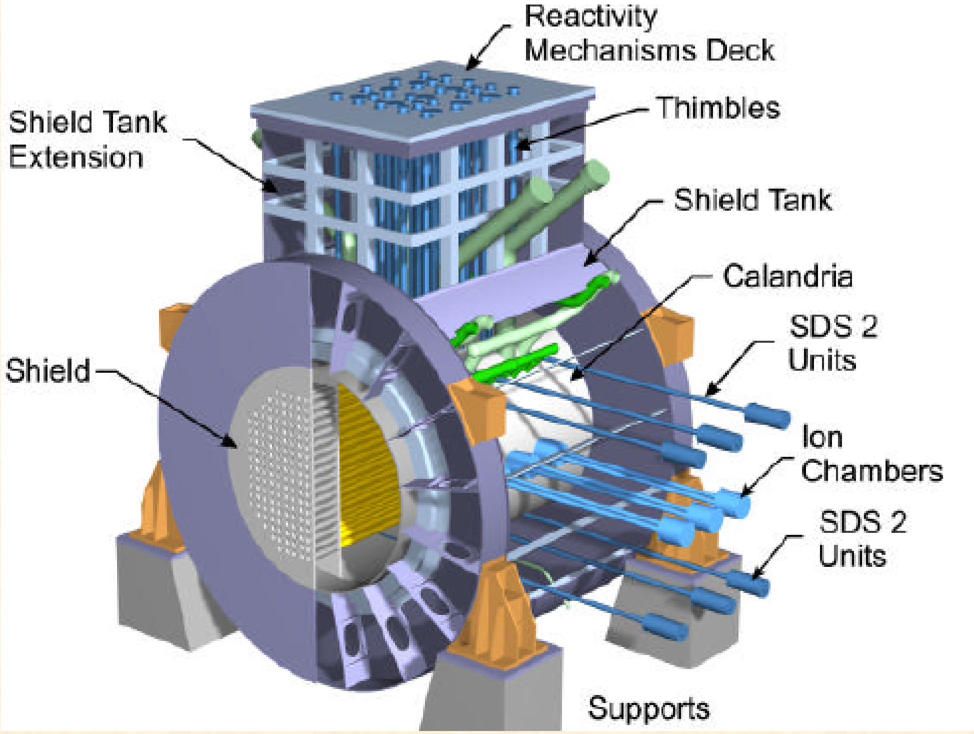
TSAR Code Module

S/U Analysis for Reactivity Responses in 1D, 2D, 3D Geometries

Example: Coolant Void Reactivity in Advanced Candu Reactor



Void Reactivity	St. Dev.
-0.002	49.8%



TSURFER Code Module

Generalized Least-Squares Consolidation of Calculated and Experimental Results

- adjust data to minimize differences in computed and measured integral experiments, using sensitivities and covariances
- propagates data adjustments to obtain application's bias and uncertainty

Application = projected CVR for ACR Bundle

Experiment = ZED-2 critical facility

Parameter	Prior	Adjusted
k (*novoid*)	1.2491	1.2479
std (*novoid*)	± 0.0067	± 0.0033
k (*void*)	1.2458	1.2445
std (*void*)	± 0.0077	± 0.0037
CVR, pcm	-212.1	-218.9
σ_{CVR} , pcm	**± 92.8**	**± 37.9**

SCALE Covariance Library

- S/U applications depend on having reasonable estimates for data covariances
- Omitted uncertainties treated as zero!
  - Under estimates response uncertainty
  - Skews data adjustments and similarity analysis
- SCALE-6 has cov data for >300 materials based on:
  - High fidelity evaluations from ENDF/B and JENDL
  - Recent high fidelity evaluations by LANL
  - Approximate values from "low fidelity" project
- Lo-Fi covariances were generated by
  - "integral method" in thermal & resonance range [ORNL]
  - nuclear model techniques in fast [BNL,LANL]

Sources of Covariance Data in SCALE-6

Source	Materials
ENDF/B-VII.0	$Gd^{152-158,160}$ Th^{232} Tc^{99} $Ir^{191,193}$
Pre-released ENDF/B-VII	$U^{233,235,238}$ Pu^{239} Li^{6}
ENDF/B-VI (or Lo-Fi ?)	Na^{23} Si^{28-29} Sc^{45} V^{51} $Cr^{50,52-54}$ Mn^{55} $Fe^{54,56-58}$ $Ni^{58,60-62,64}$ $Cu^{63,65}$ Y^{89} Nb^{93} $In^{(nat)}$ $Re^{185,187}$ Au^{197} $Pb^{206-208}$ Bi^{209} Am^{241}
JENDL	$Pu^{240-241}$
LANL Hi-Fi	H^{1-3} He^{3-4} Li^{7} Be^{9} B^{10-11} C^{12} N^{14-15} O^{16-17} F^{19}
Lo-Fi	>200 materials

Thermal Cross Sections

Nuclide	ENDF/B-VII	Integral(*)	difference
Cd-113	2.06E+4	2.06E+4 ± 1.9%	0%
Xe-135	2.63E+6	2.65E+6 ± 4.1%	-0.7%
Sm-149	4.02E+4	4.01E+4 ± 1.5%	0.2%
Np-237	1.81E+2	1.76E+2 ± 1.6%	-2.8%

Resonance Integrals

Nuclide	ENDF/B-VII	Integral(*)	difference
Cd-113	3.92E+2	3.90E+2 ± 10.3%	0.5%
Xe-135	7.65E+6	7.60E+3 ± 6.6%	0.7%
Sm-149	4.02E+4	4.01E+4 ± 5.9%	0.2%
Np-237	6.60E+2	6.40E+2 ± 7.8 %	3.0%

(*) *Atlas of Neutron Resonances*, S. F. Mughabghab

Integral Approximation For Covariance Matrix

constant that preserves integral uncertainty

covariance matrix $\mathbf{C}^{(\mathbf{rel})}_{\boldsymbol{\sigma\sigma}} \sim V\,\tilde{\mathbf{R}}$ assumed correlation matrix

- <u>*Groups in Thermal Range*</u>: E < 0.5 eV

$$V \sim \frac{\mathrm{Var}(\sigma_{2200})}{\sigma_{2200}^2} \qquad \tilde{\mathbf{R}} \sim [\mathbf{1}] \quad \text{(full correlation)}$$

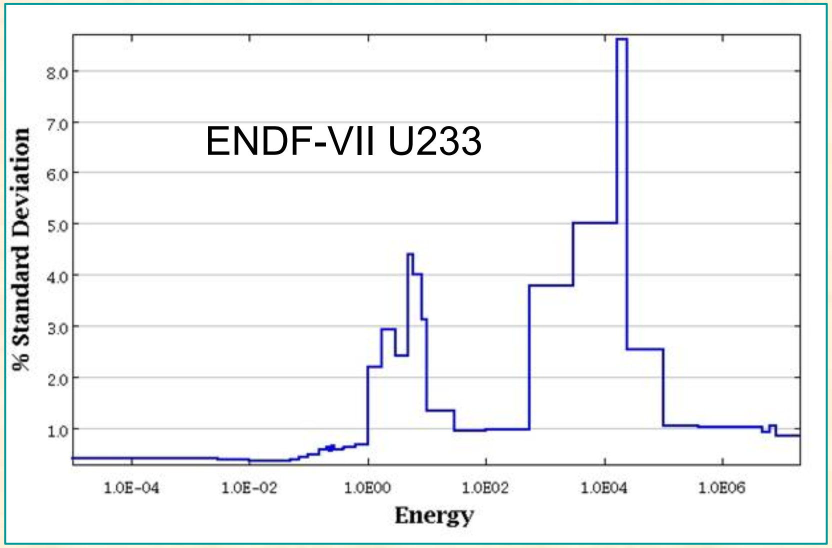
- <u>*Groups in Epithermal Range*</u>: E ε (0.5 eV, 5.0 keV)

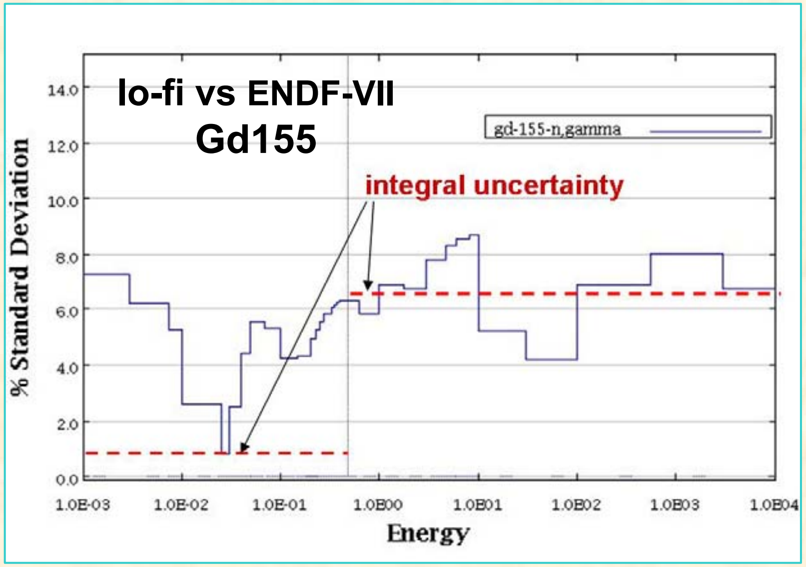
$$V \sim \frac{\mathrm{Var}(\mathrm{RI})}{(\mathrm{RI})^2} \qquad \tilde{\mathbf{R}} \sim [\mathbf{1}] \quad \text{(full correlation)}$$

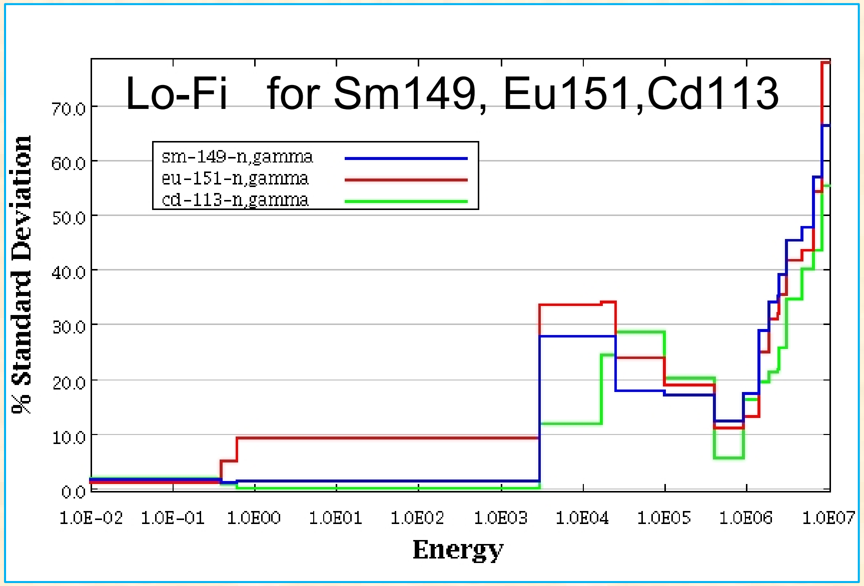
<u>*OR*</u>

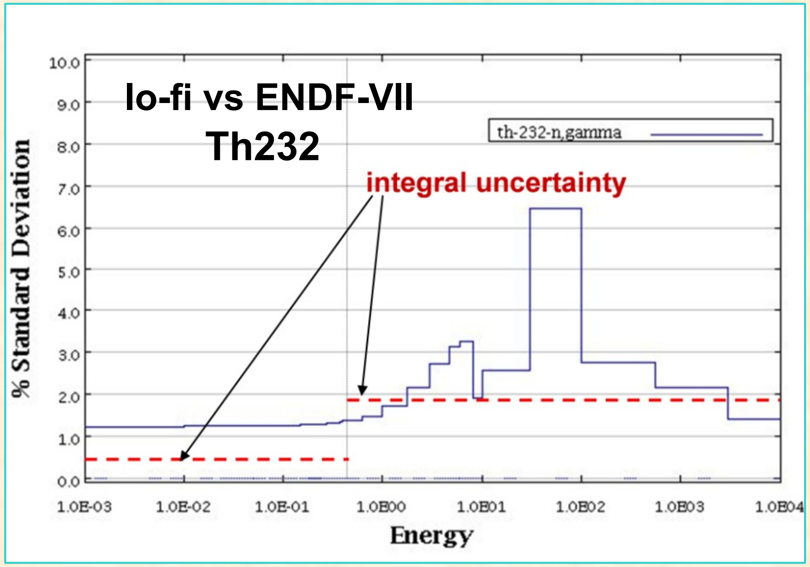
$$\begin{pmatrix} 1 & 1 & 0 & \dots \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & \\ \vdots & 0 & & \end{pmatrix} \quad \text{(tri-diagonal)}$$

Example of Uncertainties in SCALE-6









SUMMARY

- **TSUNAMI package in SCALE provides S/U methods for criticality safety and reactor physics applications**
- **Sensitivities are calculated by 1D, 2D, 3D transport methods, and include explicit + implicit effects**
- **Similarity analysis is used to select benchmark experiments to validate a design application**
- **Adjustment module combines integral experiments with calculations to reduce response uncertainty**
- **SCALE-6 has covariance data for >300 nuclides based on high-fidelity plus approximate uncertainties from the "lo-fi" work of BNL, LANL, ORNL, and ANL**