Latest Advances in the TSUNAMI Sensitivity and Uncertainty Analysis Tools Developed by ORNL

TSUNAMI

Tools for Sensitivity and UNcertainty Analysis Methodology Implementation

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UT-BATTELLE

ORNL Production-Level S/U Capabilities

- **Publicly released TSUNAMI tools in SCALE 5.0**
  - **eigenvalue S/U analysis tools**
    - **1-D discrete ordinates**
    - **3-D Monte Carlo**
  - **operation from automated sequences with problem-dependent cross section processing and “implicit effect”**
  - **cross-section-covariance data library**
  - **code for system-to-system similarity assessment**
  - **data visualization GUI and interactive HTML output**
- **TSUNAMI training for criticality code validation**
  - **8 multiday classes taught since 2004, ~150 participants**
  - **6-hour tutorial presented at 2004 ANS annual meeting**

TSUNAMI-3D Sequence

- Uses 3D Monte Carlo calculations (KENO V.a) to score spherical harmonic moments of forward and adjoint flux:

$$\tilde{\phi}^{\ell}_{g,i} = \frac{\sum_{k=1}^{K} Y^{\ell}(\Omega_{\mathbf{k}}) w_k T_{k,i}}{V_i \sum_{k=1}^{K} w_k}$$

tracklength estimator for ℓ_{th} moment, in group-g, interval-i

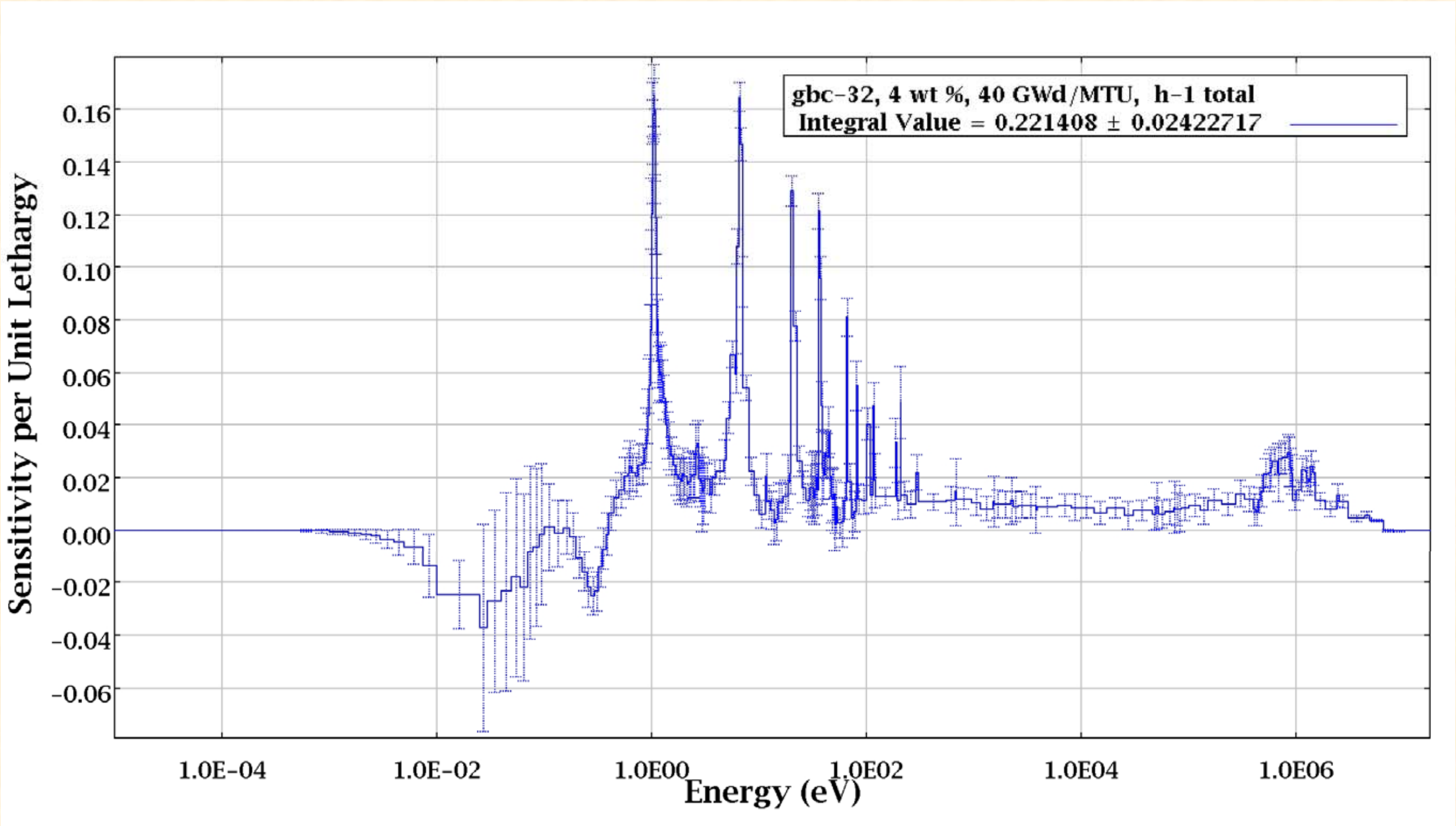
- Folds forward and adjoint moments to produce nuclide, energy & cross section dependent sensitivity profiles by spatial zone:

sensitivity coefficient for capture

$$S_{c,g}(z) \cong -\frac{\sigma_{c,g}}{D} \left\langle \Phi(\mathbf{r},E,\Omega)\, \Phi^{*}(\mathbf{r},E,\Omega) \right\rangle$$

$$\rightarrow \frac{-\sigma_{c,g}}{D} \sum_{i \in z} \sum_{\lambda} \tilde{\phi}^{\lambda}_{g,i}\, \tilde{\phi}^{*\lambda}_{g,i}\, V_i$$

Sample Sensitivity Results



Complete Sensitivity Coefficient Includes Effects of Changes in Self-Shielded Cross Sections

- The ***"explicit"*** effect is sensitivity of k_{eff} to changes in multigroup cross sections appearing transport equation

- The ***"implicit"*** effect is sensitivity of k_{eff} to cross section perturbations caused by changes in self-shielding
  - **Example: perturbation in $\sigma^{(H)}$ changes self-shielded $\sigma^{(U238)}$ => cross section data may be sensitive to changes in other data**

$$S_{\alpha_x;\alpha_j} = \frac{\alpha_j}{\alpha_x}\frac{\partial \alpha_x}{\partial \alpha_j}$$

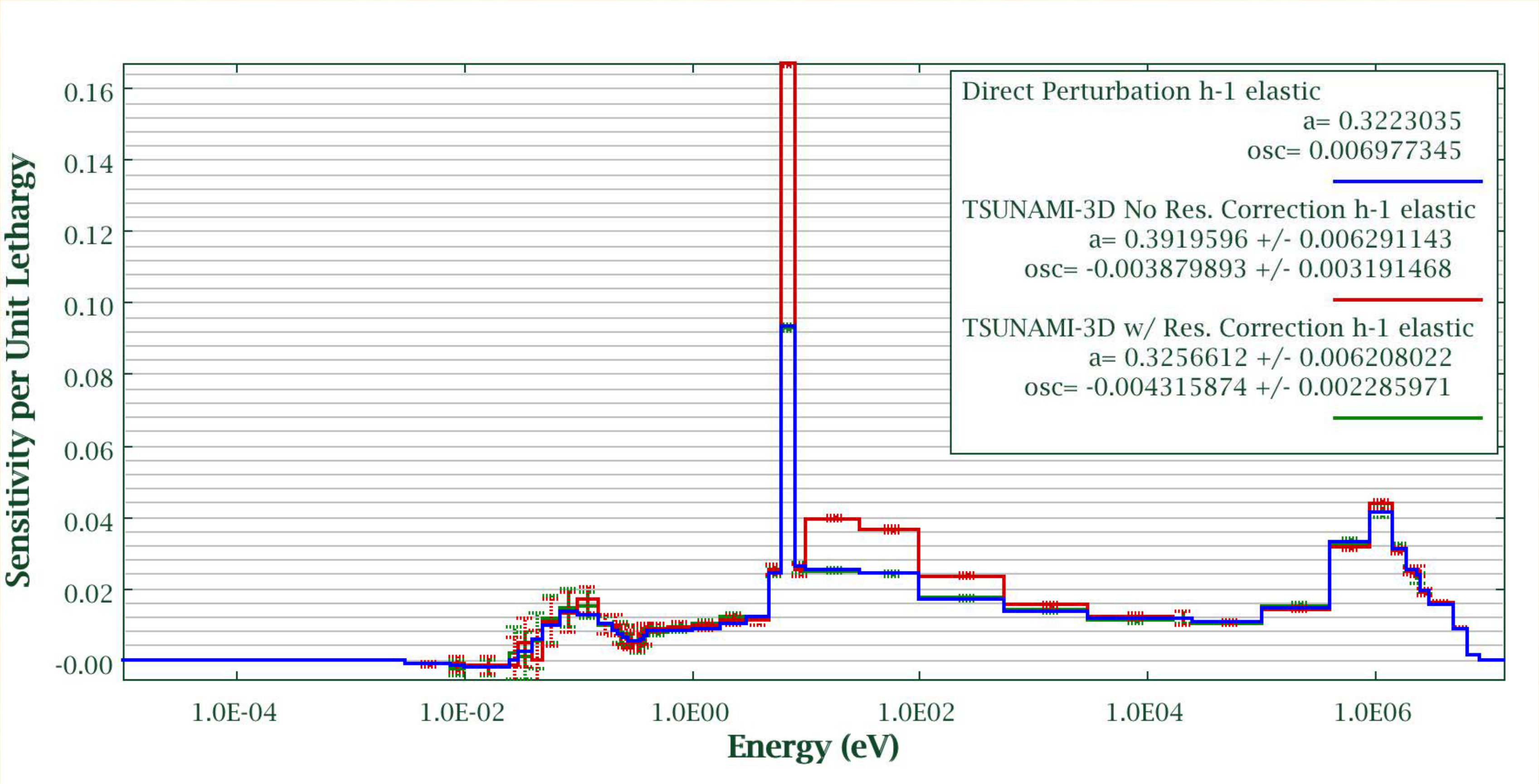
α_x = shielded cross section
α_j = data used in resonance calculation

- The implicit effect can be propagated to k_{eff} via the chain rule for derivatives and combined with the explicit to form the complete sensitivity coefficient.

Improved Results by Including Implicit Effect

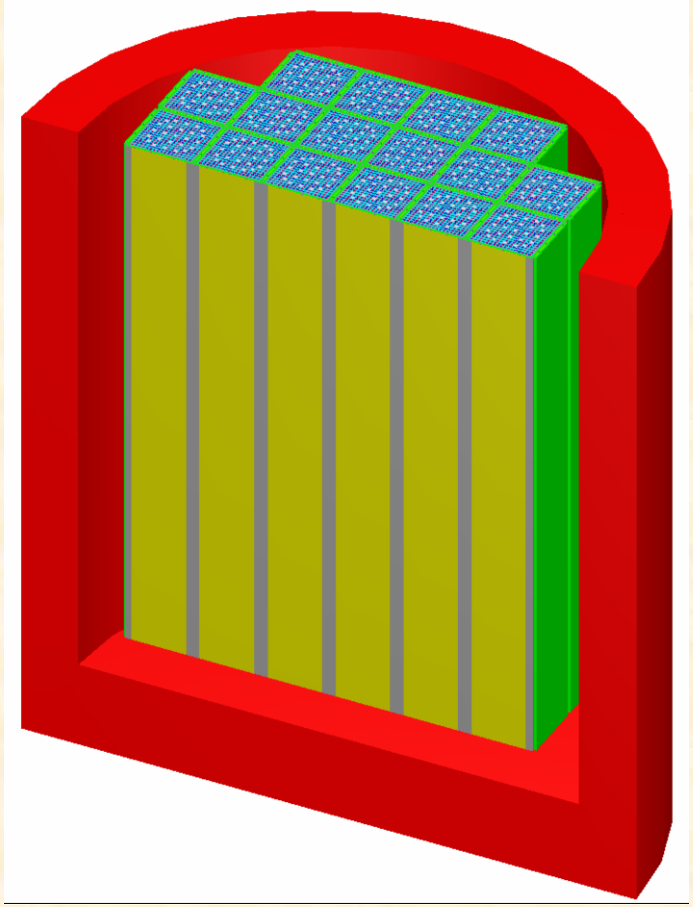
Nuclide	Reaction	Direct Perturbation Sensitivity	TSUNAMI Sensitivity	% Diff.	TSUNAMI Sensitivity (no implicit)	% Diff.
^{1}H	total	0.22	0.22	0%	0.29	27%
^{19}F	total	0.04	0.04	0%	0.05	18%
^{235}U	total	.25	0.25	0%	0.25	0%
^{238}U	total	-0.21	-0.21	0%	–0.29	39%

Sensitivity for ^{1}H Elastic, with Implicit Effect



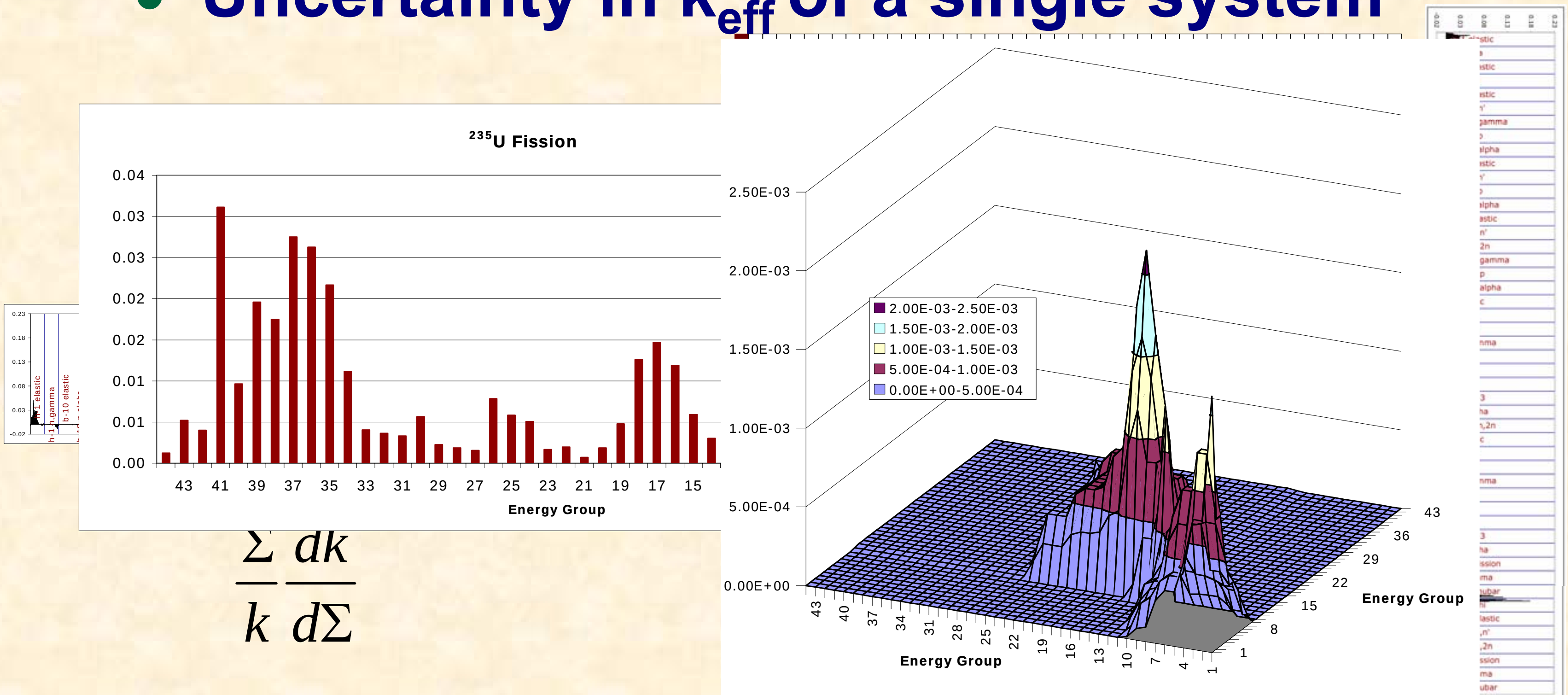
Applications of TSUNAMI-3D to Complex Models

- **Burnup Credit Cask Model**
  - **32 PWR fuel assemblies in flooded cask**
  - **18 axial burnup zones**
  - **Burned to 40 GWd/MTU; Cooled for 5 years**
  - **BORAL™ plates around each assembly**
  - **Cask filled with water**
- **Commercial Reactor Criticals (CRC)**
  - **Startup data from PWRs (Crystal River)**
  - **1/2 core models**
  - **Each pin explicitly modeled with 18 axial zones**
  - **Sensitivity coefficients for ~47,000 nuclides, ~420,000 44-group profiles**



Uncertainty Propagation

- **Uncertainty in k_{eff} of a single system**



$$\frac{\Sigma}{k}\frac{dk}{d\Sigma}$$

$$= \sigma^2$$

C_{kk}

$$\left(\frac{\Delta k}{k}\right)^2$$

$C_{\alpha\alpha}$

$$\left(\frac{\Delta \Sigma}{\Sigma}\right)^2$$

S^T

$$\frac{\Sigma}{k}\frac{dk}{d\Sigma}$$

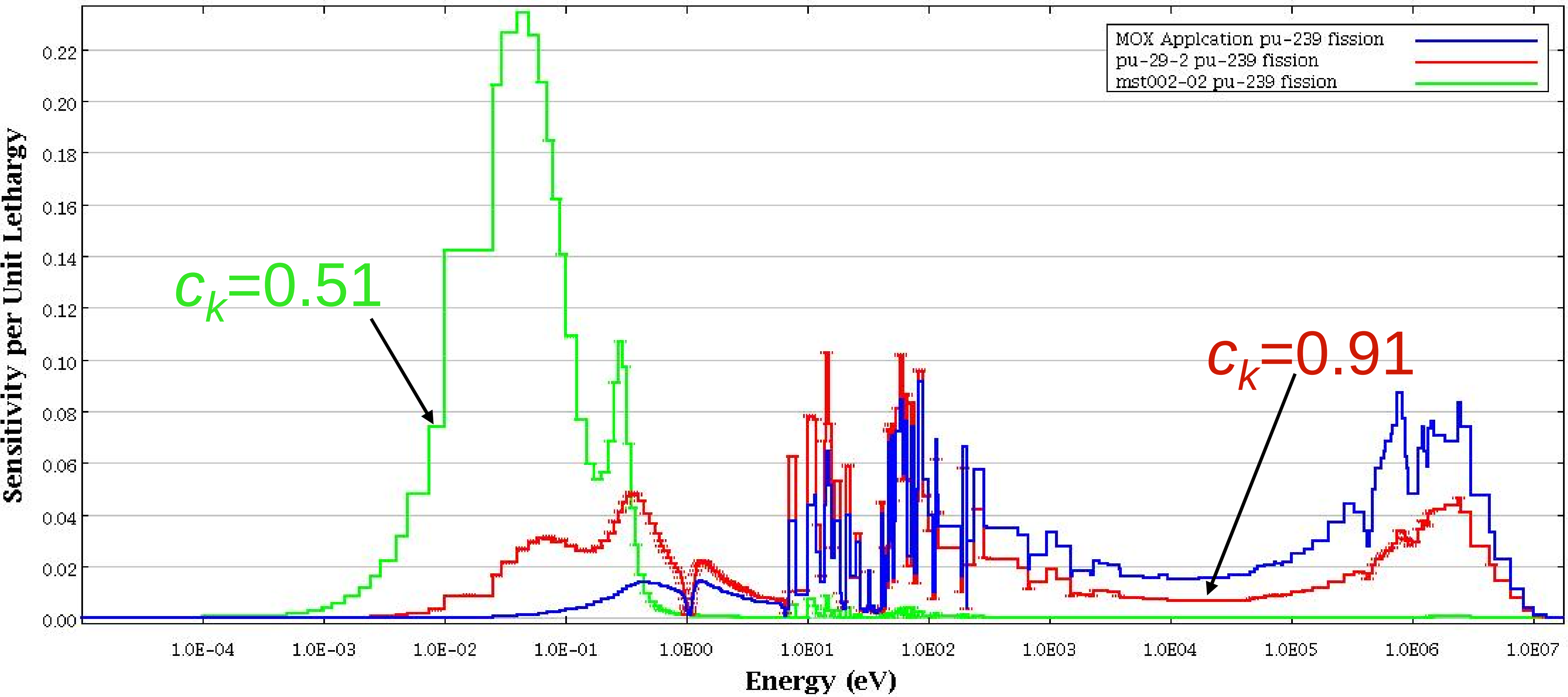
Uncertainties in k_{eff} Due to Cross Section Covariance Data

- **Uncertainties (standard deviations) in k_{eff} typically range from 0.8% (thermal) to over 2% (fast)**

Uncertainties in k_{eff} Due to Cross-Section Uncertainties

Covariance Matrix		% Δk/k
Nuclide-Reaction	**Nuclide-Reaction**	**Due to this Matrix**
^{239}Pu nubar	^{239}Pu nubar	4.0834E-01 ± 9.8836E-08
^{239}Pu chi	^{239}Pu chi	3.9044E-01 ± 1.5458E-07
^{235}U nubar	^{235}U nubar	3.1592E-01 ± 1.0725E-07
^{238}U n,gamma	^{238}U n,gamma	3.0445E-01 ± 8.8732E-07
^{241}Pu chi	^{241}Pu chi	2.7127E-01 ± 7.2082E-08
^{238}U chi	^{238}U chi	2.1686E-01 ± 6.0650E-08
^{239}Pu n,gamma	^{239}Pu n,gamma	2.0430E-01 ± 6.1635E-07
^{1}H elastic	^{1}H elastic	2.0103E-01 ± 1.5292E-05
^{239}Pu nubar	^{235}U nubar	1.7508E-01 ± 4.1615E-08
[illegible]	[illegible]	[illegible]

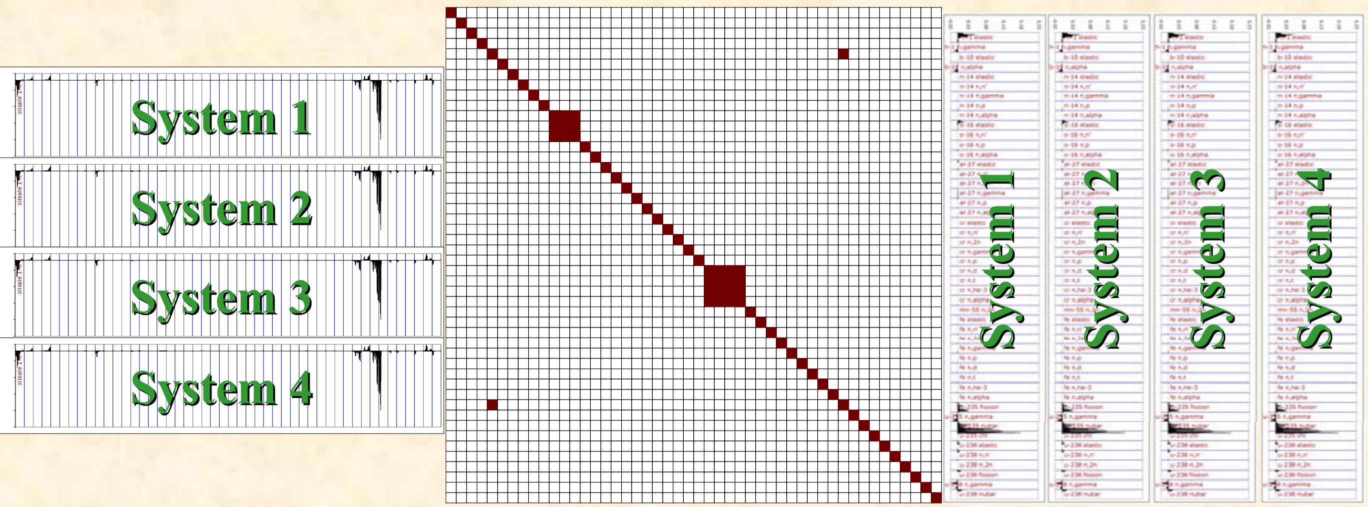
TSUNAMI Tools for System Similarity Assessment



Uncertainty Propagation (con't)

- **Uncertainty in k_{eff} for multiple systems**

Diagonal elements are variance in each system



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

S $\quad$ $C_{\alpha\alpha}$ $\quad$ S^T

Off-diagonal elements are covariance between two systems

C_{kk}

Covariance Data in ENDF/B-VI

49 of 344 evaluations have covariance data

Th-232
Pu-242
Au-197
Bi-209*
Pu-240
Am-241
V*
Co-59
Y-89*
Ti-46*,47*,48*
Na-23
U-238
Al-27
Pu-241
N-14**
Li-6**
Np-237**

Sc-45*
Cr-50,52,53,54
Fe-54,56,57,58
Ni-58,60,61,62,64
Mn-55
Cu-63*,65*
F-19
Re-185*,187*
Pb-206,207,208
Si
Nb*
In*
U-235
H-1**
O-16**
B-10**
Pu-239**

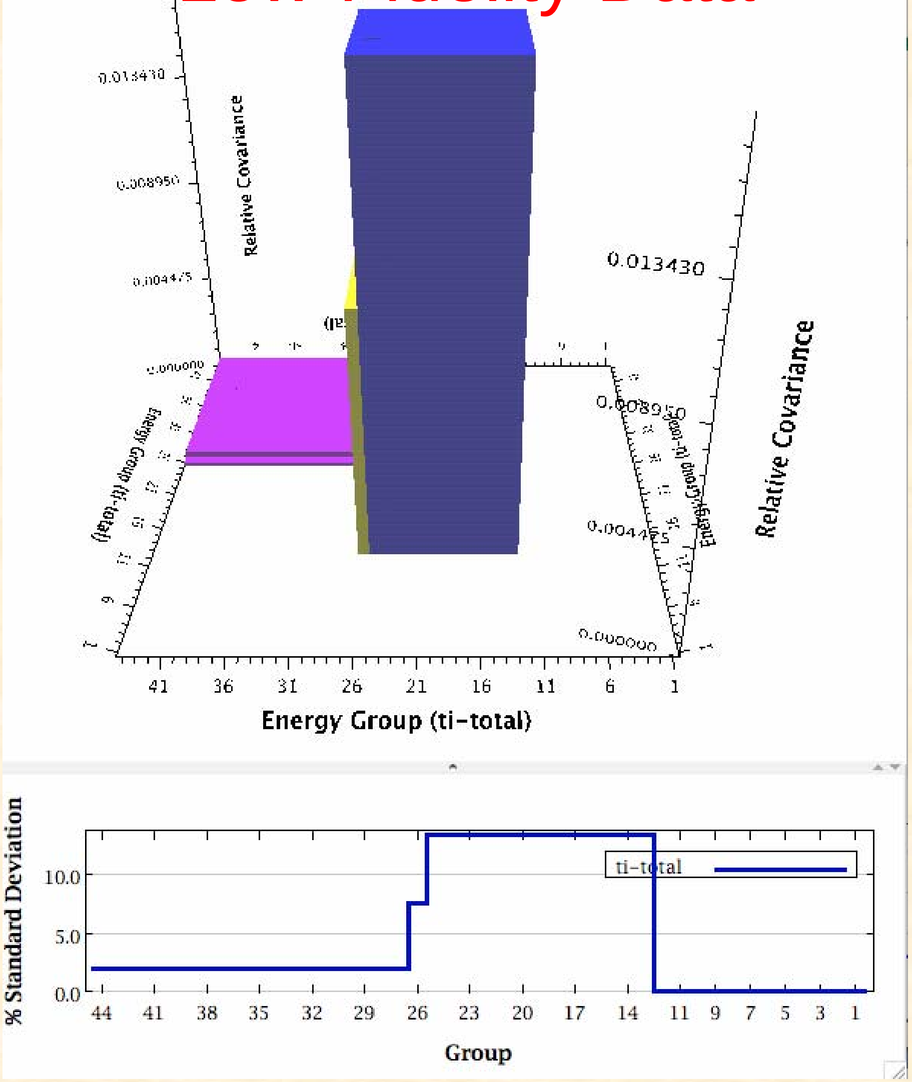
* New in ENDF/B-VI
** Present in ENDF/B-V, but not in ENDF/B-VI.

Procedure to Generate Covariance Library for Applications

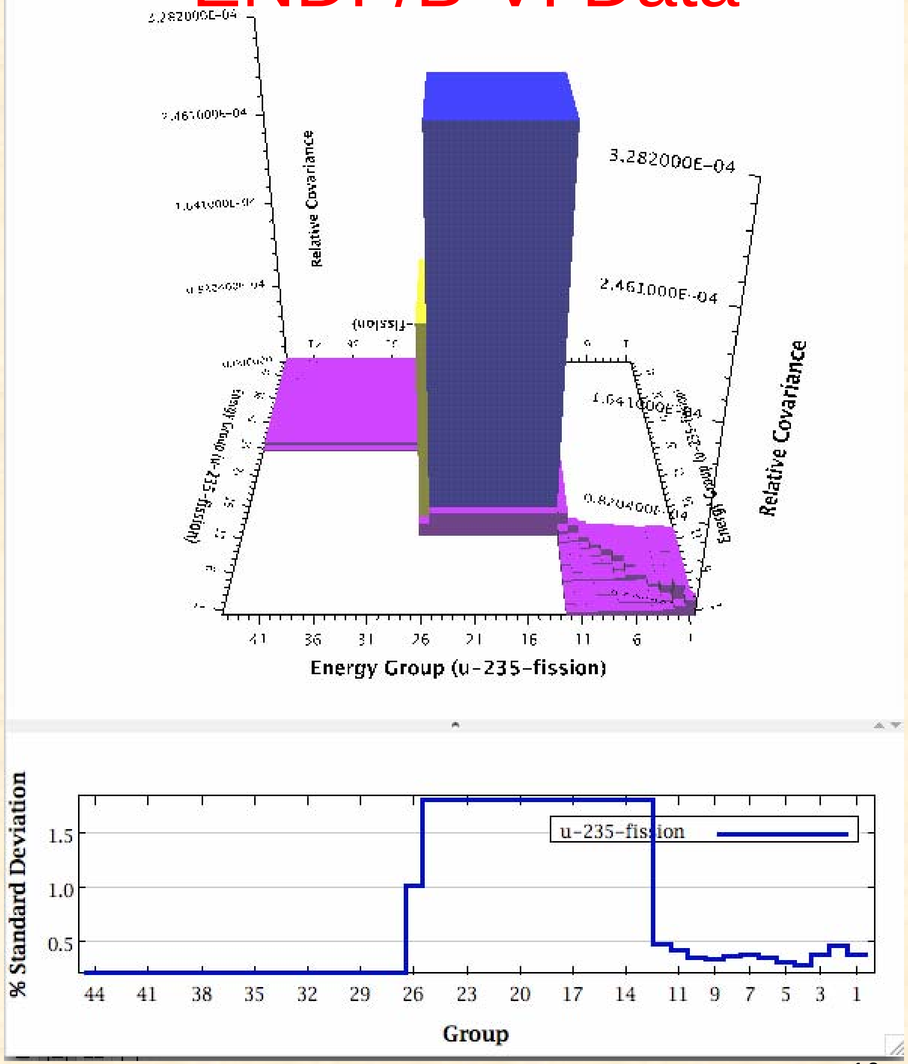
- Process all ENDF/B-VI covariances *(49 nuclides)*
- If available, use ENDF/B-V covariances for missing ENDF/B-VI data *(7 nuclides)*
- Approximate covariances of other missing nuclides by **integral measurement uncertainties -** Mughabghab data *(>250 nuclides)*
  - **σ_c, σ_f, υ covariance for E<0.5 eV based thermal data uncertainty, with full correlation**
  - **σ_c, σ_f covariance for 0.5<E<5E3 eV based on resonance integral, with full correlation**
  - **σ_s covariance for moderators based on uncertainty in potential cross section, fully correlated**
- 600 matrices in SCALE 5.0 covariance library (ENDF/B-V only)
- 2439 matrices in SCALE 5.1 covariance library

Sample SCALE 5.1 Covariance Data

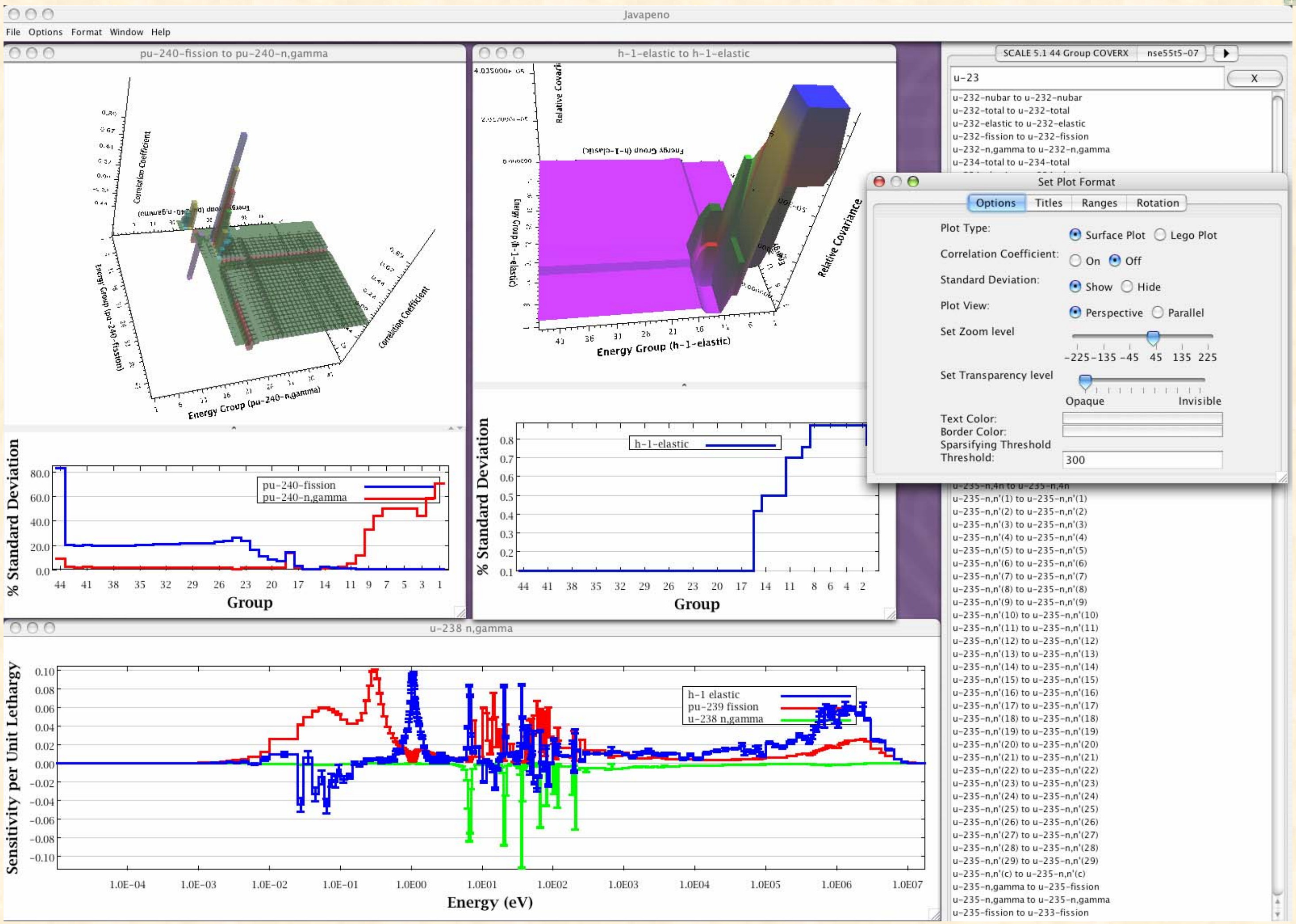
“Low-Fidelity Data”



ENDF/B-VI Data



Javapeño for SCALE 5.1



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Developmental Activities

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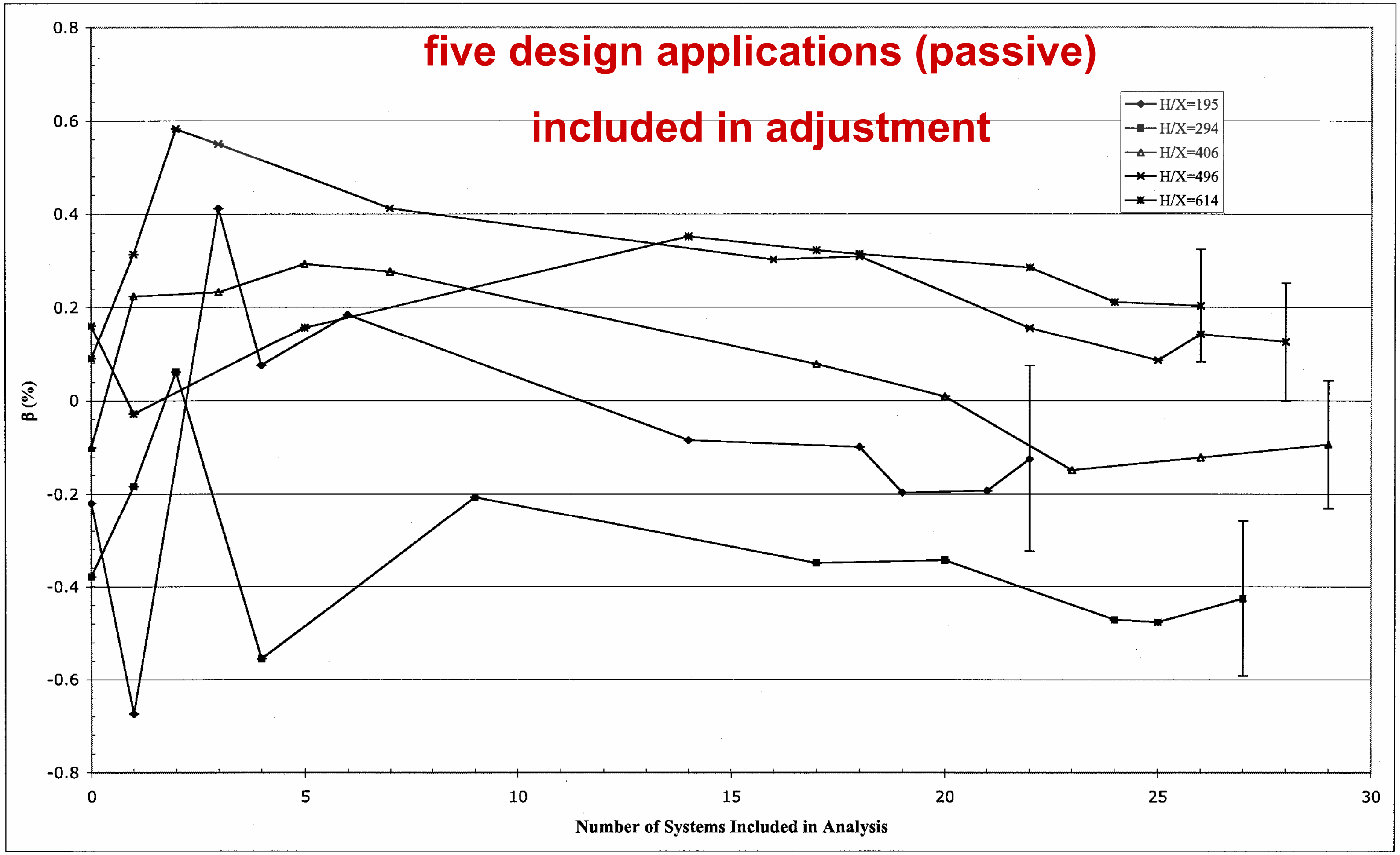
TSUNAMI Beyond SCALE 5.1

TSURFER

Performs *Generalized Linear Least-Squares (GLLS)* Analysis of Design System and Benchmark Data Base

- **Systematic procedure to consolidate calculations with measured responses**
- **Computes "best" cross-section adjustments to minimize differences in computed and measured benchmark responses**
- **Propagation of data perturbations to the design system response provides estimate of computational bias and uncertainty**
- **Allows correlations in experimental uncertainty components; filtering of benchmarks based on similarity; edit of adjusted data and covariances**

Bias Prediction Versus Number of Similar Systems ($c_k > 0.9$) in GLLS Adjustment



Reactivity Sensitivity and Uncertainty Analysis

$$S_{\rho,\alpha} = \frac{\alpha \partial \rho_{1\to 2}}{\rho_{1\to 2} \partial \alpha}$$

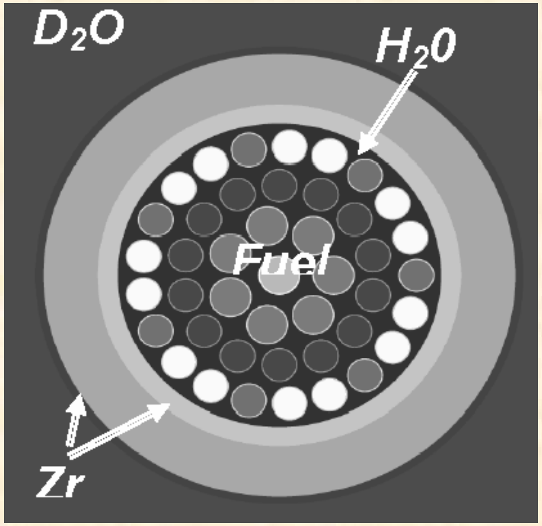
Eigenvalue Differencing Approach

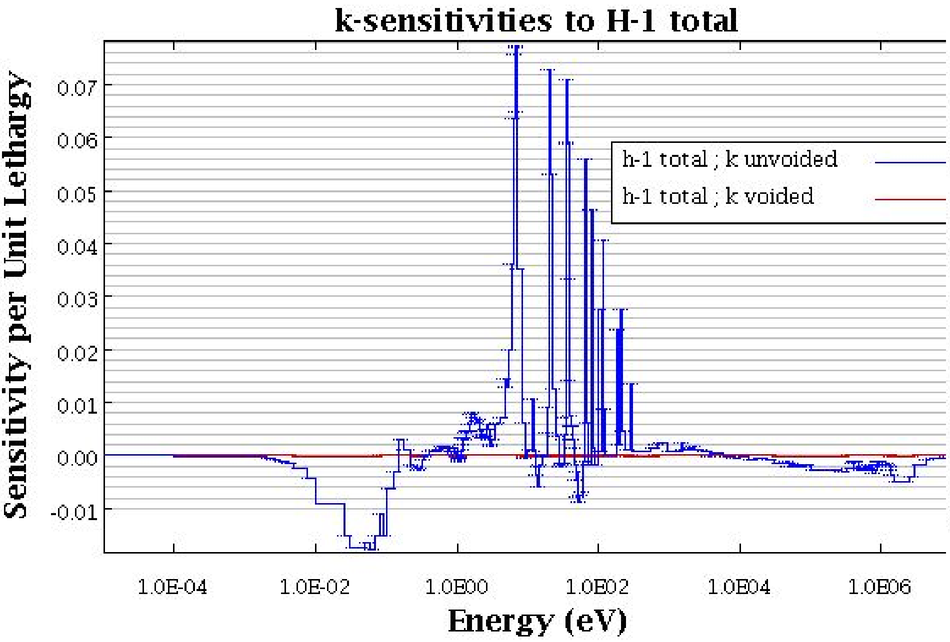
$$S_{\rho,\alpha} = \left\{ \frac{\left\langle \Phi_1^* \left(\frac{\alpha \partial L_1}{\partial \alpha} - \lambda_1 \frac{\alpha \partial P_1}{\partial \alpha} \right) \Phi_1 \right\rangle}{\rho_{1\to 2} \left\langle \Phi_1^* P_1 \Phi_1 \right\rangle} - \frac{\left\langle \Phi_2^* \left(\frac{\alpha \partial L_2}{\partial \alpha} - \lambda_2 \frac{\alpha \partial P_2}{\partial \alpha} \right) \Phi_2 \right\rangle}{\rho_{1\to 2} \left\langle \Phi_2^* P_2 \Phi_2 \right\rangle} \right\}$$

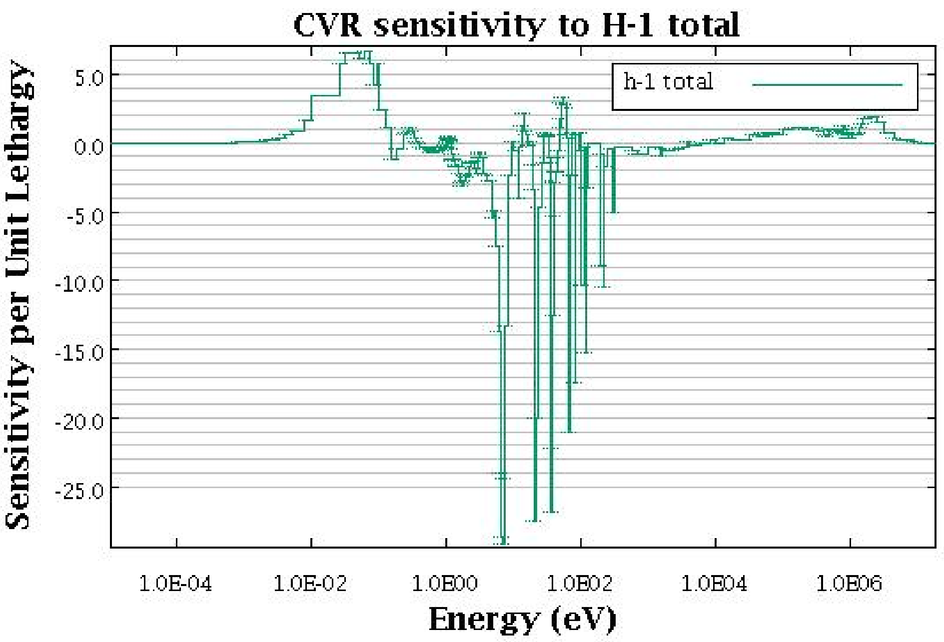
Uncertainty in Reactivity

$$\sigma_\rho^2 = \left(\frac{\lambda_1 \sigma_{\lambda_1}}{\rho_{1\to 2}} \right)^2 + \left(\frac{\lambda_2 \sigma_{\lambda_2}}{\rho_{1\to 2}} \right)^2 - 2 \frac{\sigma_{\lambda_1,\lambda_2}}{\sigma_{\lambda_1} \sigma_{\lambda 2}} \left(\frac{\lambda_1 \sigma_{\lambda_1}}{\rho_{1\to 2}} \right) \left(\frac{\lambda_2 \sigma_{\lambda_2}}{\rho_{1\to 2}} \right)$$

Application to ACR-700 CVR





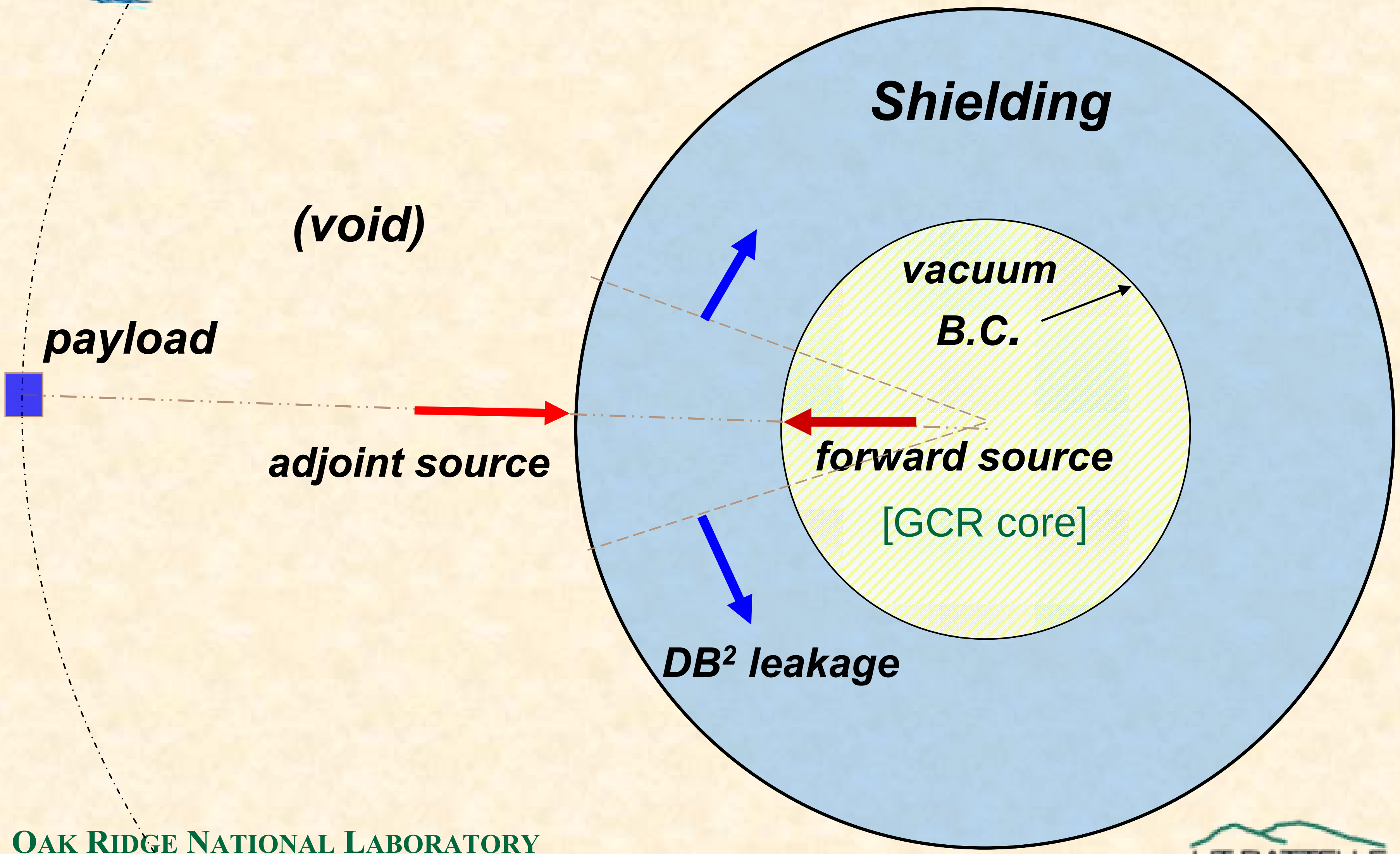


ACR-700 Uncertainties

TABLE V
Response Uncertainties Due to Available Nuclear Data Covariances

Response	Relative Standard Deviation (%)
Multiplication factor for state 1	0.80
Multiplication factor for state 2	0.84
Coolant void reactivity (CVR)	49.8

Space Reactor Spherical Model



Response Uncertainty Analysis for Space-Shielding

Shield Design	Response ; Uncertainty %	Identified Major Contributors to Uncertainty
front SS316 B4C Be + B4C SS316 Water+LiOH SS316 back	φ>1MeV 6.01%	o-16 n,n'
		h-1 elastic
		o-16 elastic
		o-16 n,alpha
		li-6 elastic
		fe-56 n,n'
	Si γ-Kerma 1.34%	fe-56 n,gamma
		cr-53 n,gamma
		ni-58 n,gamma
		mn-55 n,gamma
	Peak Heating 0.28%	b-10 n,alpha
		fe-56 elastic

Overview of ORNL Lab-Directed R&D Projects on the Strategic Use of High Performance Computing for Modeling Complex Phenomena

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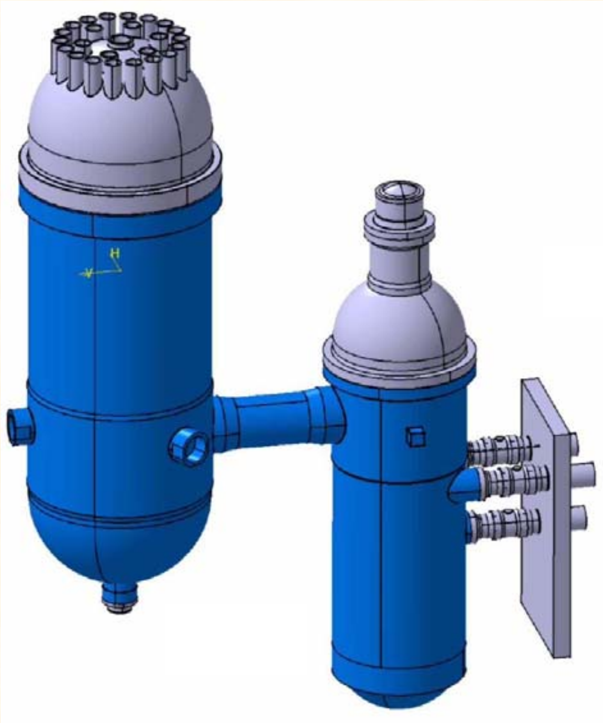
Tools for Sensitivity and UNcertainty Analysis Methodology Implementation

Kevin Clarno

Global Nuclear Energy Simulator for Reactors - GNES-R

- **Explore scientific phenomena**
  - **Complex interaction of nuclear, mechanical, chemical, & structural processes in fission reactors**
- **Simulate severe accidents**
  - **Multi-physics transients with advanced materials at high temperature and pressure in a changing radiation spectrum**
- **Optimize nuclear designs**
  - **Nuclear facilities are expensive: cost & time**
  - **Radiation activation prevents retrofits**



- **Leverage both ORNL & INL resources**

ORNL	INL
Nuclear analysis and simulation Computer science and mathematics 2 year, 5 people	Thermal-fluid simulation for reactors Nuclear reactor accident modeling Two 3 year, 5 people

Working together we can utilize intellectual and financial resources across institutions

- **Computer Science and Math** — **ORNL**
  - **Integrate interoperability and scientific tools from the SciDAC program** — **ANL, U-Tenn**
- **Radiation Transport** — **ORNL - GA Tech**
  - **Develop a high-fidelity neutral-particle radiation transport code** — **U-Tenn**
- **Fluid Dynamics & Heat Transfer** — **INL**
  - **Develop a multi-phase, non-isothermal CFD code** — **ANL**
  - **Multi-material, non-isothermal, chemically-reactive**

LDRDs ↑

Future Work ↓

- **Structural-dynamics** — **(TBD)**
  - **Fluid-structure, elasto-plastic mechanics**
  - **Impact dynamics**
- **Multi-scale materials modeling** — **(TBD)**

Proposed ORNL/LANL R&D Under DOE SciDAC

- **Integrate advanced TSUNAMI eigenvalue S/U techniques into CE-KENO and MCNP**
- **Develop production-level sensitivity version of ORIGEN**
- **End goal: Production level depletion-perturbation-theory code sequence for advanced reactor design**
- **Propagate and accumulate uncertainties throughout calculation**