TSUNAMI Methods for Validation, Gap Analysis and Experiment Design

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Verification and Validation for Nuclear Systems Analysis Workshop

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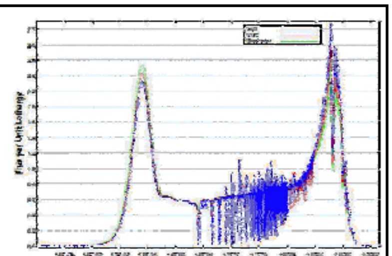
Criticality Safety Assessment

- **ANS/ANSI 8.24 Standard requires validation of computational methods with comparison to experimental data that are similar to the safety application.**
- **Bias and uncertainty in bias must be quantified with defensible methods.**
- **Subcriticality of safety application must be ensured.**
- **An Upper Subcritical Limit (USL) is established as maximum allowed *computed* value of k_{eff} for safety application.**

Uses of TSUNAMI for Criticality Safety and Reactor Physics Validation

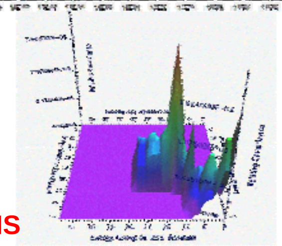
- **Uncertainty quantification for applications and benchmark experiments**
  - **Uncertainty due to cross section covariance data should bound most computational bias**
- **Rigorous assessment of similarity between applications and benchmarks**
- **Bias and bias uncertainty determination by projection of experimental bias to application**
  - **Trending bias as a function of experiment-application similarity**
  - **Data adjustment to quantify bias in application**
- **Gap analysis – quantification of uncertainty in application that is not covered by benchmarks (penalty assessment)**
- **Design of optimized experiments to quantify bias present in gap.**

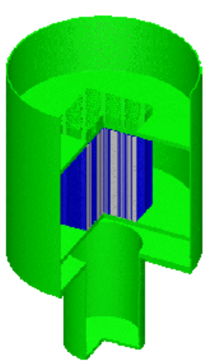
TSUNAMI-3D in SCALE 5.1



CENTRMST/PMCST

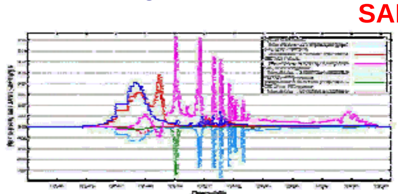
Continuous energy transport for multigroup cross-section preparation with "implicit effect", up to 40% contribution for thermal/intermediate systems





KENO V.a

Forward/Adjoint multigroup Monte Carlo flux calculation with angular moments



SAMS

Sensitivity coefficient generation
Uncertainty propagation from cross-section covariance data to k_{eff}

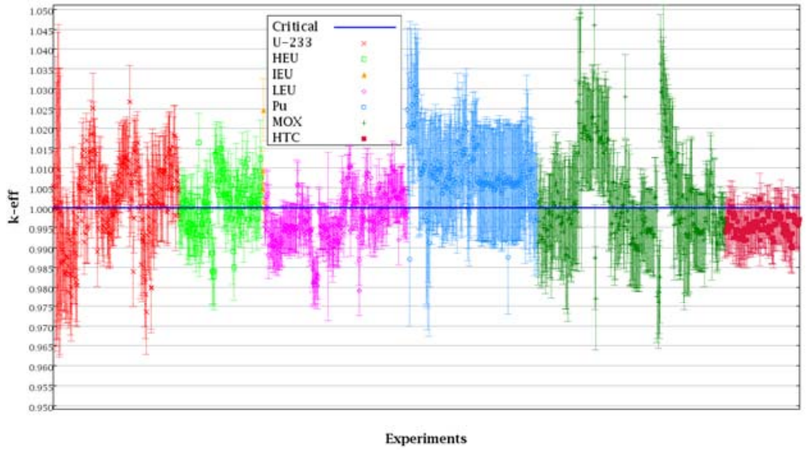
SCALE Covariance Library

- 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 has Cov data for >250 materials based on:
  - High fidelity evaluations from ENDF/B and JENDL
  - Recent high fidelity evaluations by LANL
  - Approximate values fro "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}
ENDF/B-VI	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} $Pb^{206-208}$ B^{209} Am^{241}
JENDL	$Pu^{240-241}$
LANL Hi-Fi	H^{1-3} He^{3-4} Li^{6-7} Be^{9} B^{10-11} C^{12} N^{14-15} O^{16-17} F^{19}
Lo-Fi	~ 200 materials

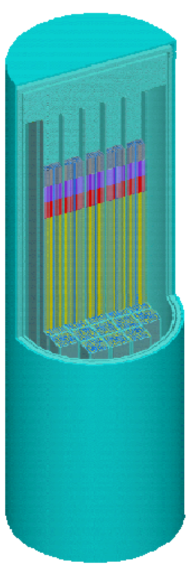
k_{eff} and Uncertainty for 1378 Critical Experiments

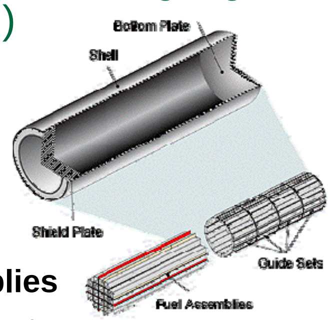


Statistical agreement with k_{eff} = 1.0 – near perfect Gaussian distribution

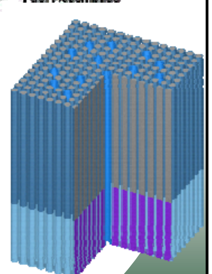
- 68% agree within 1 σ
- 95% agree within 2 σ
- 98% agree within 3 σ

Yucca Mountain Transportation, Aging and Disposal Canister (TAD)





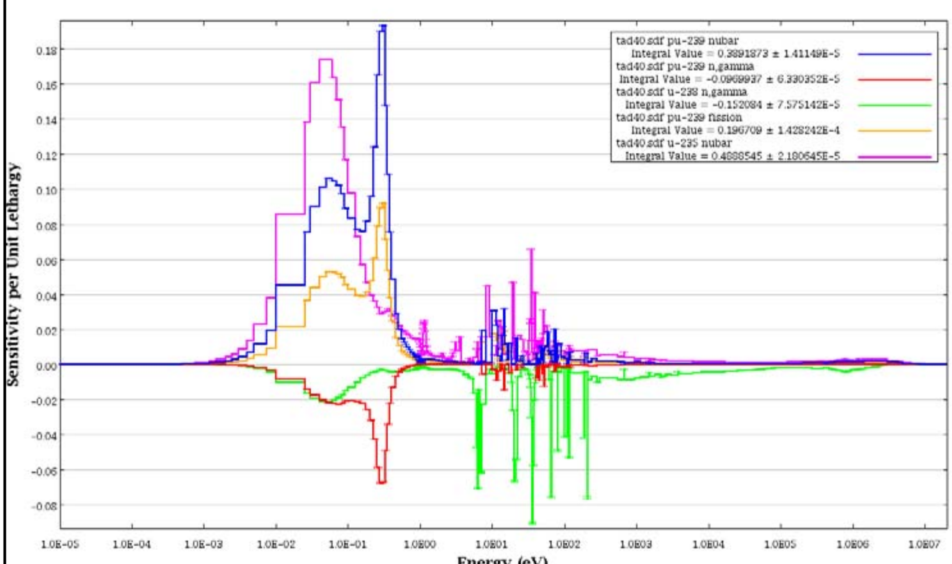
- **21 15 × 15 PWR Assemblies**
- **Initial enrichment of 4 wt-%**
- **Burned to 40 GWD/MT**
- **Flooded waste package surrounded by tuff**
- **Stainless steel sheaths and borated steel plates**



Nuclides in TAD Model

Spent Fuel		Cladding		Moderator	Steel Sheaths		Borated Steel		Tuff
^{16}O	^{233}U	^{16}O	^{112}Sn	^{1}H	C	^{54}Fe	^{10}B	^{55}Mn	^{16}O
^{95}Mo	^{234}U	^{50}Cr	^{114}Sn	^{16}O	^{14}N	^{56}Fe	^{11}B	^{54}Fe	^{23}Na
^{99}Tc	^{235}U	^{52}Cr	^{115}Sn		Si	^{57}Fe	C	^{56}Fe	Mg
^{101}Ru	^{236}U	^{53}Cr	^{116}Sn		^{31}P	^{58}Fe	^{14}N	^{57}Fe	^{27}Al
^{103}Rh	^{238}U	^{54}Cr	^{117}Sn		^{32}S	^{58}Ni	Si	^{58}Fe	Si
^{109}Ag	^{237}Np	^{54}Fe	^{118}Sn		^{50}Cr	^{60}Ni	^{31}P	^{59}Co	^{31}P
^{143}Nd	^{238}Pu	^{56}Fe	^{119}Sn		^{52}Cr	^{61}Ni	^{32}S	^{58}Ni	K
^{145}Nd	^{239}Pu	^{57}Fe	^{120}Sn		^{53}Cr	^{62}Ni	^{50}Cr	^{60}Ni	Ca
^{147}Sm	^{240}Pu	^{58}Fe	^{122}Sn		^{54}Cr	^{64}Ni	^{52}Cr	^{61}Ni	Ti
^{149}Sm	^{241}Pu	Zr	^{124}Sn		^{55}Mn	Mo	^{53}Cr	^{62}Ni	^{55}Mn
^{150}Sm	^{242}Pu						^{54}Cr	^{64}Ni	^{54}Fe
^{151}Sm	^{241}Am								^{56}Fe
^{152}Sm	^{242}Am								^{57}Fe
^{151}Eu	^{243}Am								^{58}Fe
^{153}Eu									
^{155}Gd									

Sensitivity Profiles for TAD



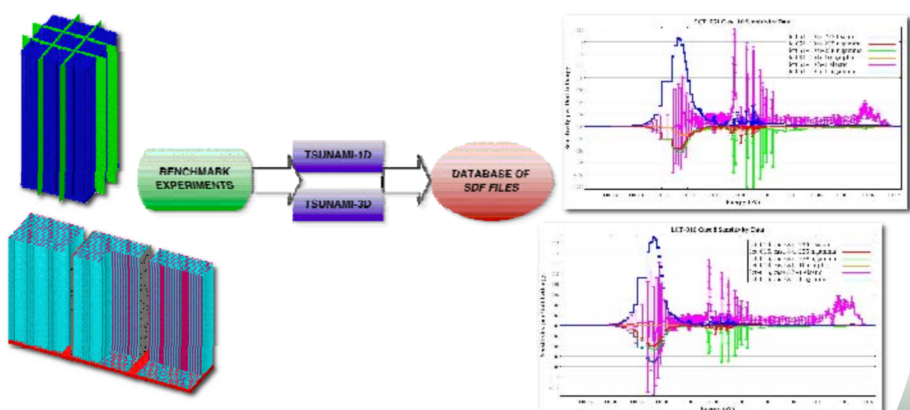
Uncertainty Assessment

the relative standard deviation of k_{eff} (% $\Delta k/k$) is: 0.5982 ± 0.0001 percent

contributions to uncertainty in k_{eff} (% $\Delta k/k$) by individual energy covariance matrices:

Covariance Matrix		% Δk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{239}Pu nubar	^{239}Pu nubar	4.0032E-01 ± 7.5161E-06
^{239}Pu n,gamma	^{239}Pu n,gamma	2.2350E-01 ± 8.7365E-05
^{238}U n,gamma	^{238}U n,gamma	2.2281E-01 ± 1.0662E-04
^{239}Pu fission	^{239}Pu fission	1.5511E-01 ± 4.8605E-05
^{235}U nubar	^{235}U nubar	1.3980E-01 ± 3.5216E-06

Identify and Analyze Benchmark Experiments to Quantify Bias in Application



Correlation Coefficient (c_k)

(a.k.a. representativity factor)

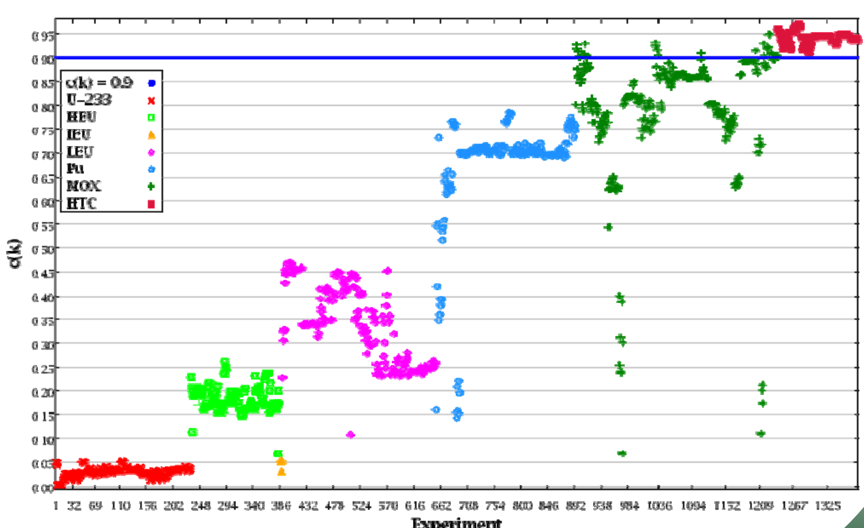
- **Quantifies degree of shared variance in k_{eff} between design application and benchmark experiment.**

$$c_k = \frac{\sigma_{ae}^2}{\sigma_a \sigma_e}$$

Covariance between Experiment (e) and Application (a) due to all nuclides and reactions

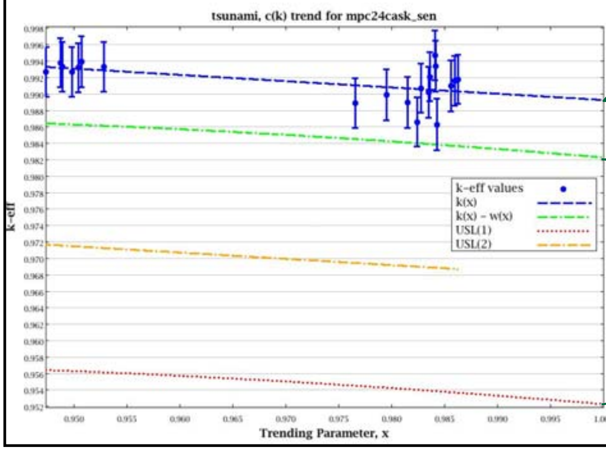
Standard deviations for Application (a) and Experiment (e) due to all nuclides and reactions

c_k Values for 1378 Experiments Relative to TAD Canister

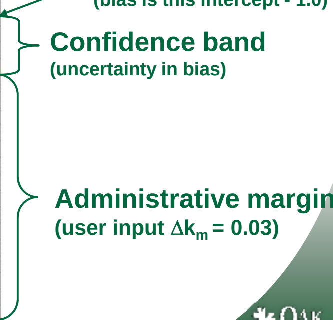


Projection of Bias to Application

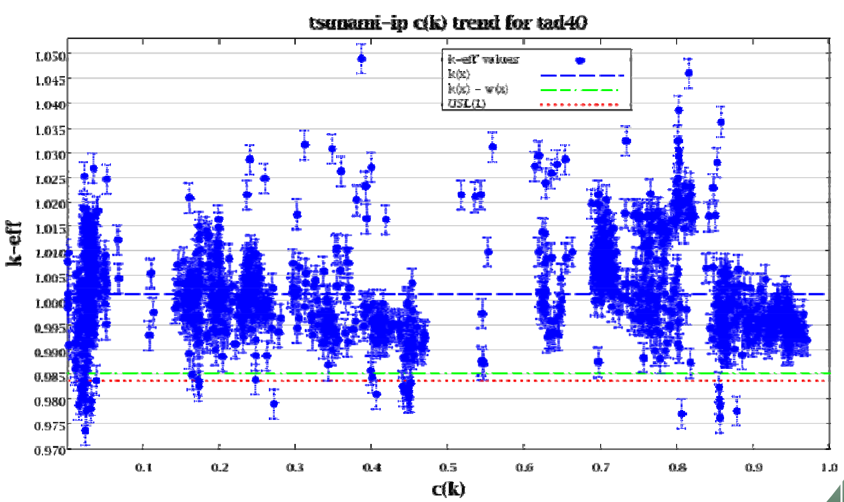
Examine normality of data
Perform regression/extrapolation



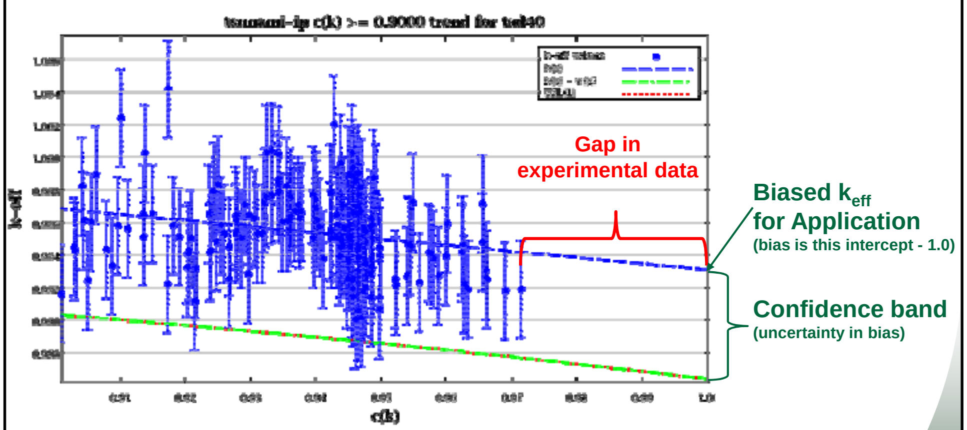
Biased k_{eff} for Application
(bias is this intercept - 1.0)



TAD Bias Assessment with USLSTATS using all 1378 Experiments



Improved TAD Bias Assessment with USLSTATS using only Best Experiments



note administrative margin is set to 0.0 here

Gap Analysis for TAD

the relative standard deviation of k_{eff} (% $\Delta k/k$) due to uncovered sensitivity data is: 0.1829 ± 0.0000 percent

contributions to uncertainty in k_{eff} (% $\Delta k/k$) by individual energy covariance matrices:

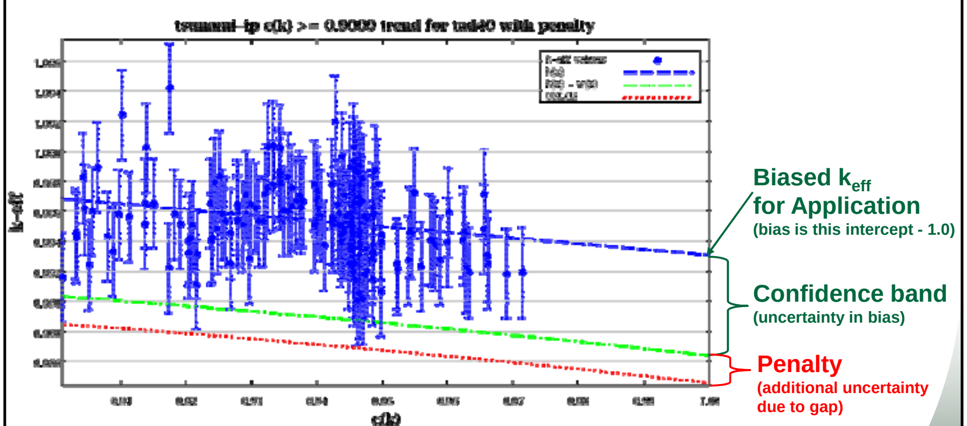
Covariance Matrix		% $\Delta k/k$
Nuclide-Reaction	**Nuclide-Reaction**	**Due to this Matrix**
^{239}Pu nubar	^{239}Pu nubar	7.0692E-02 ± 5.5661E-06
^{239}Pu n,gamma	^{239}Pu n,gamma	6.5976E-02 ± 6.9402E-05
^{239}Pu fission	^{239}Pu fission	6.2445E-02 ± 4.1232E-05
^{56}Fe n,gamma	^{56}Fe n,gamma	5.1023E-02 ± 5.5337E-05
^{235}U fission	^{235}U fission	5.0409E-02 ± 3.0036E-05
^{238}U n,gamma	^{238}U n,gamma	4.7994E-02 ± 9.7189E-05

Fission Product Uncertainties

- **With few exceptions, fission products are absent from experimental database and ENDF covariance data.**
- **Quantification of bias not possible because of lack of available experimental data.**
- **Bias can only be conservatively bounded by uncertainty quantification – or penalty.**
- **Fission product penalty is 0.07% Δk/k of 0.18% Δk/k total penalty**

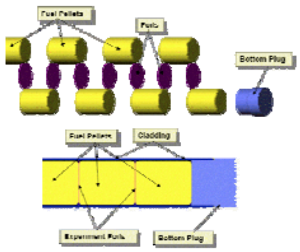
Nuclide	Reaction	Penalty Contribution %Δk/k
^{143}Nd	n,gamma	4.18E-02
^{103}Rh	n,gamma	2.69E-02
^{145}Nd	n,gamma	2.30E-02
^{149}Sm	n,gamma	2.20E-02
^{101}Ru	n,gamma	2.13E-02
^{99}Tc	n,gamma	1.47E-02
^{151}Sm	n,gamma	1.37E-02
^{147}Sm	n,gamma	1.12E-02
^{153}Eu	n,gamma	1.02E-02
^{152}Sm	n,gamma	9.08E-03
^{150}Sm	n,gamma	5.99E-03
^{95}Mo	n,gamma	5.35E-03
^{109}Ag	n,gamma	3.40E-03
^{155}Gd	n,gamma	2.75E-03

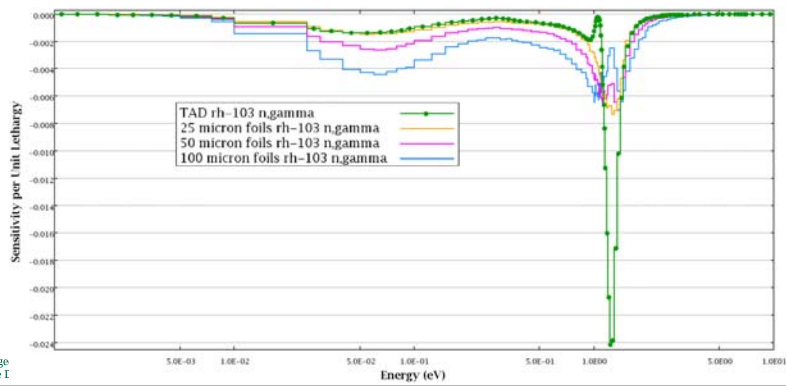
Addition of Penalty to Upper Subcritical Limit



note 1σ penalty applied here, could be 2 or 3σ for improved confidence

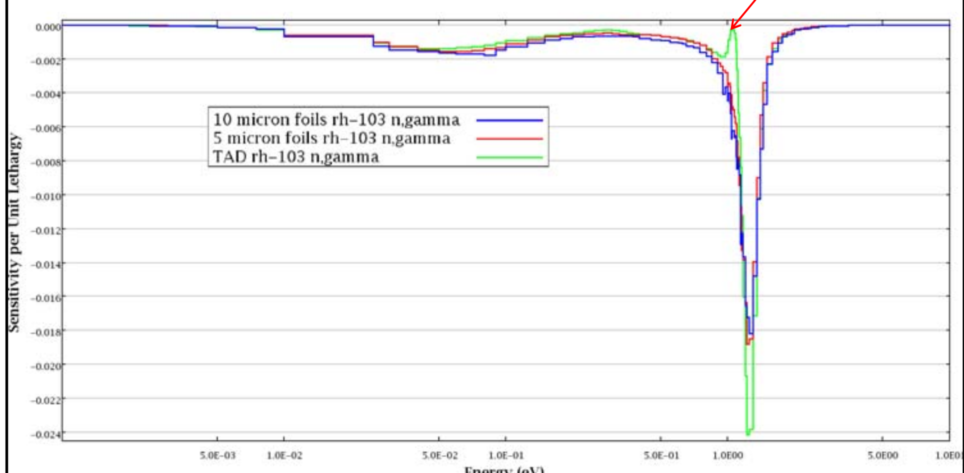
^{103}Rh in SNL BUCCX – LEU-COMP-THERM-079





Experiment Design with TSUNAMI – Optimize Foil Thickness

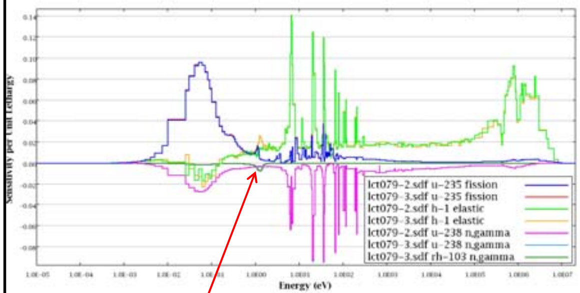
flux suppression from ^{240}Pu



Determine Bias Due Only to Replacement Material by Examining Pairs of Criticals

computed k_{eff}
lct79-2 no foils
0.9911
lct79-3 25 micron foils
0.9917

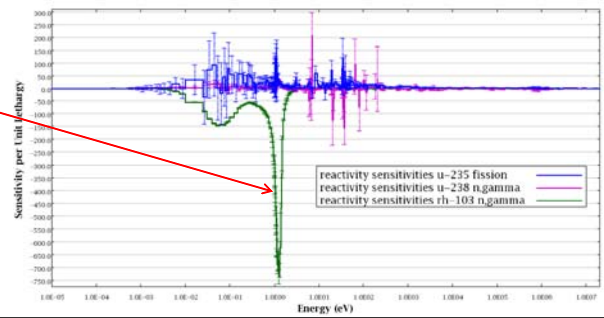
reactivity difference
60 pcm



k_{eff} sensitivity

^{103}Rh

ρ sensitivity

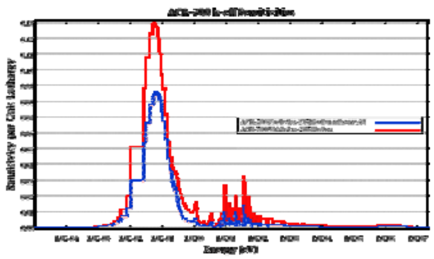


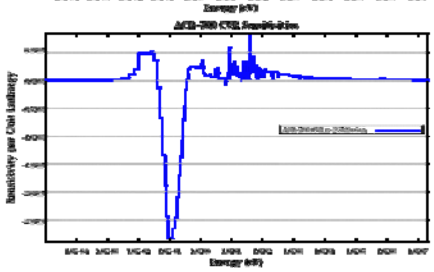
Data Adjustment Tool TSURFER

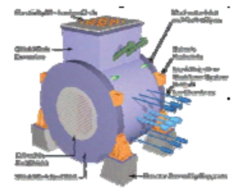
Generalized Linear Least-Squares (GLLS)

- **Simultaneously examines measured and calculated data and adjusts integral experiment values within their uncertainties and cross sections within their uncertainties to minimize differences between measured and computed results.**
- **Uses TSUNAMI sensitivity data for uncertainty propagation and to determine optimum adjustments**
- **Can consolidate useful data from different types of experiments that each contribute to the validation of the application**
  - **adjust to k_{eff} of 1.0 or reactivity difference to 0.0**
- **Once adjustments that minimize biases in experiments are computed, the adjustments are projected to the application via the sensitivity coefficients to predict its bias.**
- **Adjusted data are not used for further calculations, only to predict the bias.**
- **Can only make adjustments where experiments are available.**

Coolant Void Reactivity for ACR-700

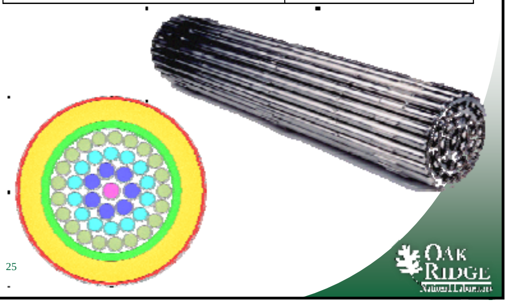






Response Uncertainties Due to Nuclear Data Covariances

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



Growing Use

- **The relatively easy-to-use TSUNAMI codes, GUIs, documentation, training courses and user support have brought sensitivity and uncertainty analysis into the mainstream.**
- **Distributed as part of SCALE by RSICC and NEA Data Bank.**
- **OECD/NEA Expert groups:**
  - **Uncertainty Analysis in Methods (UAM)**
  - **Uncertainty Analysis in Criticality Safety Assessment (UACSA)**
- **Recent and upcoming TSUNAMI training courses:**
  - **January 2008, NRC Headquarters, Washington, D.C. – 2 day refresher**
  - **February 2008, NEA Headquarters, Paris – 5 days**
  - **April 2008, WSMS Offices, SRNL – 2 day refresher**
  - **October 2008, NEA course hosted by KFKI, Budapest, Hungary – 5 days**
  - **November 2008, ORNL – 4 days**

Questions?

http://www.ornl.gov/scale/tsunami