Bias Assessment of ^{233}U Systems Using SCALE TSURFER

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^{233}U Downblending at ORNL

- Operations being designed to downblend materials stored at Radiochemical Development Facility (RDF)
  - Highly-enriched ^{233}U downblended with ^{238}U
- Aqueous process will be used
- K. R. ELAM, L. L. GILPIN, and B. W. STARNES, "Integrating Criticality Safety in Design of ^{233}U Downblending Process," *Trans. Am. Nucl.Soc.*, **100**, 343-344 (2009).

SCALE TSUNAMI Analysis

- ORNL staff used the SCALE TSUNAMI tools to provide a demonstration evaluation of critical experiments considered for use in validation of current and anticipated operations involving ^{233}U at the RDF.
- Reported in ORNL/TM-2008/196 issued in January 2009.
- Similarity assessment and c_k analysis presented at ANS in Winter 2009.
- Today we present the TSURFER bias assessment of two representative safety analysis models provided by RDF staff.

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

ORNL/TM-2008/196

Application of the SCALE TSUNAMI Tools for the Validation of Criticality Safety Calculations Involving ^{233}U

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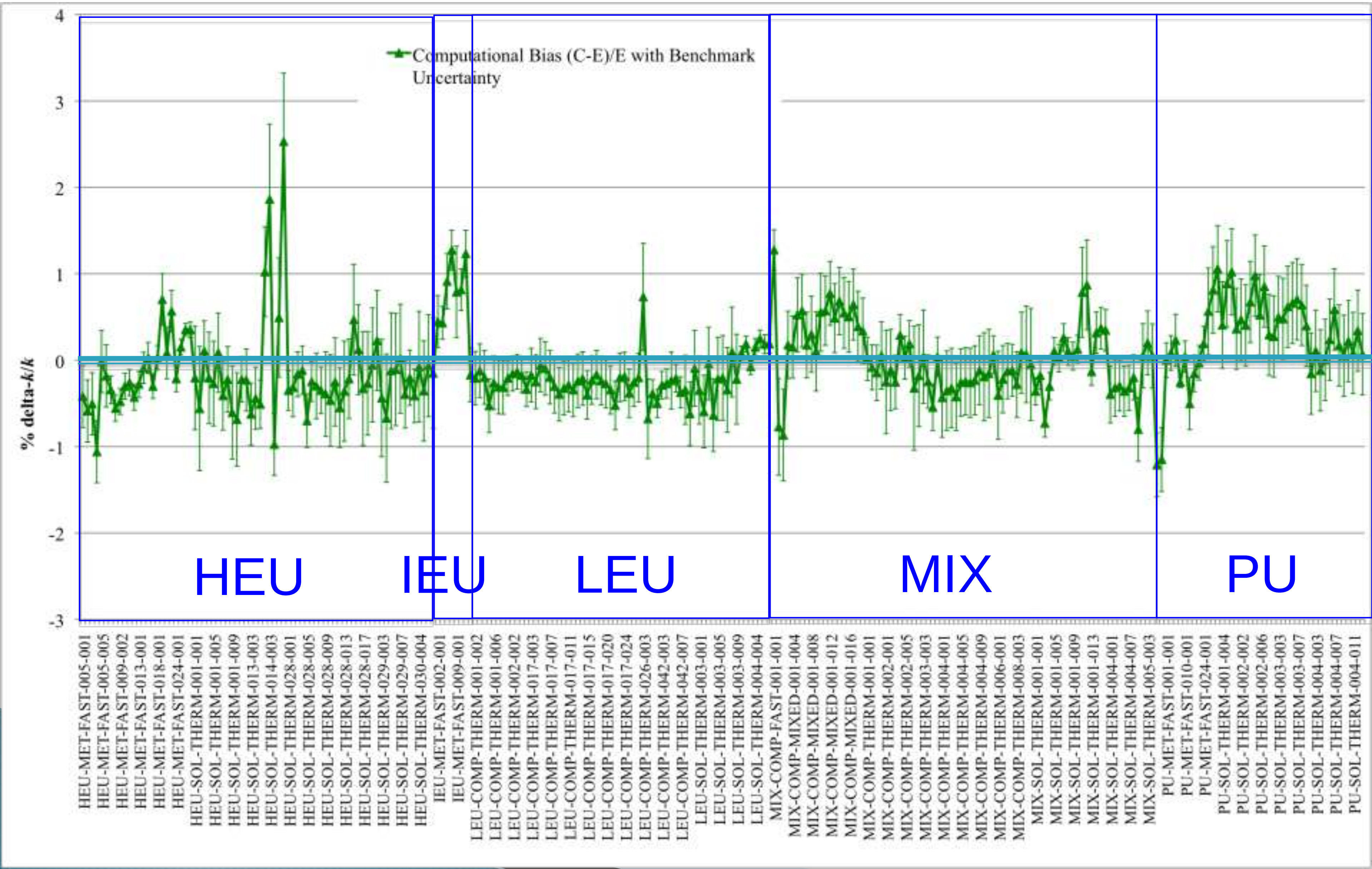
Computational Biases and Their Bounds

- Premise of SCALE/TSUNAMI validation concept for criticality safety applications
  - Computational biases are primarily caused by errors in cross-section data
  - Errors are bounded by cross-section uncertainties represented in covariance data
- SCALE provides sensitivity analysis tools to accurately and conveniently produce the sensitivity of k_{eff} and reactivity responses using explicit 3D Monte Carlo models
- SCALE sensitivity data are distributed through the ICSBEP
- Comprehensive covariance library distributed with SCALE

275 Benchmark Experiments

SCALE 6 ENDF/B-VII.0



275 Benchmark Experiments

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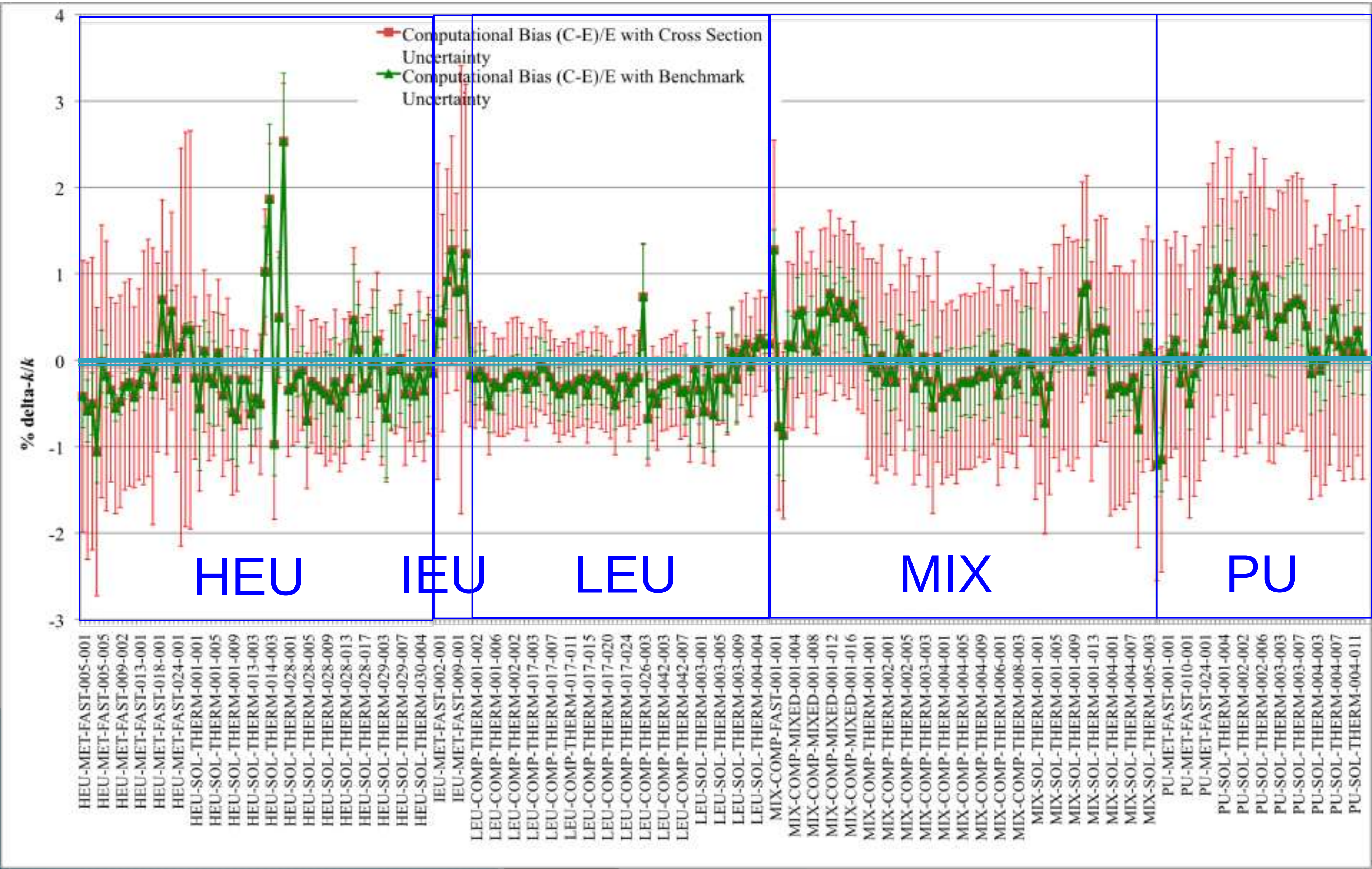


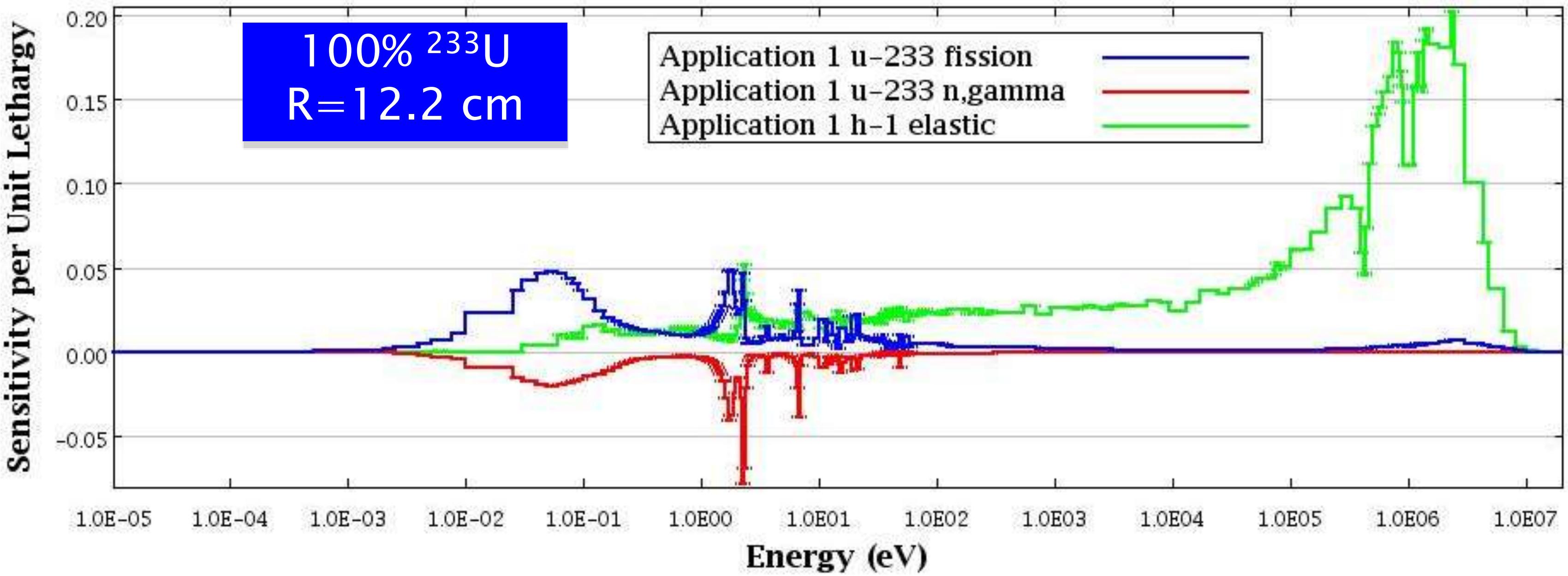
Generalized Linear Least Squares Approach to Bias and Bias Uncertainty Quantification

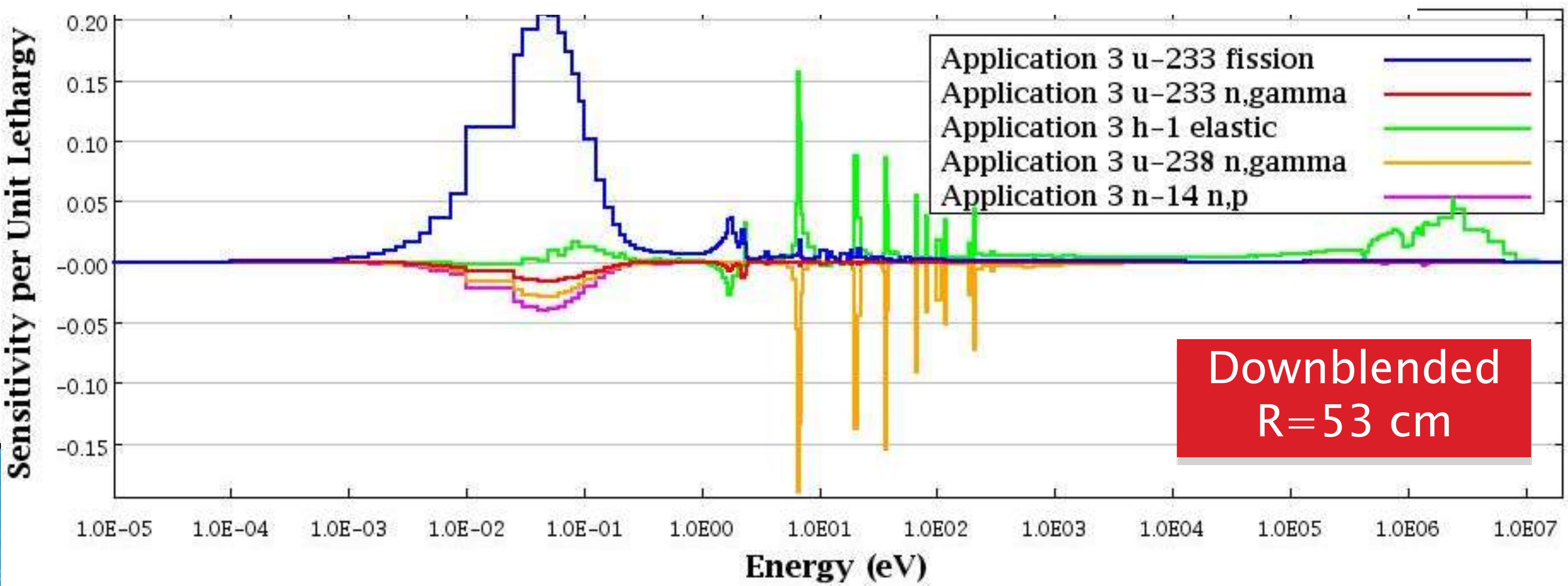
- *T*ool for *S*/*U* analysis of *R*esponse *F*unctionals using *E*xperimental *R*esults
  - Biases are observed as differences between benchmark and calculated k_{eff} values.
  - Benchmark values have uncertainties, some of which are correlated between different systems.
  - Calculated values have uncertainties, primarily due to uncertainties in the cross sections. These are correlated between systems that use the same cross sections.
  - Taking into account the uncertainties and correlations, a consistent set of of data can be formed that eliminates biases for the benchmarks, within a known uncertainty.
  - Where the cross sections and covariance data are modified, the modifications can be used to project biases from the benchmarks to a bias and bias uncertainty for targeted application systems.

^{233}U Application Models

- Application 1
  - 12.2 cm radius sphere of 220 g U per liter uranyl nitrate solution
  - U is 100 wt % ^{233}U
  - Reflector – 0.25 cm thick Type 304 stainless steel tank and 2 cm of water.
  - EALF is 0.282 eV
  - k_{eff} calculated for this system is 1.0028 ± 0.0002.
  - 82 experiments with $c_k \geq 0.95$
- Application 3
  - 53.0 cm radius sphere of 600 g U per liter uranyl nitrate solution, 80° C
  - U is 3 wt % ^{233}U, 0.2 wt % ^{235}U, and 96.8 wt % ^{238}U.
  - Reflector – 0.25 cm thick Type 304 stainless steel tank and 2 cm of water
  - EALF is 0.0631 eV
  - k_{eff} calculated for this system is 0.9690 ± 0.0002.
  - No experiments with $c_k \geq 0.7$

Sensitivity Profiles





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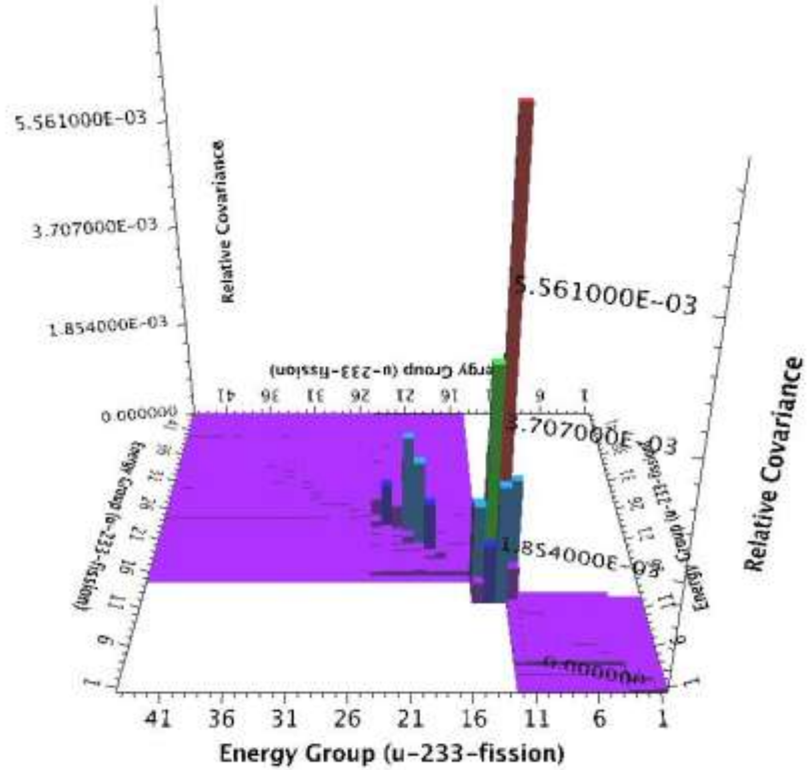
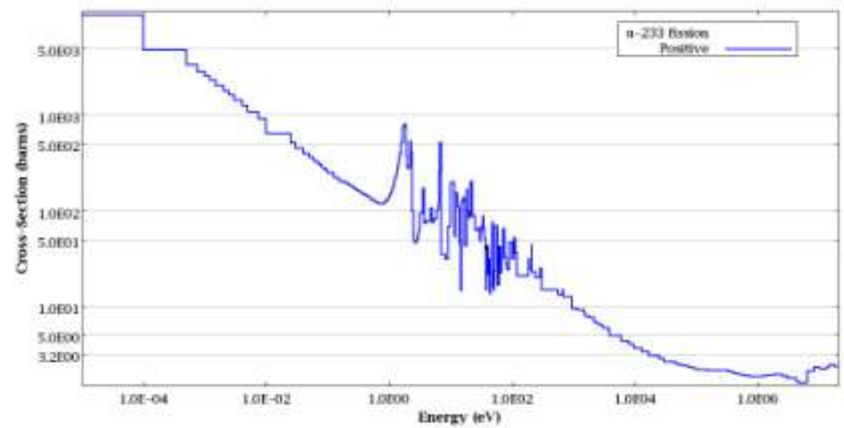
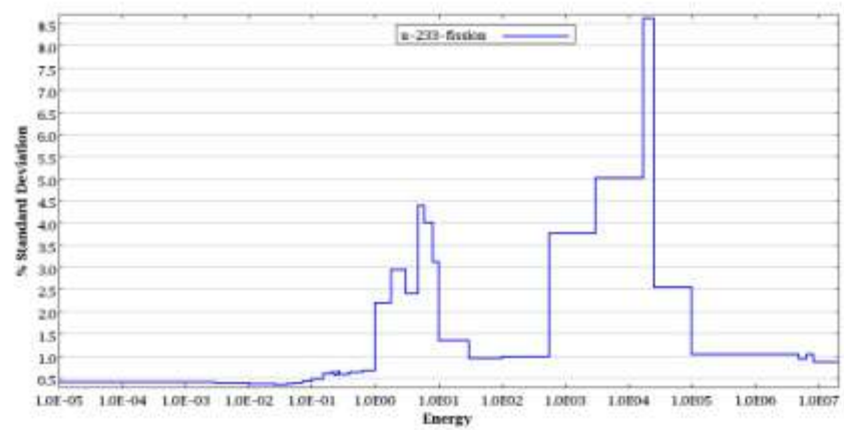
Covariance Data – ^{233}U Fission







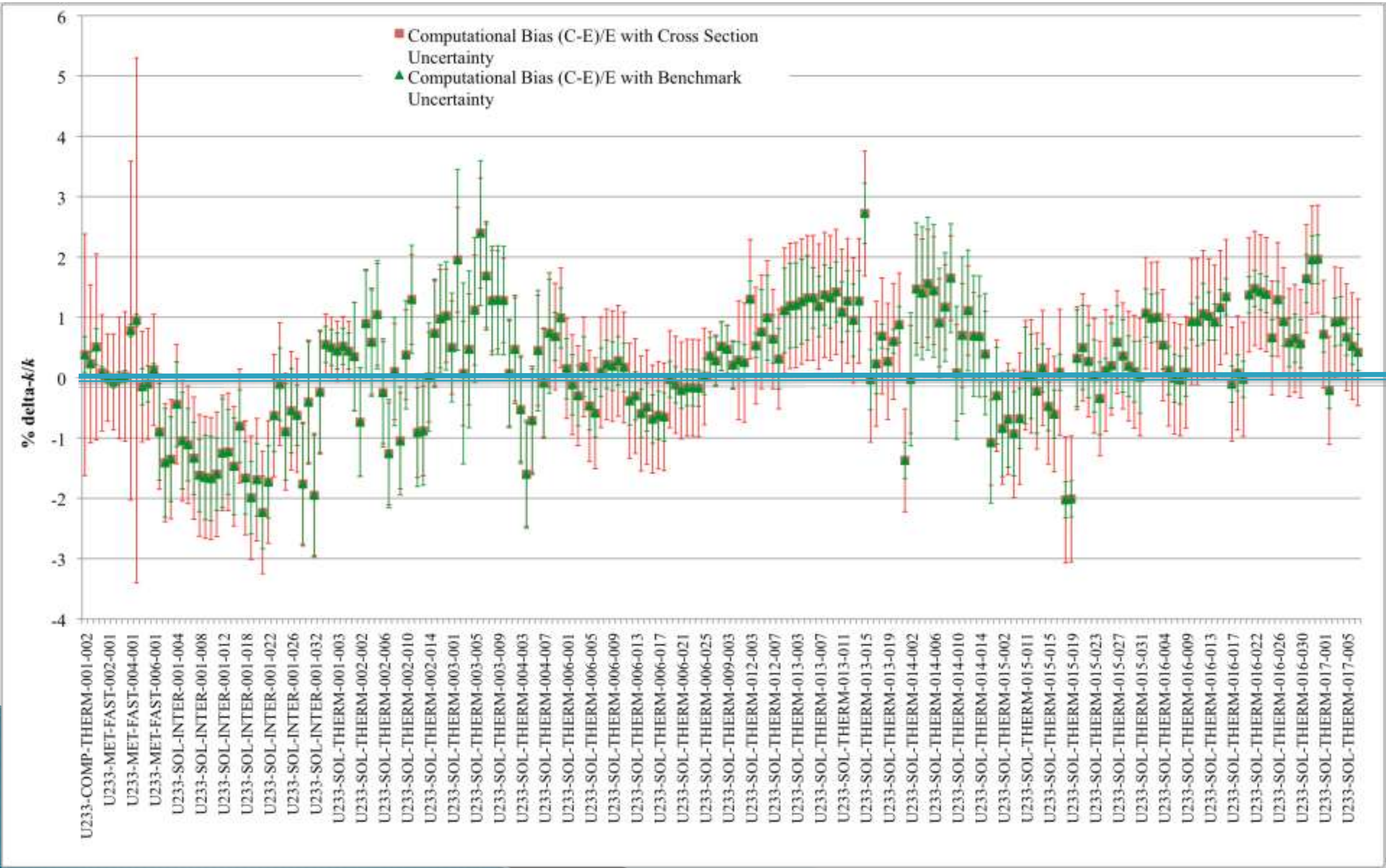
Uncertainty in Applications due to Covariance Data

System	Standard deviation (%)	Top six contributors to standard deviation (%)	
Application 1	0.937	^{233}U χ to ^{233}U χ	0.819
		^{1}H elastic to ^{1}H elastic	0.320
		^{16}O elastic to ^{16}O elastic	0.194
		^{233}U n,γ to ^{233}U n,γ	0.174
		^{233}U nubar to ^{233}U nubar	0.145
		^{233}U fission to ^{233}U fission	0.117
Application 3	0.515	^{14}N n,p to ^{14}N n,p	0.346
		^{238}U n,γ to ^{238}U n,γ	0.233
		^{233}U fission to ^{233}U fission	0.173
		^{1}H n,γ to ^{1}H n,γ	0.145
		^{233}U χ to ^{233}U χ	0.136
		^{233}U nubar to ^{233}U nubar	0.135

Analysis Methods

- SCALE 5.1 TSUNAMI tools TSUNAMI-3D, TSUNAMI-1D were used to generate k_{eff} sensitivity data for the applications and 672 critical experiments from 101 ICSBEP evaluations
  - 232 ^{233}U configurations
  - 28 mixed U/Pu configurations
  - 153 high uranium enrichment configurations
  - 255 low uranium enrichment configurations
- Pre-release SCALE 6.0 TSURFER Code was applied to 1066 benchmarks as a demonstration of the technique

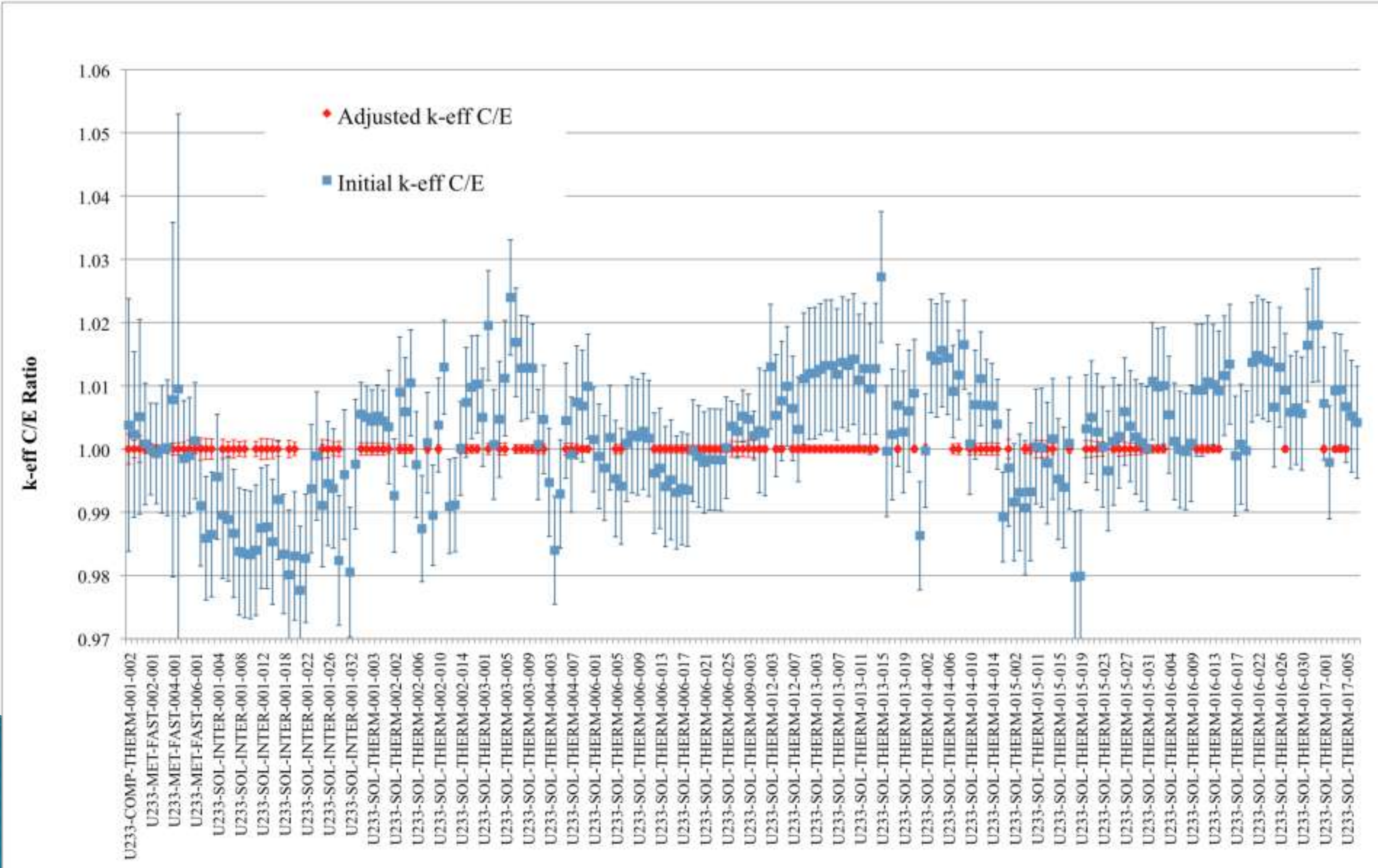
^{233}U Systems from 2009 ICSBEP Handbook Distribution k_{eff} C/E and Experimental Uncertainty



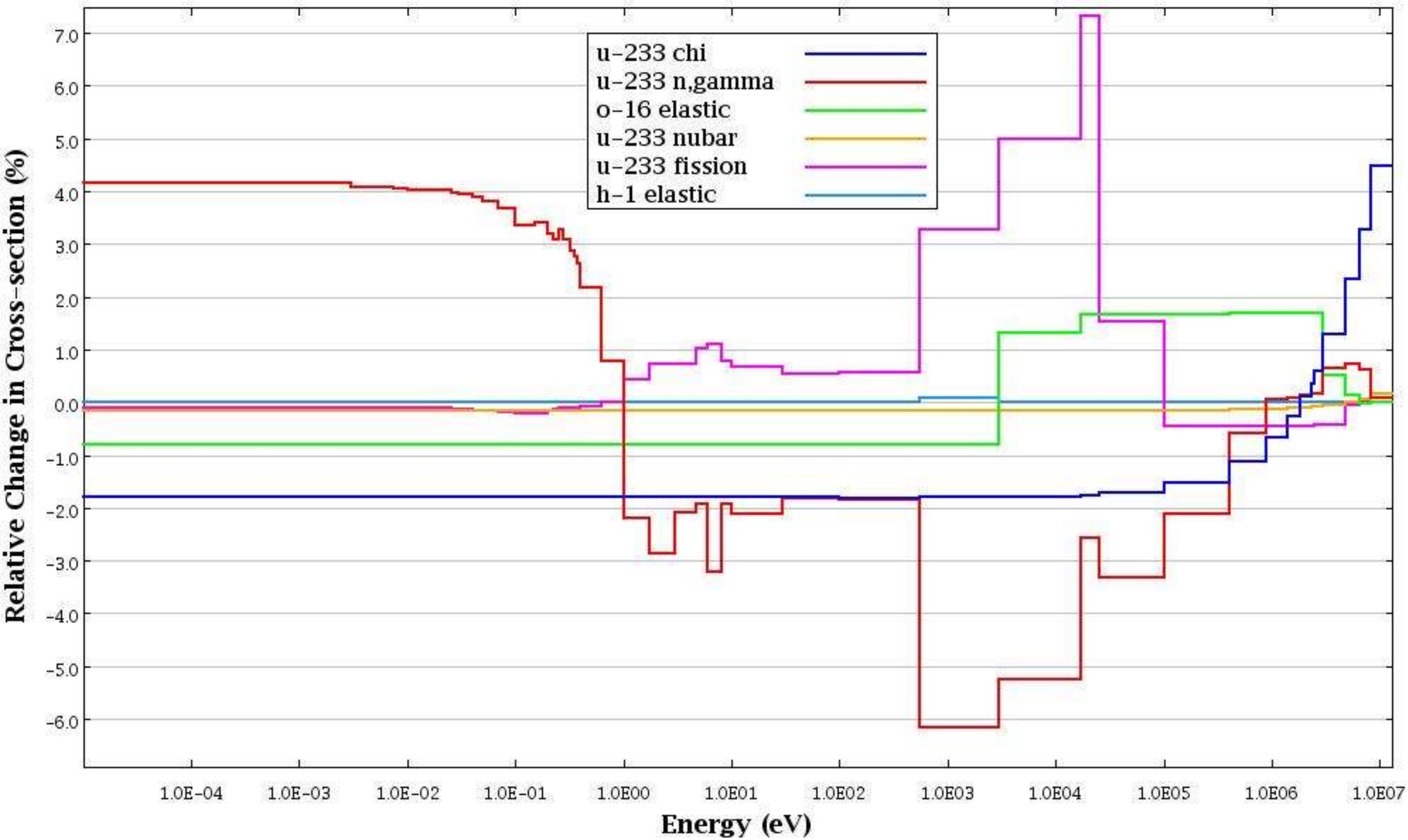
Consistency Assessment

- TSURFER minimizes experimental and calculated differences by adjusting:
  - Measured data, within uncertainties
  - Cross sections, within uncertainties, which impact computed values through sensitivities
- All identified correlations are taken into account
- χ^2 – number of standard deviations a data point moves
  - Typical target is to not move any data point by more than 1.2 χ^2
- Cross section adjustments are constrained by all experiments that use the same cross sections in the same spectrum

Initial and TSURFER Adjusted C/E



Cross Section Adjustments

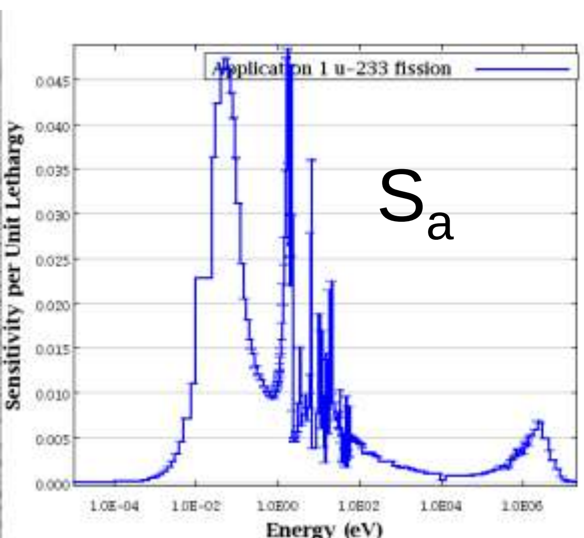


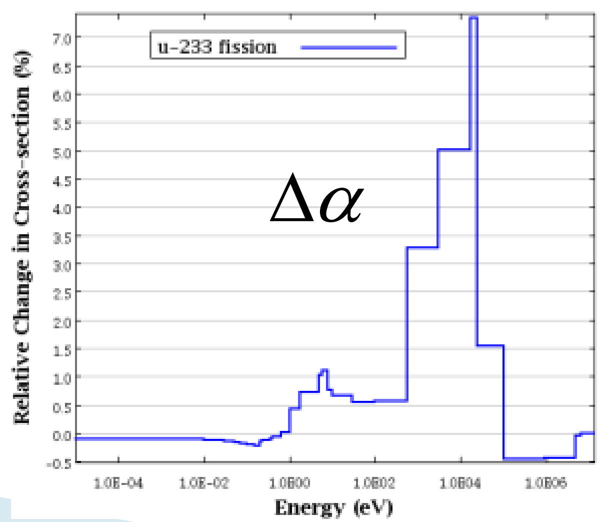
Bias Quantification

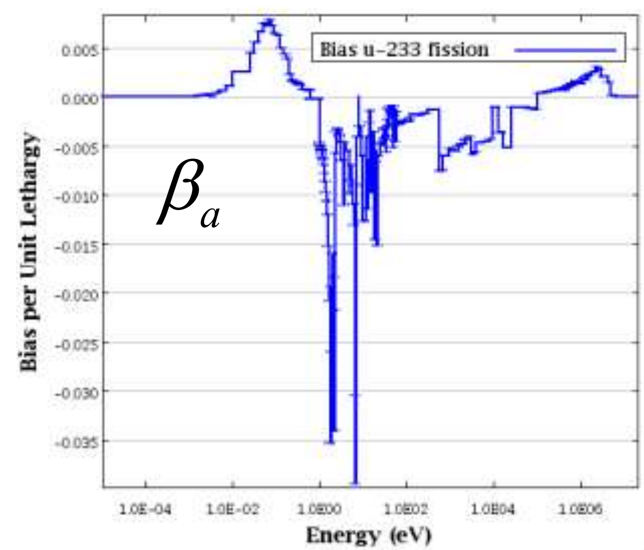
- Project adjustments in input parameter to bias in application via sensitivity coefficients.
- Determine post-adjustment uncertainty in application as uncertainty in bias.

Bias : $\beta_a \approx -\mathbf{S}_a(\Delta\alpha)$

Uncertainty (1σ): $\boldsymbol{\sigma}^2_{\boldsymbol{\beta}_\mathbf{a}} = \mathbf{S}_\mathbf{a}\mathbf{C}_{\boldsymbol{\alpha}'\boldsymbol{\alpha}'}\mathbf{S}^\mathbf{T}_\mathbf{a}$



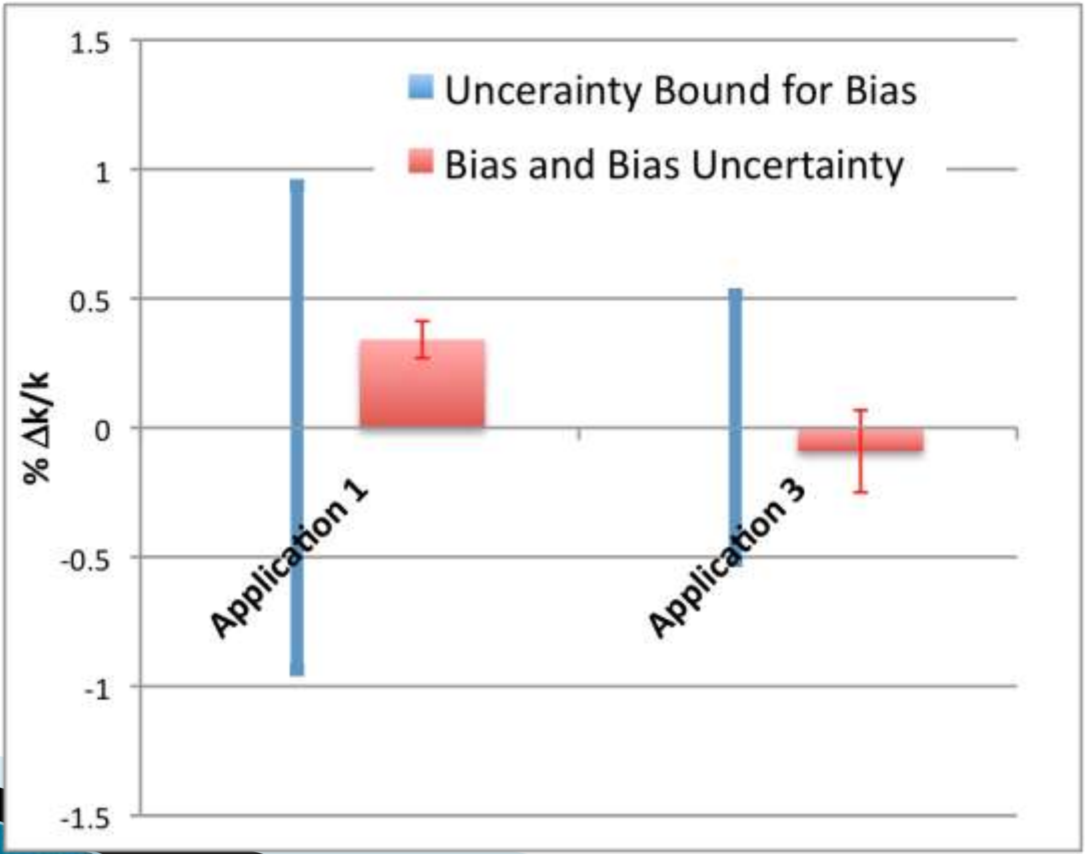




Bias and Bias Uncertainty

Application	Bias (% Δ*k*/*k*)	Bias uncertainty (% Δ*k*/*k*)
1	0.341	0.071
3	-0.091	0.159

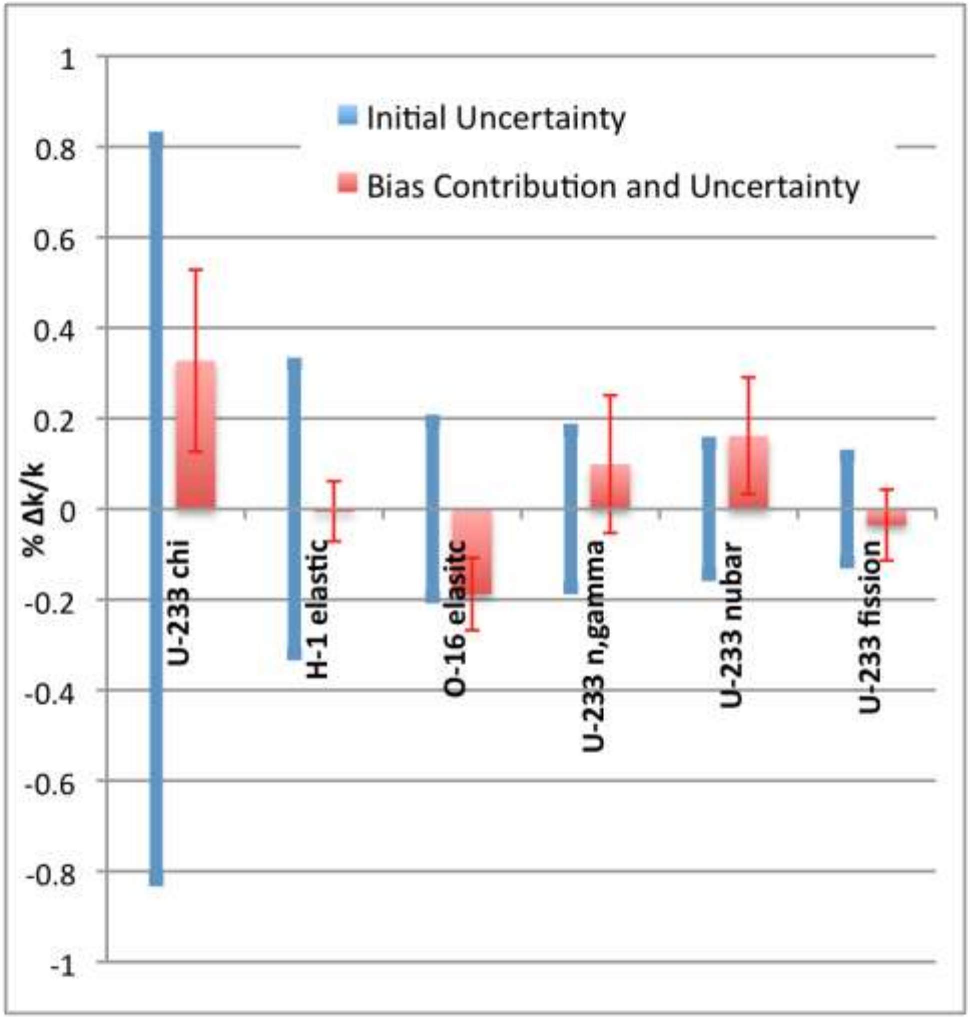
Recall: no similar experiments for Application 3, but TSURFER can combine information from many experiments



Bias and Bias Uncertainty Contributions

Contributions to Bias for Application 1 (100% ^{233}U)

Nuclide	Reaction	Contribution to bias % $\Delta k/k$
^{233}U	chi	3.2738E-01
^{233}U	n,γ	9.8989E-02
^{16}O	elastic	-1.8796E-01
^{233}U	nubar	1.6175E-01
^{233}U	fission	-3.5477E-02
^{233}U	n,n'	-3.7597E-02
^{233}U	elastic	6.2944E-03
^{56}Fe	n,γ	6.4198E-03
^{14}N	n,p	6.1571E-03
^{1}H	n,γ	5.4157E-03
^{1}H	elastic	-4.9899E-03



Bias Uncertainty Assessment

- Where experimental data are inconsistent or not available, cross section uncertainties remain after the adjustment procedure as an uncertainty in the bias.
- The adjusted covariance data provides a detailed assessment of bias uncertainties.

System	Standard deviation (%)	Top six contributors to standard deviation (%)	
Application 1	0.071	^{233}U chi to ^{233}U chi	0.201
		^{233}U n,γ to ^{233}U chi	-0.198
		^{233}U nubar to ^{233}U chi	-0.157
		^{233}U n,γ to ^{233}U n,γ	0.152
		^{233}U nubar to ^{233}U nubar	0.129
		^{16}O elastic to ^{233}U chi	-0.080
Application 3	0.159	^{233}U fission to ^{233}U fission	0.132
		^{233}U nubar to ^{233}U nubar	0.120
		^{14}N n,p to ^{14}N n,p	0.104
		^{233}U fission to ^{233}U nubar	-0.100
		^{1}H n,γ to ^{233}U fission	-0.086
		^{238}U n,γ to ^{238}U n,γ	0.078

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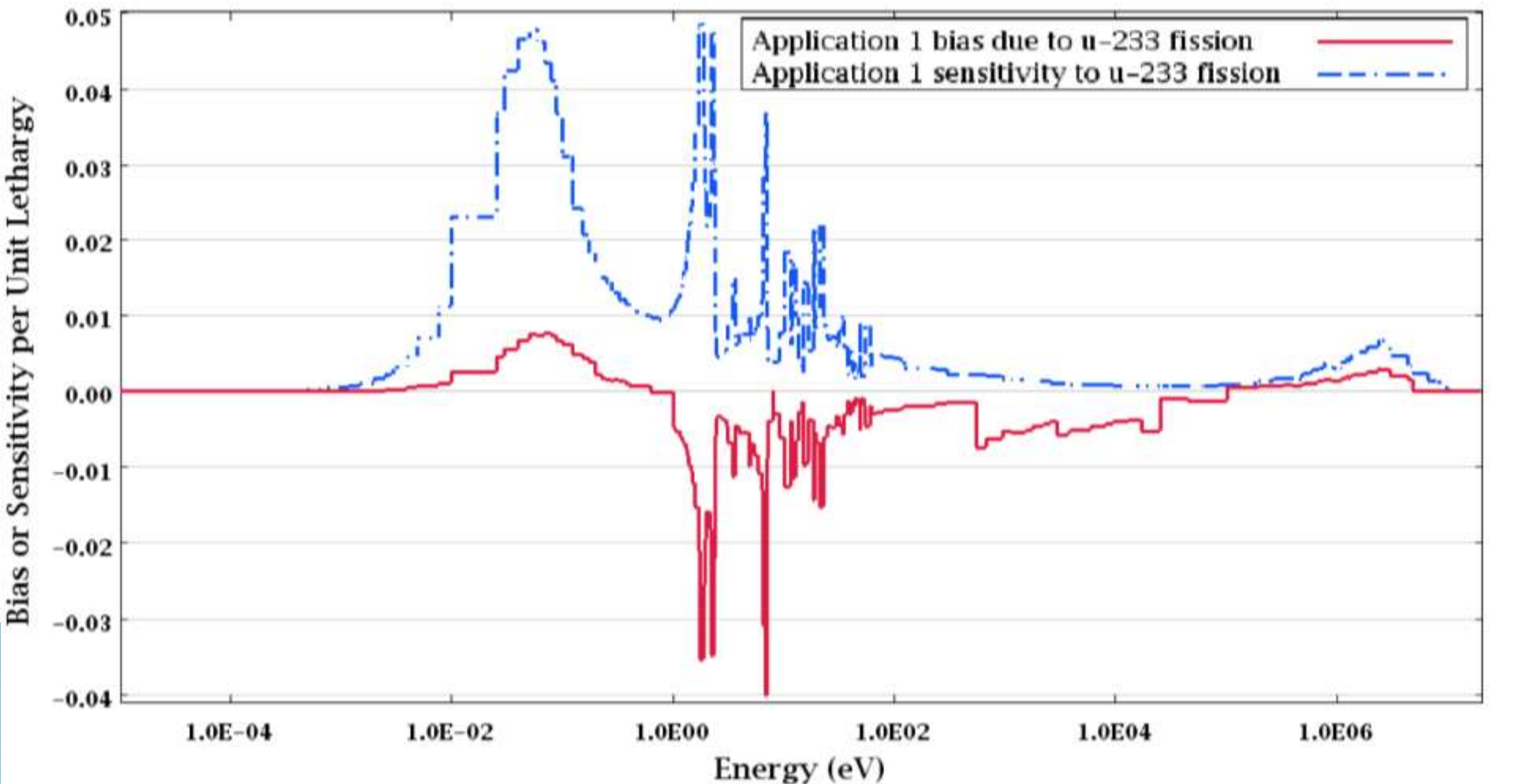
Energy-Dependent Bias

- Multiplying change in cross section by sensitivity to the cross section produces an energy-dependent bias assessment.



Conclusions

- TSURFER provides a unique tool for bias and bias uncertainty assessment.
- Sources of bias from many different experiments testing different materials can be simultaneously assessed using consistency or “assimilation” methods.
- Details of sources of bias and bias uncertainty can be quantified on a nuclide-reaction specific basis.