SCALE Resonance Parameter Sensitivity Coefficient Calculations

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UNM NUCLEAR ENGINEERING

OAK RIDGE National Laboratory

Dr. Mark L. Williams

(1951 - 2018)

EDUCATION

PhD Nuclear Engineering, University of Tennessee, Knoxville, TN, 1979
MS Nuclear Engineering, Georgia Institute of Technology, Atlanta, GA, 1974
BS Engineering Science, Louisiana State University, Baton Rouge, LA, 1972

PROFESSIONAL EXPERIENCE

OAK RIDGE NATIONAL LABORATORY (ORNL), Oak Ridge, Tennessee
Distinguished Research Staff, Nuclear Reactor and Systems Division 2003-2018
LOUISIANA STATE UNIVERSITY (LSU), Baton Rouge, Louisiana
Professor of Physics and Astronomy 1983-2003
OAK RIDGE NATIONAL LABORATORY, Oak Ridge, Tennessee
Research Staff, Neutron Physics Division 1974-1983

Eugene Wigner Award Winner 2016

The award honors Williams for innovative contributions to **resonance self-shielding theory** and development of continuous-energy deterministic transport calculations for lattice physics applications; for his leadership in the development and **generation of cross section covariance data; and for his advancements in sensitivity/uncertainty methods**, including implicit sensitivity treatment and depletion perturbation theory for coupled neutron/nuclide fields.

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Introduction

- Next-generation nuclear reactor designers rely on the availability of high-fidelity modeling and simulation (M&S) tools.
- Significant uncertainties (more than 50%) exist in key actinide neutron cross sections.
- Critical experiments have been performed to help data scientists verify the accuracy of their evaluations.
- Our goal is to formalize comparisons with benchmark experiment data by developing a mathematically rigorous method for assimilating the results of criticality experiments to improve the fidelity of nuclear data evaluations and nuclear data uncertainty estimates.

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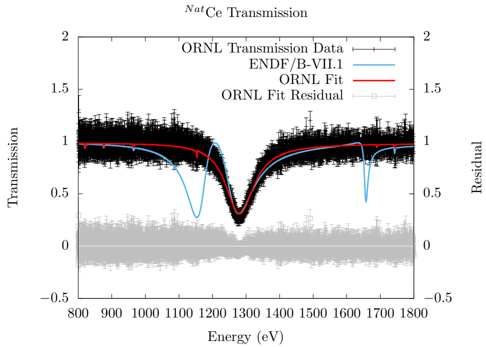
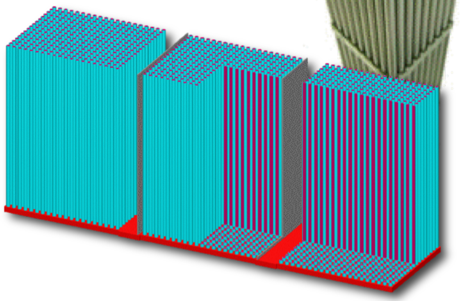
Introduction

- Nuclear data evaluators do not consider critical experiment results when generating nuclear data.

Differential Nuclear Data Measurements



Integral Benchmark Critical Experiments

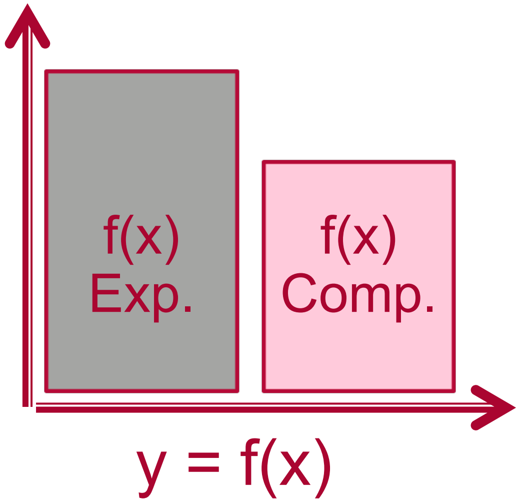


Nuclear Data Evaluation

Experimental Data Assimilation

Monte Carlo radiation transport M&S tools are extremely high fidelity, relying mostly on first principle assumptions.

- **Premise:**
  Disagreement between experimental results and high-fidelity M&S tools is caused primarily by errors in nuclear data.
- **Corollary:**
  We can calibrate nuclear data evaluations by comparing experimental and computed results.



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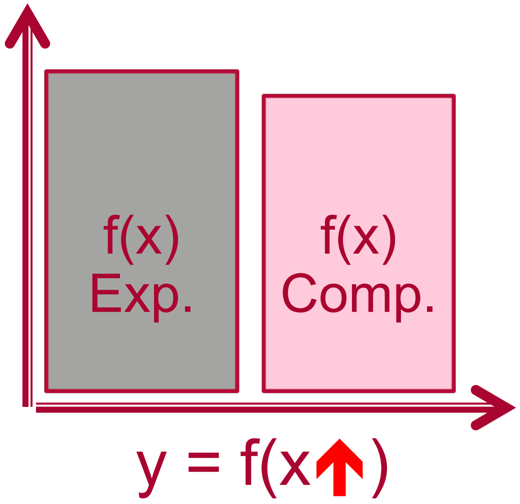

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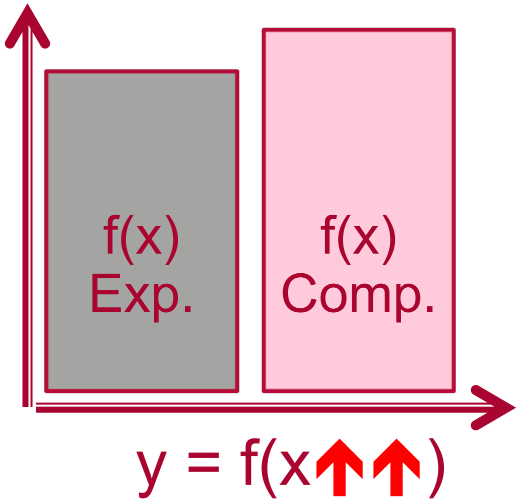

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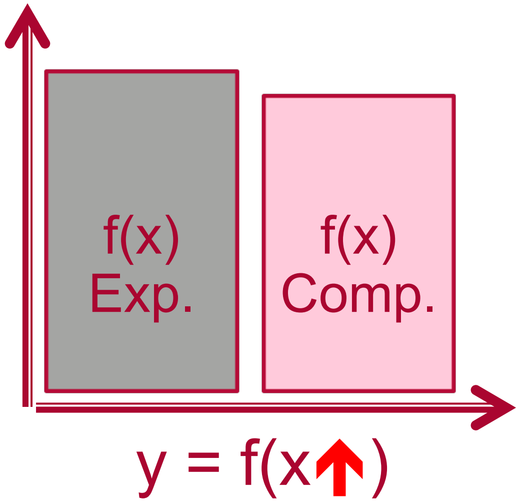

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TSURFER Tools for Data Adjustment and Experimental Data Assimilation

TSURFER: *T*ool for *S*/*U* analysis of *R*esponse *F*unctionals using *E*xperimental *R*esults

Uses sensitivity information to **consistently** adjust nuclear cross section data and reconcile biases between integral experiment results and computational predictions.

$$S_{f(x),x} = \frac{\partial f(x) / f(x)}{\partial x / x}$$

Modified cross section and cross section uncertainty data is used to anticipate computational biases in criticality safety applications.

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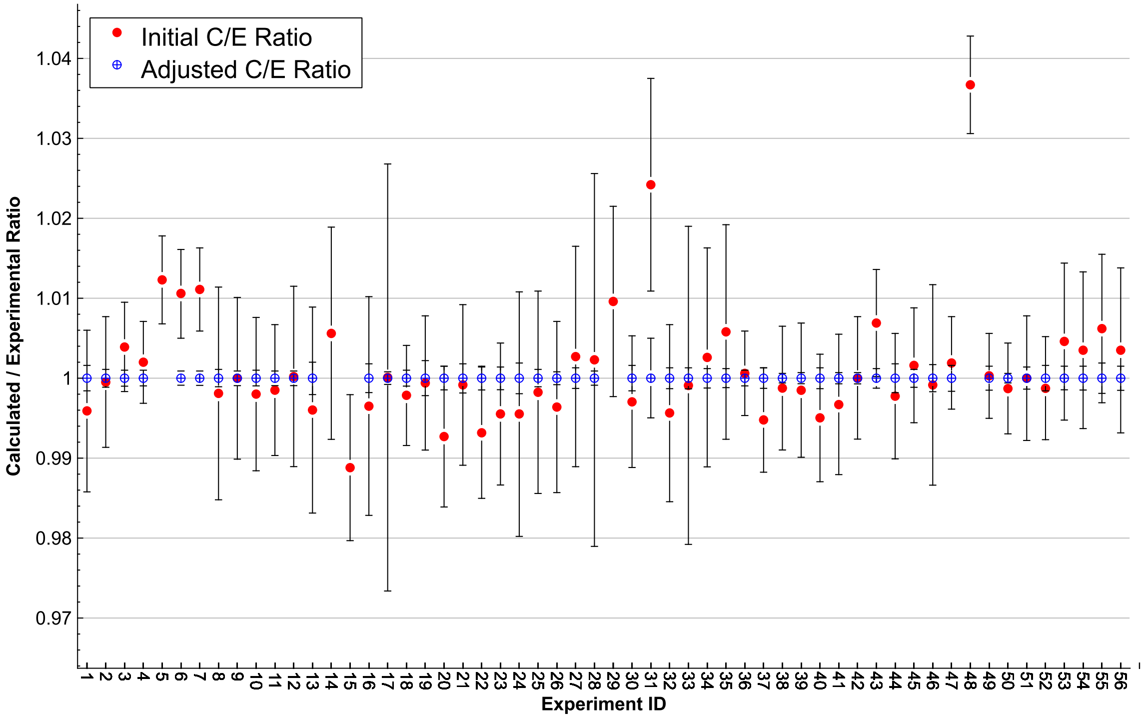
Data Assimilation/Calibration

- Experimental benchmark data (E) is used to improve the accuracy of the initial computed responses (C).
- This assimilation consistently adjusts the underlying nuclear data.



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TSURFER Cross Section Adjustments

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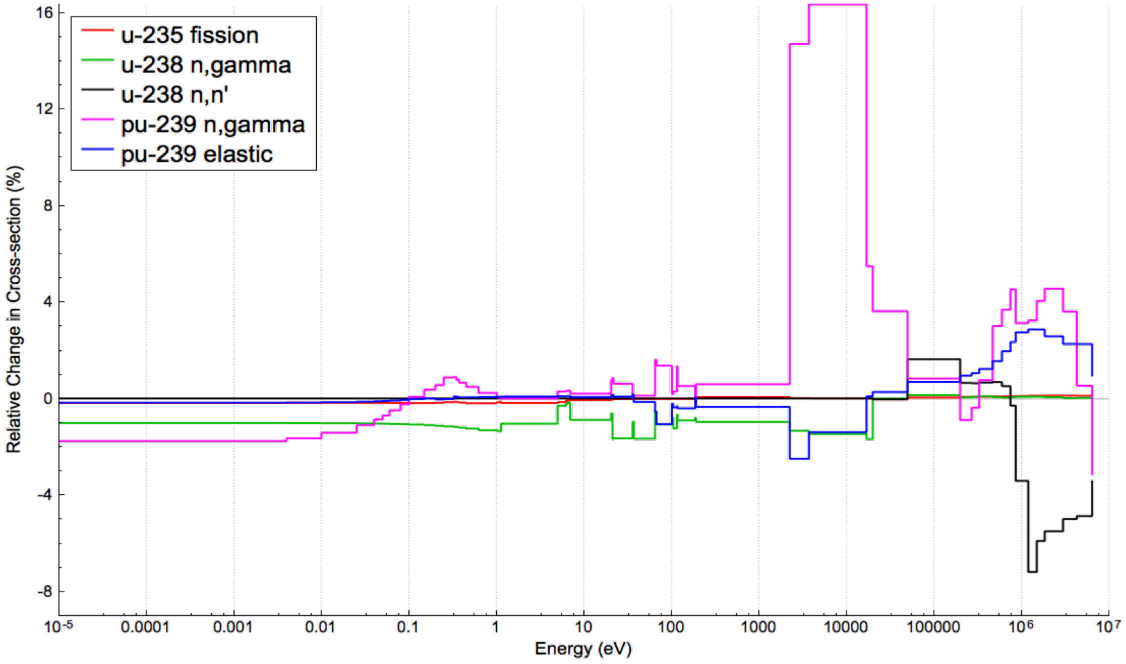

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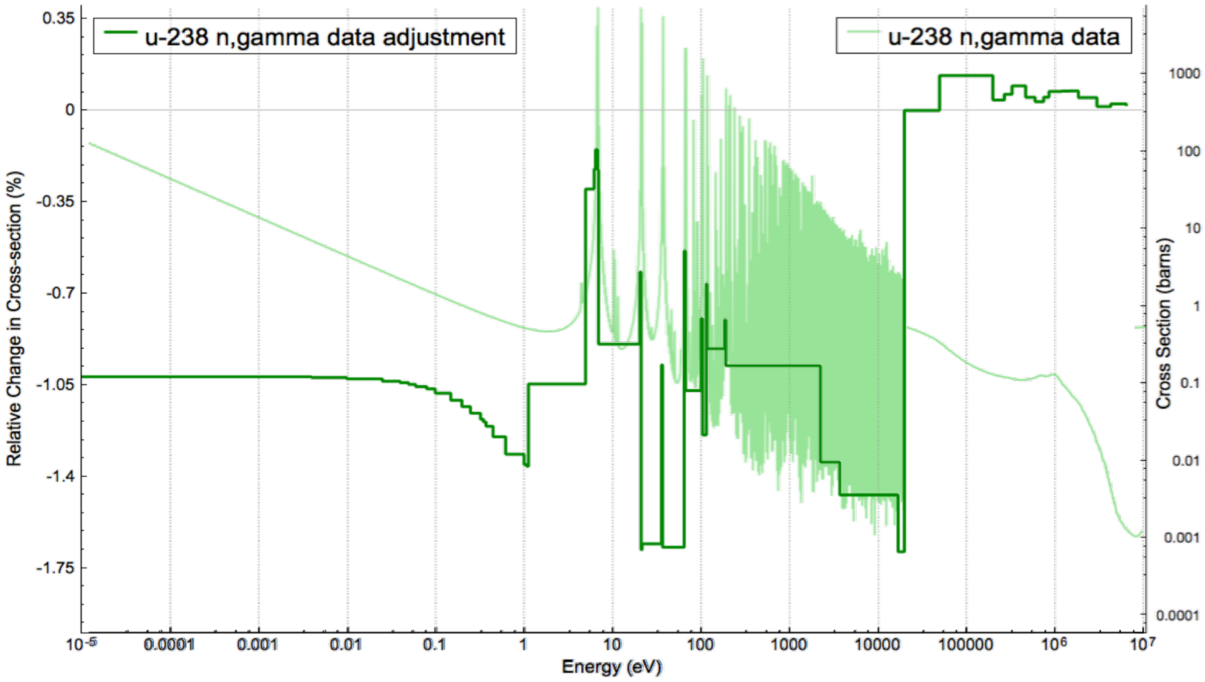
Realistic Cross Section Adjustments?

- TSURFER adjusts multigroup (i.e. energy-averaged) cross sections.
- This approach cannot generate usable nuclear data evaluations.



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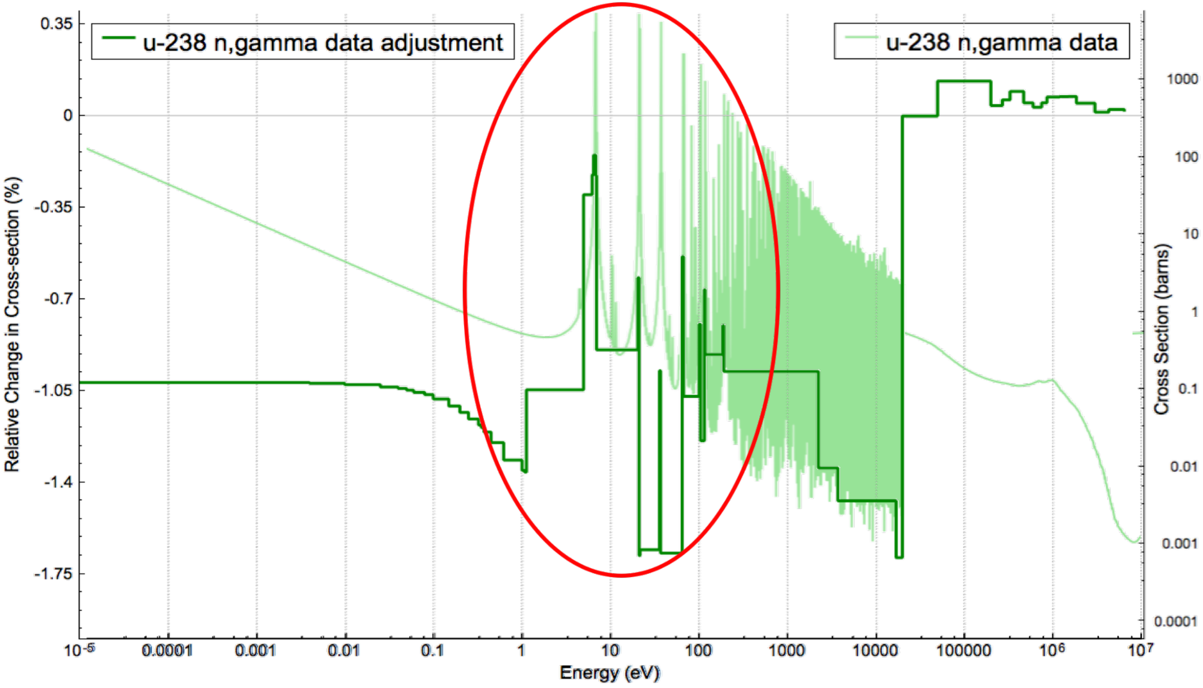

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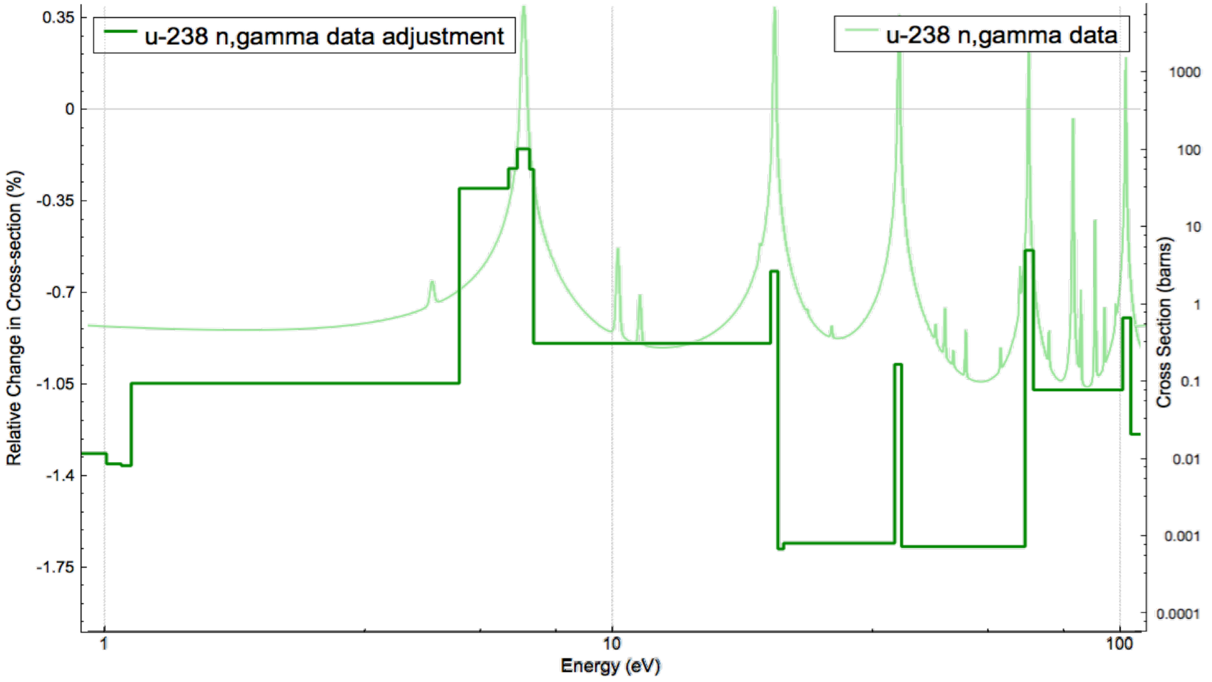

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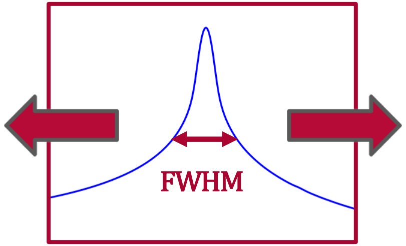
Our Research Plan

- **Task 1:** Develop a resonance parameter sensitivity capability.
- **Task 2:** Modify TSURFER to assimilate experimental data by adjusting fundamental nuclear data.
- **Task 3:** Evaluate the accuracy of nuclear data and nuclear covariance adjustments.

Task 1:

$$S_{f(x),\,FWHM} = \frac{\partial f(x) / f(x)}{\partial FWHM / FWHM}$$

Task 2:



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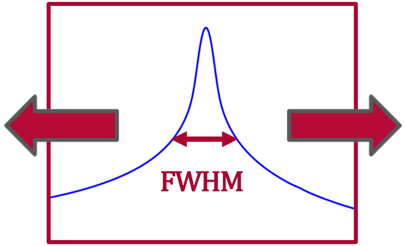

Task 3:

Methodology

- TSUNAMI-3D was used to compute the resonance parameter sensitivity coefficients (using the CLUTCH method) via the Chain Rule.

$$S_{R,\Sigma_x} = \frac{\delta R / R}{\delta \Sigma_x / \Sigma_x} \quad \Rightarrow \quad S_{R,\Gamma} = \frac{\delta R / R}{\delta \Gamma / \Gamma} = \frac{\delta R / R}{\delta \Sigma_x / \Sigma_x} \times \frac{\delta \Sigma_x / \Sigma_x}{\delta \Gamma / \Gamma}$$

- The sensitivity of cross sections to resonance parameters was estimated using the AMPX Cross Section Processing Code.

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Methodology: Caveats

- Computing resonance parameter sensitivities significantly increases the number of sensitivity tallies.
  - Multigroup-binned sensitivity tallies use ~252 energy bins / isotope.
  - Isotope nuclear data evaluations can contain more than 10,000 evaluated resonance parameters per isotope.
- The AMPX sensitivity estimates were obtained using direct-difference calculations.
  - Performing this many cross section calculations significantly increased the simulation runtime.
  - The potential exists to mitigate this runtime penalty using multipole cross section methods.

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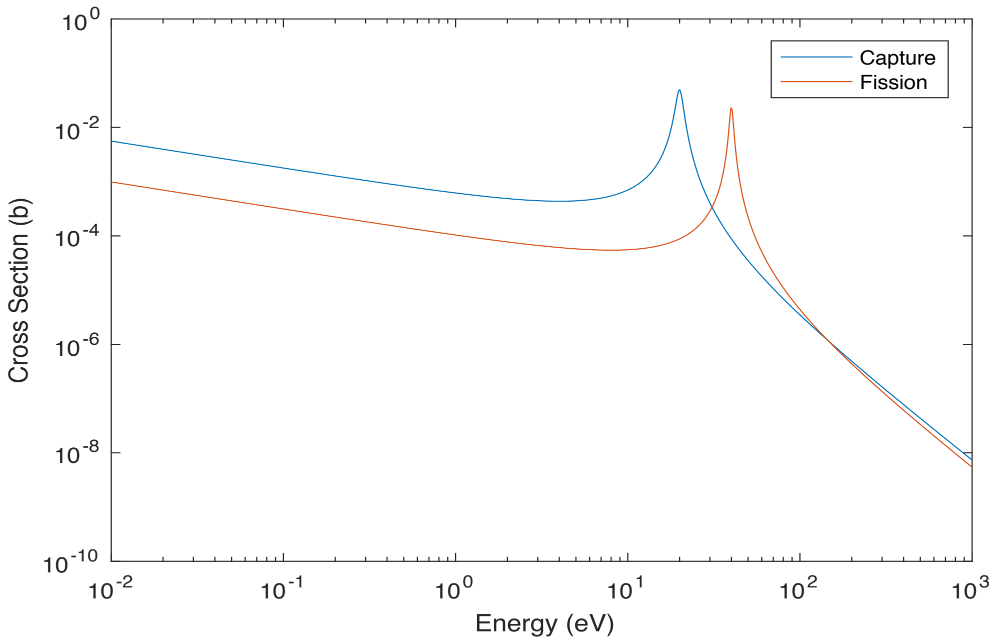
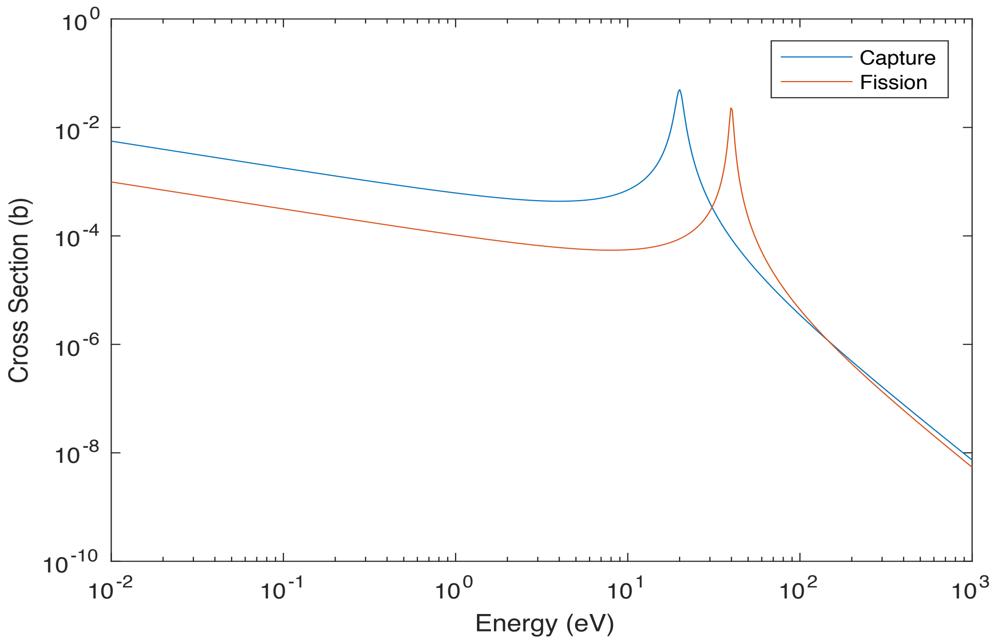
Results

- Proof of principle was tested using a model of an infinitely homogenous system with three fictitious isotopes.
- The three isotopes are defined to have purely scattering, absorbing, or fissioning cross sections.



Results

- The **fission** and **capture** isotopes each contain one resonance.
- The energy of the fission resonance was set to 40 eV.
- The energy of the capture resonance was varied from 20 eV to 60 eV to test whether the methodology accurately predicts sensitivity coefficients for overlapping resonances.



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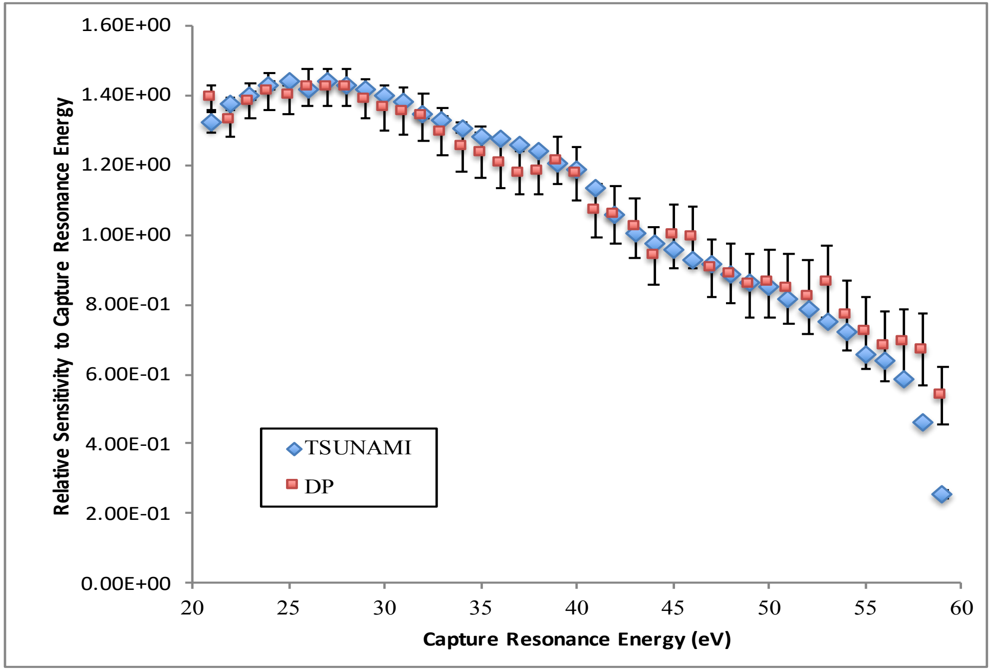
Results

- Good agreement was observed between the TSUNAMI resonance parameter sensitivity coefficient estimates and reference direct perturbation (DP) results.



Conclusions

- This work has demonstrated proof of principle for a methodology to compute the sensitivity of integral experiment responses to evaluated nuclear data.
- Future work includes:
  - Testing this methodology for a more complete set of verification problems.
  - Improving the efficiency of the AMPX sensitivity algorithms.
  - Completing modifications to the TSURFER data assimilation code to generate adjusted continuous-energy cross section libraries.

Questions?

Please contact:

Chris Perfetti
cperfetti@unm.edu

"All models are wrong, but some are useful."

– Professor George E. P. Box