Methods for Sensitivity and Uncertainty Analysis in Nuclear Engineering Applications

Dr. Christopher M. Perfetti
Assistant Professor
Nuclear Engineering Department
University of New Mexico

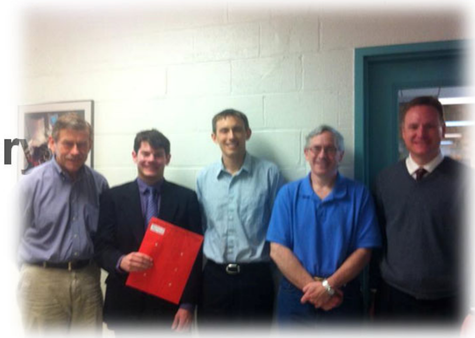
NUCLEAR ENGINEERING

Presentation Outline

- Part 1 – Introduction to Sensitivity Coefficients
- Part 2 – Applications of Sensitivity Analysis
  - Design Optimization
  - Uncertainty Quantification
  - Benchmark Experiment Selection
  - Experimental Data Assimilation
- Part 3 – Current Research

About Me

- Born and raised in Florida
- Education:
  - 2007: B.S. in Nuclear Engineering, University of Florida
  - 2008: M.S. in Nuclear Engineering, University of Florida
  - 2012: PhD. in Nuclear Engineering, University of Michigan
- 2012-2018: R&D Scientist, Oak Ridge National Laboratory
- 2018-Present: Assistant Professor, University of New Mexico



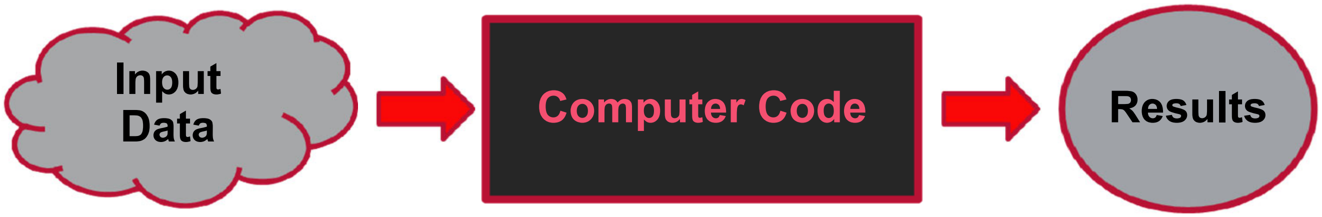
NUCLEAR ENGINEERING

Presentation Outline

- Part 1 – Introduction to Sensitivity Coefficients
- Part 2 – Applications of Sensitivity Analysis
  - Design Optimization
  - Uncertainty Quantification
  - Benchmark Experiment Selection
  - Experimental Data Assimilation
- Part 3 – Current Research

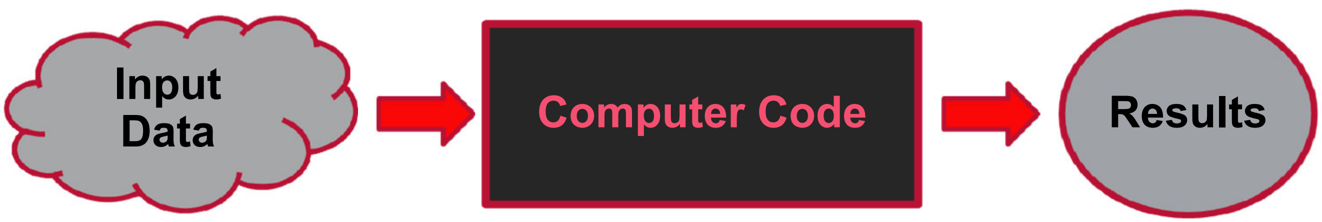
Sensitivity Analysis and Uncertainty Propagation

Sensitivity coefficients provide insight on the sources and impact of uncertainty in nuclear engineering models.



Sensitivity Analysis and Uncertainty Propagation

Sensitivity coefficients provide insight on the sources and impact of uncertainty in nuclear engineering models.



Input Information:
Nuclear Data (Σ), Atom Densities (N), Material Densities (ρ)

Input Uncertainty:
ΔΣ, ΔN, Δρ

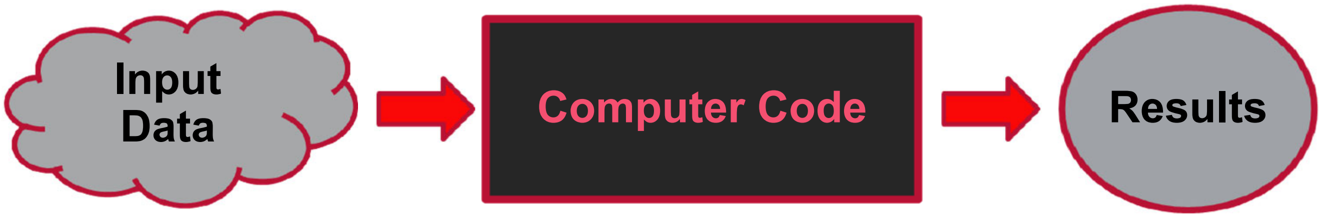
Output Information:
k_{eff}, Dose Rate, *Fission Rate, etc…*

Output Uncertainty:
Δk_{eff}, Δ Dose Rate, ΔFission Rate

NUCLEAR ENGINEERING

Sensitivity Analysis and Uncertainty Propagation

Sensitivity coefficients provide insight on the sources and impact of uncertainty in nuclear engineering models.



Input Information:
Nuclear Data (Σ), Atom Densities (*N*), Material Densities (ρ)

Input Uncertainty:
$\Delta\Sigma, \Delta N, \Delta\rho$

$$\frac{\delta k_{\mathrm{eff}}/k_{\mathrm{eff}}}{\delta\Sigma/\Sigma}$$

Output Information:
k_{eff}, Dose Rate, *Fission Rate, etc…*

Output Uncertainty:
Δk_{eff}, Δ Dose Rate, ΔFission Rate

NUCLEAR ENGINEERING

Introduction to Sensitivity Coefficients

- Sensitivity coefficients describe the fractional change in a response that is due to perturbations, or uncertainties, in system parameters.

$$S_{R,\Sigma_x} = \frac{\delta R/R}{\delta \Sigma_x/\Sigma_x}$$

- The SCALE TSUNAMI code calculates sensitivity coefficients for critical eigenvalue or reaction rate ratio responses:

$$R = k_{eff} \qquad R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}$$

NUCLEAR ENGINEERING

Introduction to Sensitivity Coefficients

- Sensitivity coefficients describe the fractional change in a response that is due to perturbations, or uncertainties, in system parameters.

$$S_{R,\Sigma_x} = \frac{\delta R/R}{\delta \Sigma_x/\Sigma_x}$$

- The SCALE TSUNAMI code calculates sensitivity coefficients for critical eigenvalue or reaction rate ratio responses:

$$R = k_{eff}$$

$$R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}$$

Introduction to Sensitivity Coefficients

- Eigenvalue sensitivity coefficient calculations in TSUNAMI are calculated using the First-Order Perturbation Equation.

$$S_{k,\Sigma_x} = \Sigma_x \frac{< \Phi^* \left(\lambda \frac{\delta F}{\delta \Sigma_x} - \frac{\delta B}{\delta \Sigma_x} \right) \Phi >}{\lambda < \Phi^* F \Phi >}$$

Introduction to Sensitivity Coefficients

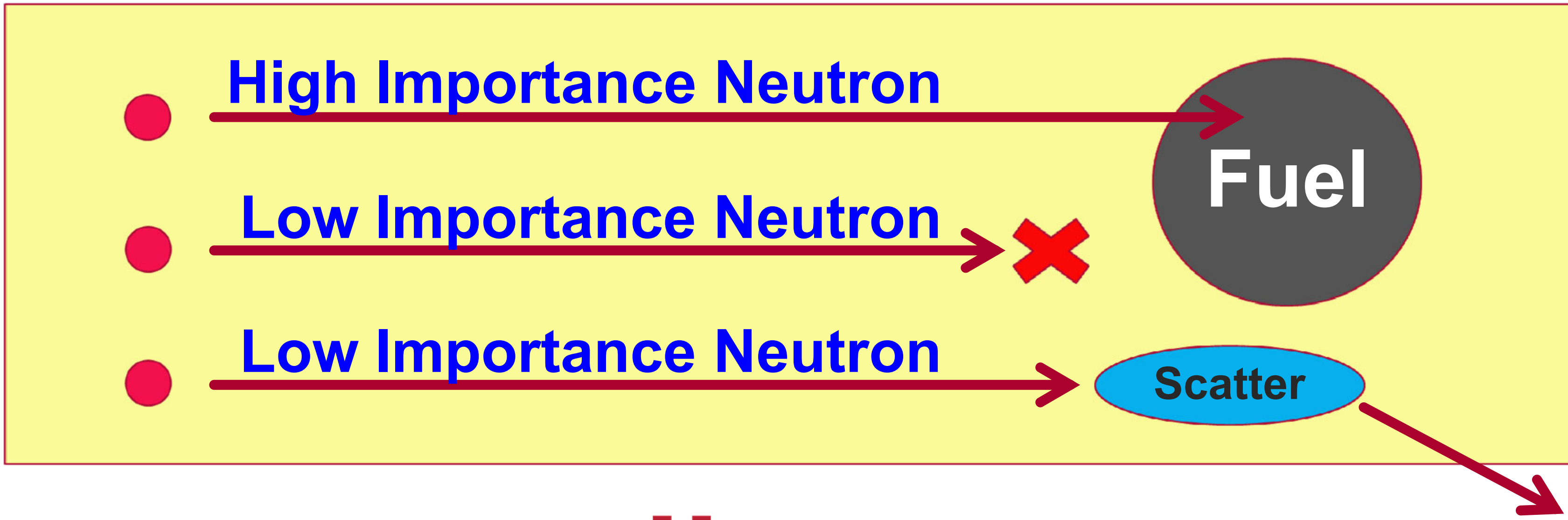
- For a sample capture reaction ($cap.$), the First-Order Perturbation Equation reduces to:

$$S_{k,\Sigma_{cap.}} = \frac{< \Phi^* \, \Sigma_{cap.} \Phi >}{\frac{1}{k} < \Phi^* \, \Sigma_f \Phi >}$$

- Tallying reaction rates is relatively straightforward for a Monte Carlo code.
- Tallying the adjoint flux (Φ^*) is more challenging.

What is the Adjoint Flux?

- The adjoint flux, or "importance," describes how much a neutron will contribute to a response.



Introduction to Sensitivity Coefficients

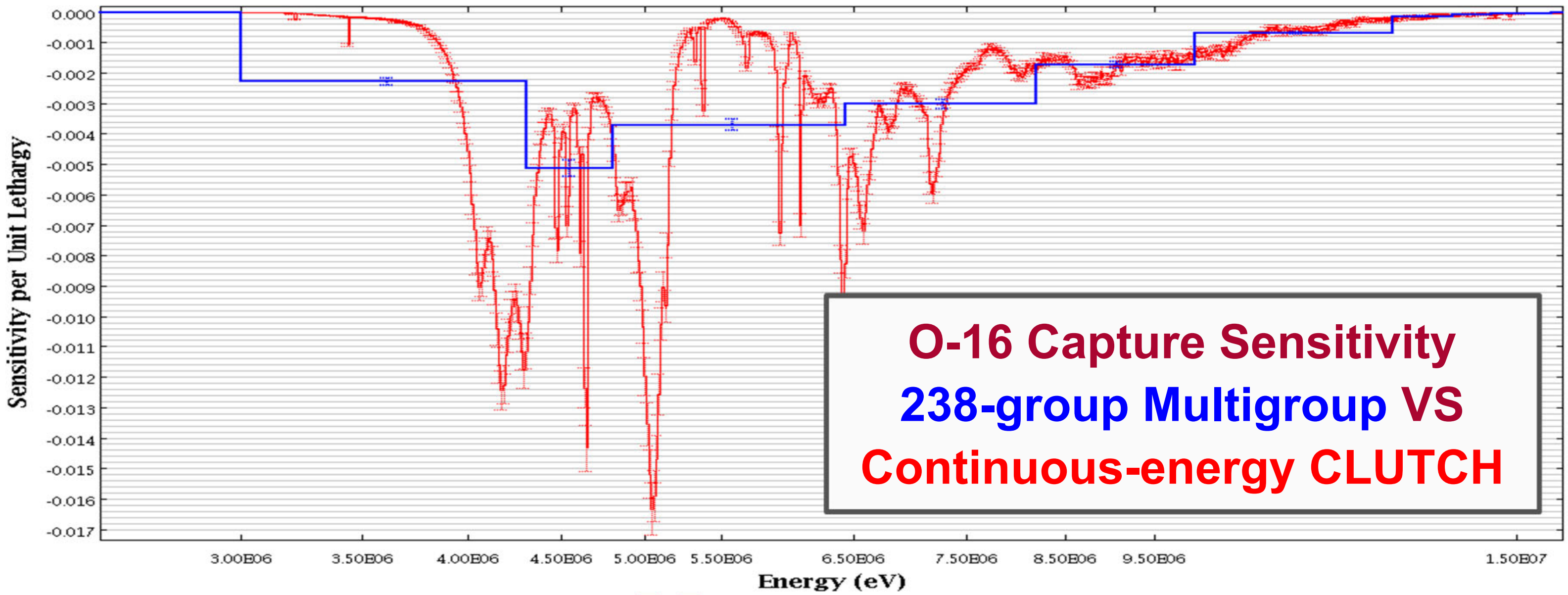
- For a sample capture reaction ($cap.$), the First-Order Perturbation Equation reduces to:

$$S_{k,\Sigma_{cap.}} = \frac{< \Phi^* \, \Sigma_{cap.} \Phi >}{\frac{1}{k} < \Phi^* \, \Sigma_f \Phi >}$$

- Tallying reaction rates is relatively straightforward for a Monte Carlo code.
- Tallying the adjoint flux (Φ^*) is more challenging.

Continuous-Energy Resolution

- Continuous-energy capabilities allow for a better understanding what phenomena contribute a system's uncertainty.



NUCLEAR ENGINEERING

Presentation Outline

- Part 1 – Introduction to Sensitivity Coefficients
- Part 2 – Applications of Sensitivity Analysis
  - Design Optimization
  - Uncertainty Quantification
  - Benchmark Experiment Selection
  - Experimental Data Assimilation
- Part 3 – Current Research

Advanced Sensitivity Methods: Generalized Perturbation Theory

- Generalized Perturbation Theory (GPT) calculates sensitivity coefficients for responses that can be expressed as the ratio of reaction rates.

$$S_{R,\Sigma_x} = \frac{\delta R/R}{\delta \Sigma_x/\Sigma_x} \qquad R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}$$

- Calculating generalized sensitivity coefficients requires solving an inhomogeneous, or generalized, adjoint equation:

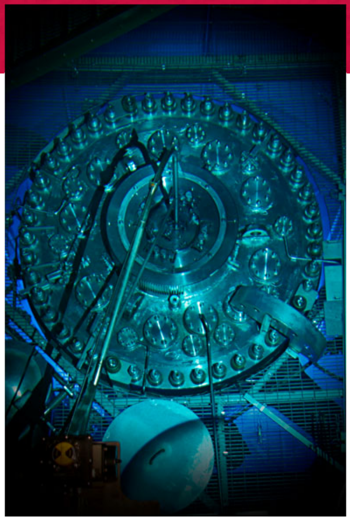
$$(L^* - \lambda P^*)\Gamma^* = S^*$$

- Applications for GPT sensitivity/uncertainty analysis include:
  - Relative Powers
  - Isotope Conversion Ratios
  - Multigroup Cross Sections

NUCLEAR ENGINEERING

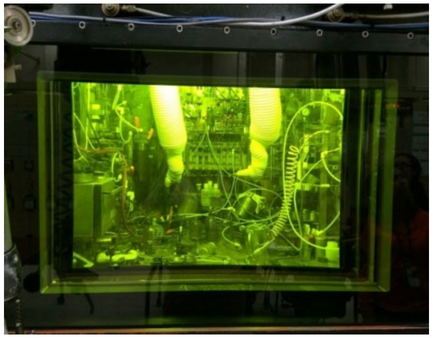
+ C. M. Perfetti, B. T. Rearden, "Development of a Generalized Perturbation Theory Method for Uncertainty and Sensitivity Analysis using Continuous-Energy Monte Carlo Methods," *Nucl. Sci. Eng.*, 182, *3*, 354–368 (2016).

Isotope Production Opportunities



- The High Flux Isotope Reactor (HFIR) at ORNL provides one of the highest intensity neutron fluxes.
- HFIR can provide unique isotopes, some of which have no alternative U.S. production source, including:

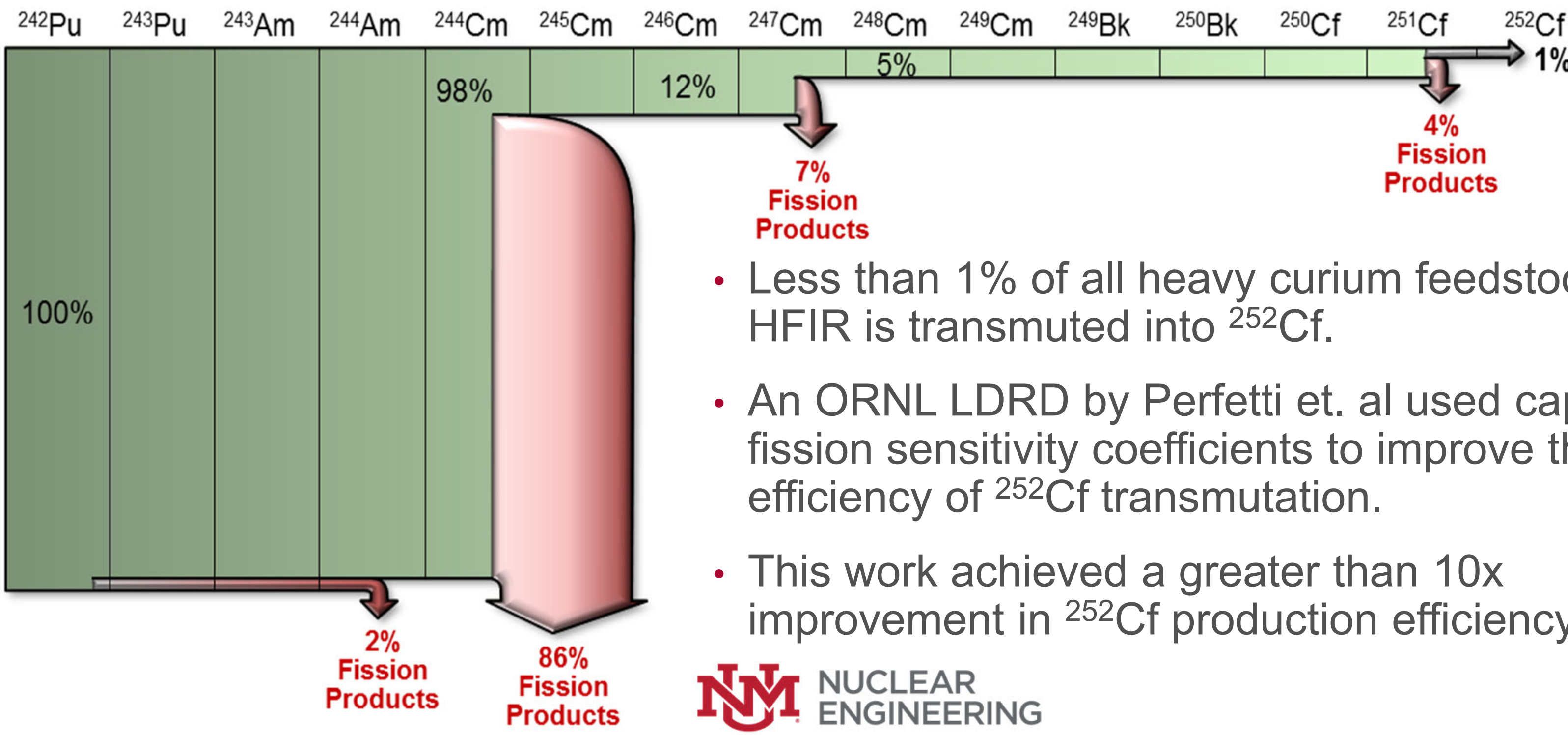
- **^{14}C** useful in medical applications such as studying diabetes, gout, anemia, and acromegaly
- **^{63}Ni** explosives detection, airport security
- **^{229}Th** provides ^{225}Ac for α-particle cancer therapy
- **^{238}Pu** radioisotope power for space exploration
- **^{254}Es** production of super-heavy elements
- **^{252}Cf** source of neutrons for nuclear reactor startup, study of materials with neutron diffraction, oil well logging, and neutron spectroscopy



NUCLEAR ENGINEERING

Sensitivity Applications: Design Optimization

The Long Road to ^{252}Cf



- Less than 1% of all heavy curium feedstock in HFIR is transmuted into ^{252}Cf.
- An ORNL LDRD by Perfetti et. al used capture-to-fission sensitivity coefficients to improve the efficiency of ^{252}Cf transmutation.
- This work achieved a greater than 10x improvement in ^{252}Cf production efficiency.

NUCLEAR ENGINEERING

Presentation Outline

- Part 1 – Introduction to Sensitivity Coefficients
- Part 2 – Applications of Sensitivity Analysis
  - Design Optimization
  - Uncertainty Quantification
  - Benchmark Experiment Selection
  - Experimental Data Assimilation
- Part 3 – Current Research

NUCLEAR ENGINEERING

Sensitivity Applications:
Uncertainty Quantification

- Sensitivity coefficients can be combined with cross section uncertainties to quantify the uncertainty in a response.

$$S_{k,\Sigma_x} \cdot Cov_{\Sigma_x,\Sigma_y} \cdot S_{k,\Sigma_y}^T = \sigma_k^2$$

The Sandwich Equation

Sensitivity Applications: Uncertainty Quantification

- Sensitivity coefficients can be combined with cross section uncertainties to quantify the uncertainty in a response.

$$S_{k,\Sigma_x} \cdot Cov_{\Sigma_x,\Sigma_y} \cdot S^T_{k,\Sigma_y} = \sigma_k^2$$

$$\uparrow \qquad \uparrow \qquad \uparrow \qquad \uparrow$$

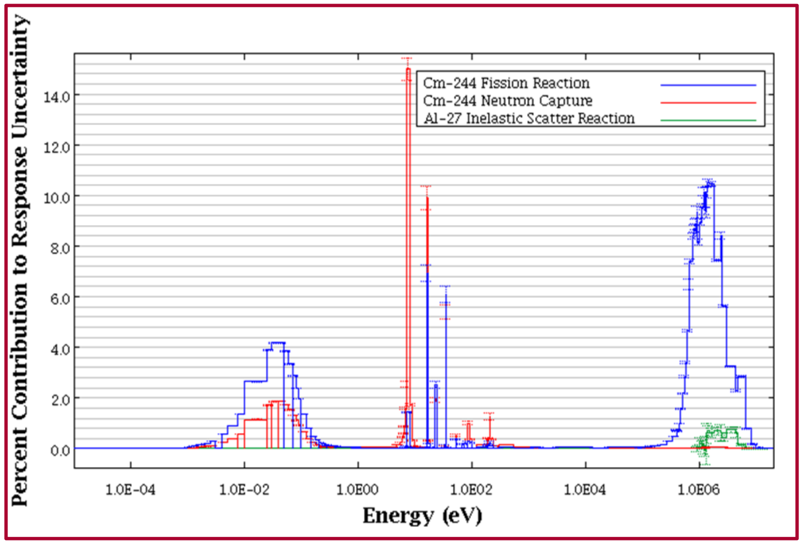
$$\left(\frac{\delta k/k}{\delta\Sigma/\Sigma}\right) \qquad \left(\frac{\Delta\Sigma}{\Sigma}\right)^2 \qquad \left(\frac{\delta k/k}{\delta\Sigma/\Sigma}\right) \qquad \left(\frac{\Delta k}{k}\right)^2$$

The Sandwich Equation

Identifying Nuclear Data Needs

- Sensitivity-based uncertainty analyses offer insight on which reactions and neutron energies contribute the most uncertainty to responses of interest.

Reaction Contributions to the Uncertainty in the ^{244}Cm Conversion Ratio	
^{244}Cm Fission Reaction	17.62%
^{244}Cm Neutron Capture	4.96%
^{27}Al Inelastic Scatter Reaction	0.72%
^{244}Cm Elastic Scatter Reaction	0.59%
^{1}H Elastic Scatter Reaction	0.56%
Total Data-Induced Uncertainty	**18.33%**



Energy-dependent contributions to the uncertainty in the ^{244}Cm conversion ratio.

Presentation Outline

- Part 1 – Introduction to Sensitivity Coefficients
- Part 2 – Applications of Sensitivity Analysis
  - Design Optimization
  - Uncertainty Quantification
  - Benchmark Experiment Selection
  - Experimental Data Assimilation
- Part 3 – Current Research

Sensitivity Applications:

Benchmark Similarity Assessment for Next-Generation Reactor Systems

- The similarity coefficient, *c(k)* or c_k, describes the amount of nuclear data-induced uncertainty that is shared by two systems.

$$S_{R_1,\Sigma_x} \cdot Cov_{\Sigma_x,\Sigma_y} \cdot S^T_{R_2,\Sigma_y} = \sigma^2_{R_1,R_2}$$

$$S_{R_1,\Sigma_x} \Leftarrow \left(\frac{\delta R/R}{\delta\Sigma/\Sigma}\right), \quad Cov_{\Sigma_x,\Sigma_y} \Leftarrow (\Delta\Sigma/\Sigma)^2, \quad S^T_{R_2,\Sigma_y} \Leftarrow \left(\frac{\delta R/R}{\delta\Sigma/\Sigma}\right), \quad \sigma^2_{R_1,R_2} \Leftarrow (\Delta R/R)^2$$

$$c_k = \frac{\sigma^2_{R_1,R_2}}{\sigma_{R_1}\sigma_{R_2}}$$

Sensitivity Applications:

Benchmark Similarity Assessment for Next-Generation Reactor Systems

- The similarity coefficient, *c(k)* or c_k, describes the amount of nuclear data-induced uncertainty that is shared by two systems.

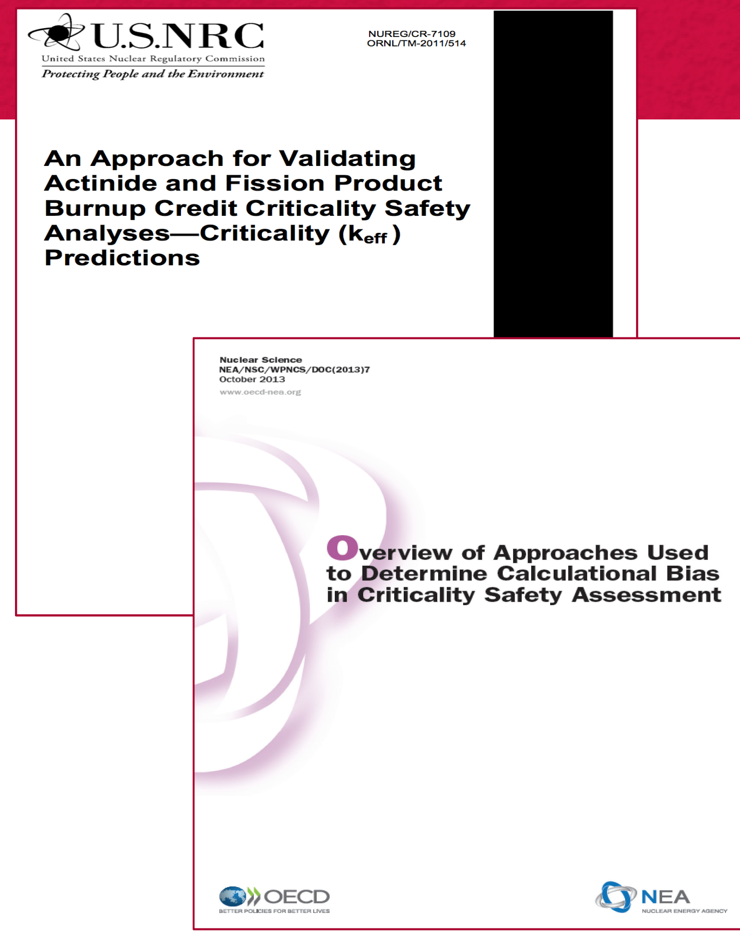
$$S_{R_1,\Sigma_x} \cdot Cov_{\Sigma_x,\Sigma_y} \cdot S^T_{R_2,\Sigma_y} = \sigma^2_{R_1,R_2} \rightarrow c_k = \frac{\sigma^2_{R_1,R_2}}{\sigma_{R_1}\sigma_{R_2}}$$

$$\left(\frac{\delta R/R}{\delta\Sigma/\Sigma}\right) \qquad (\Delta\Sigma/\Sigma)^2 \qquad \left(\frac{\delta R/R}{\delta\Sigma/\Sigma}\right) \qquad (\Delta R/R)^2$$

- The TSUNAMI-IP code calculates c_k values between a target application and reference benchmark experiments.

TSUNAMI in Practice

- U.S. Nuclear Regulatory Commission
  - Nuclear Materials Safety and Safeguards, Nuclear Reactor Regulation, Office of New Reactors
- U.S. DOE / Areva / Duke Energy
  - Mixed Oxide Fuel Fabrication Facility
- Candu Energy
  - ACR-1000 Design Validation
- Atomic Energy of Canada, Ltd.
  - ACR-700 NRC Review/PIRT
- U.S. DOE
  - Yucca Mountain post-closure criticality safety
- Global Nuclear Fuels
  - Transportation package licensing
- Svensk Kärnbränslehantering AB
  - Swedish used fuel repository
- Organization for Economic Cooperation and Development, Nuclear Energy Agency
  - International Expert Groups



NUCLEAR ENGINEERING

Presentation Outline

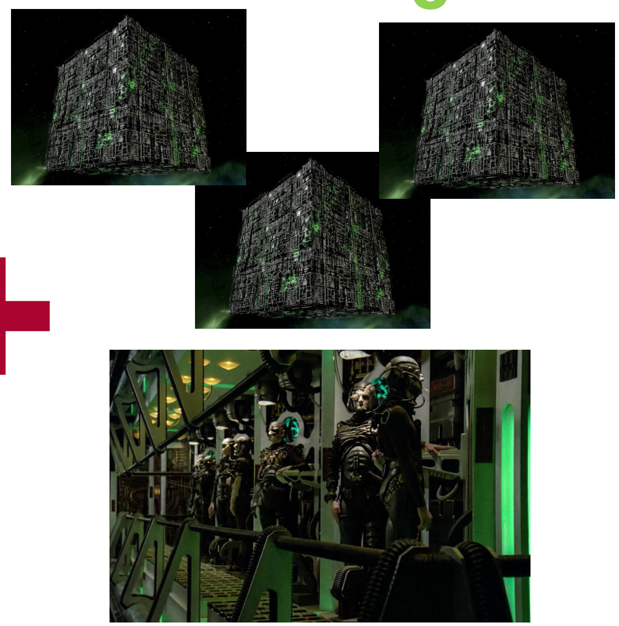
- Part 1 – Introduction to Sensitivity Coefficients
- Part 2 – Applications of Sensitivity Analysis
  - Design Optimization
  - Uncertainty Quantification
  - Benchmark Experiment Selection
  - Experimental Data Assimilation
- Part 3 – Current Research

Data Assimilation

Data

+

The Borg



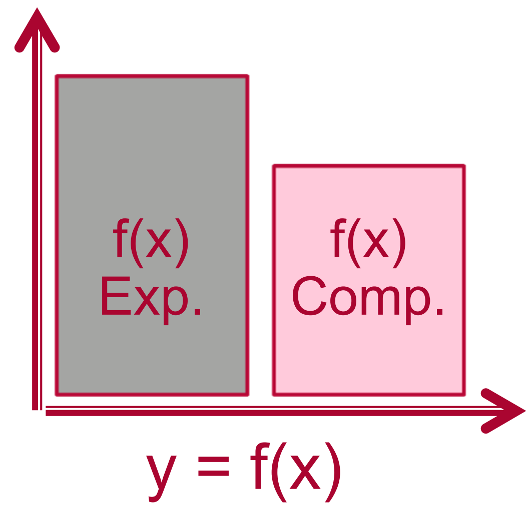
=

Data Assimilation

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.

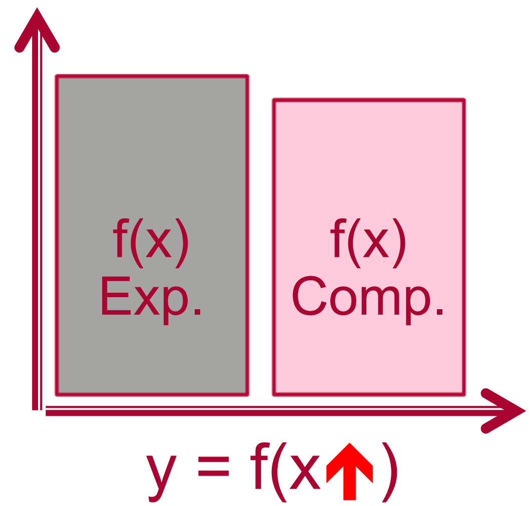


NUCLEAR ENGINEERING

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.

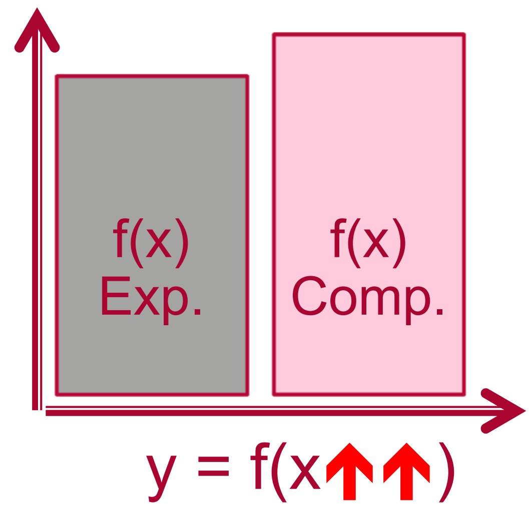


NUCLEAR ENGINEERING

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.

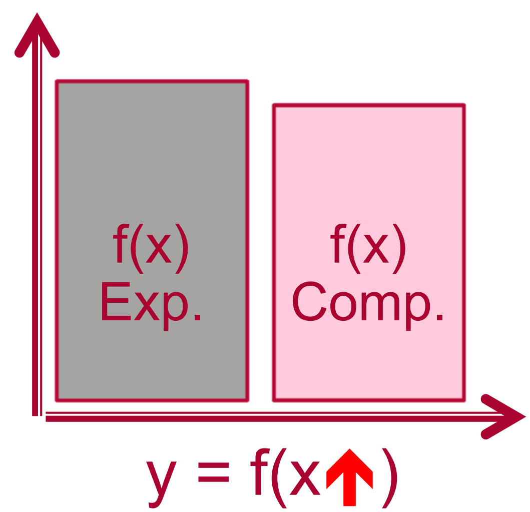


NUCLEAR ENGINEERING

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.



NUCLEAR ENGINEERING

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.

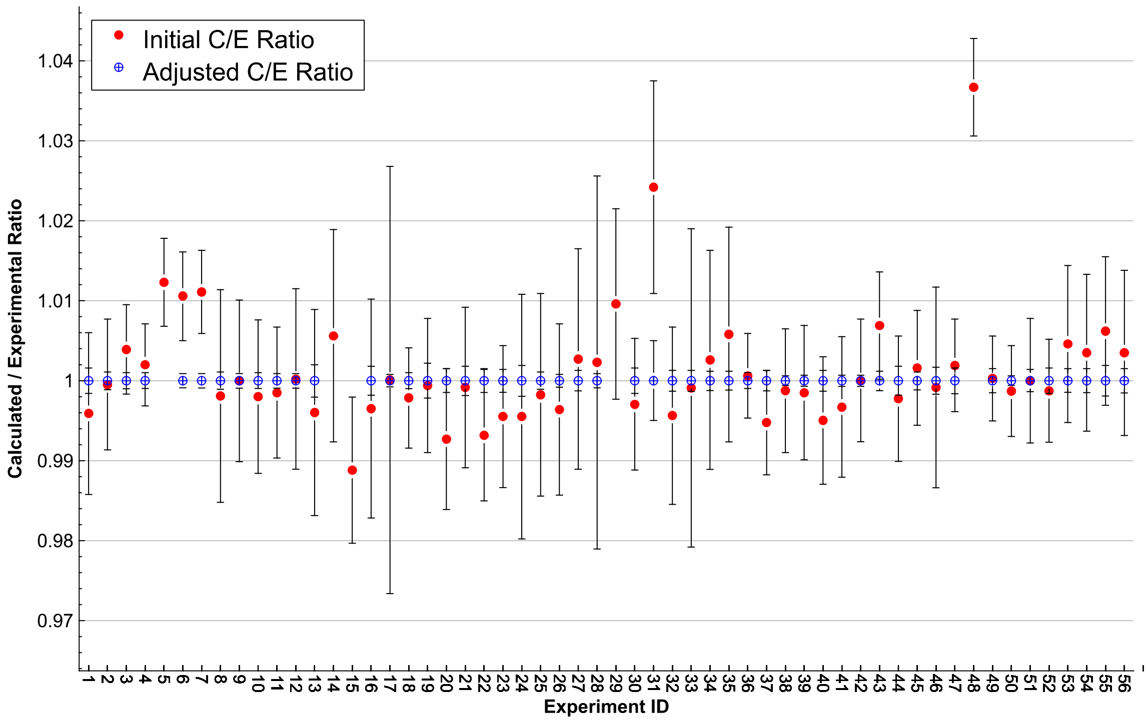
$$S_{f(x),x} = \frac{\partial f(x) / f(x)}{\partial x / x}$$

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

NUCLEAR ENGINEERING

Data Assimilation and Calibration

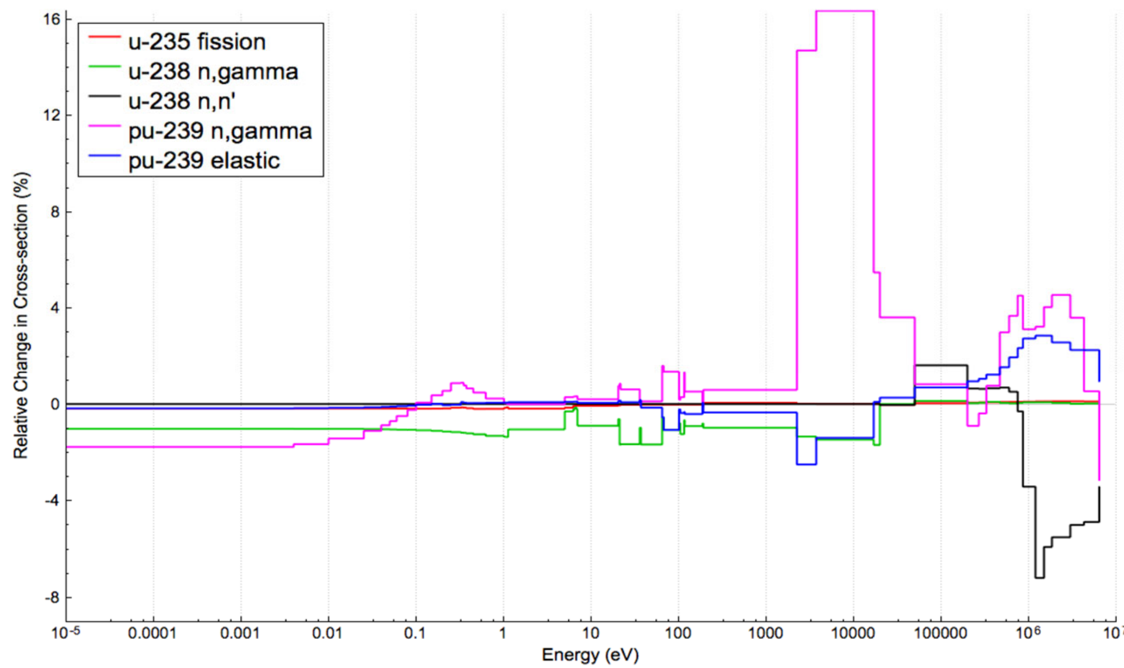
- Experimental benchmark data (E) is used to improve the accuracy of the initial computed responses (C).
- This assimilation consistently adjusts the underlying nuclear data.



NUCLEAR ENGINEERING

TSURFER Cross Section Adjustments

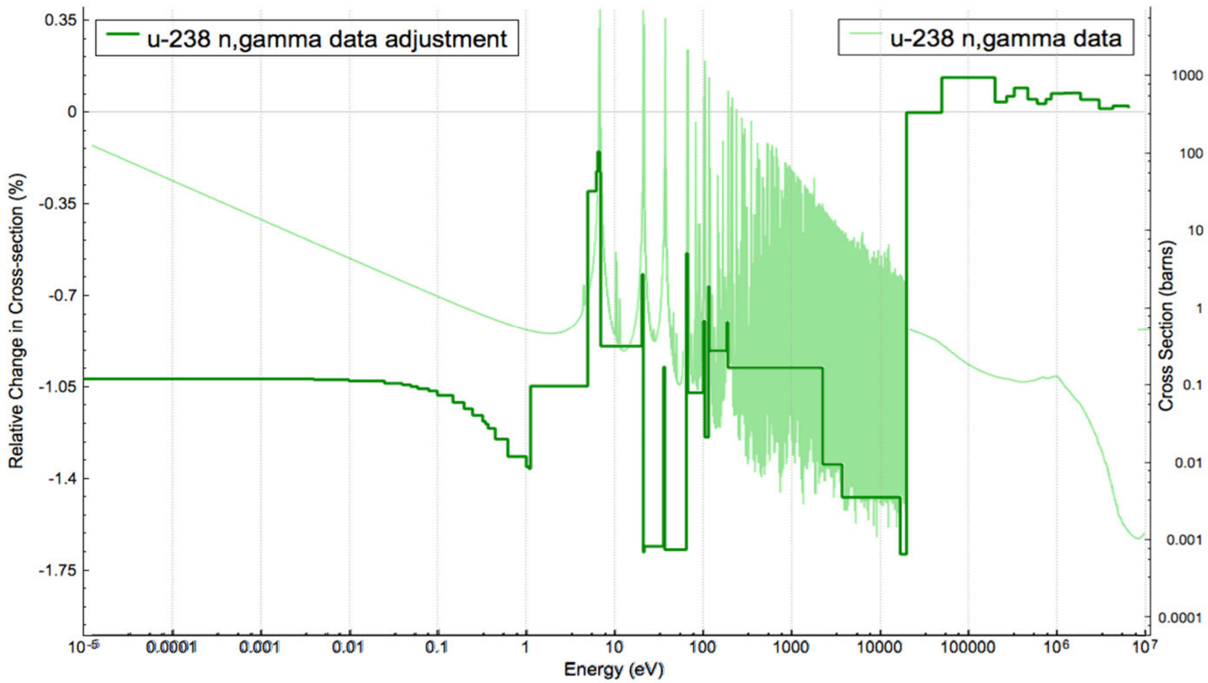
- Experimental benchmark data (E) is used to improve the accuracy of the initial computed responses (C).
- This assimilation consistently adjusts the underlying nuclear data.



NUCLEAR ENGINEERING

Realistic Cross Section Adjustments?

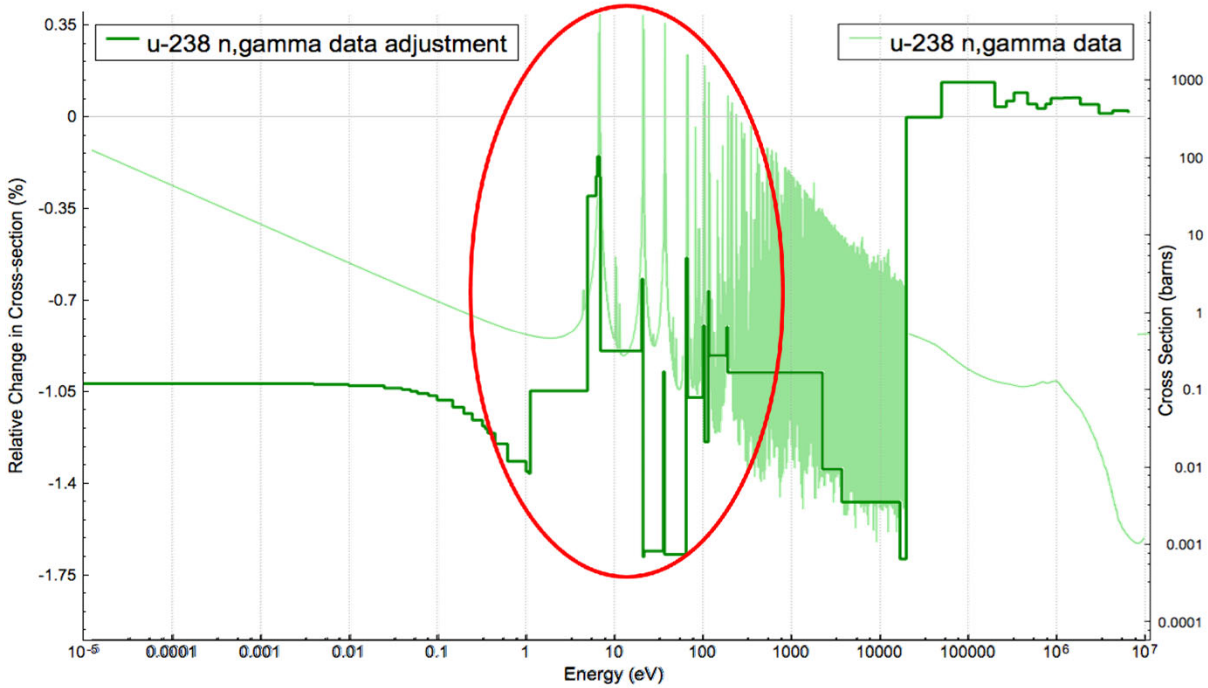
- TSURFER adjusts multigroup (i.e. energy-averaged) cross sections.
- This approach cannot generate usable nuclear data evaluations.



NUCLEAR ENGINEERING

Realistic Cross Section Adjustments?

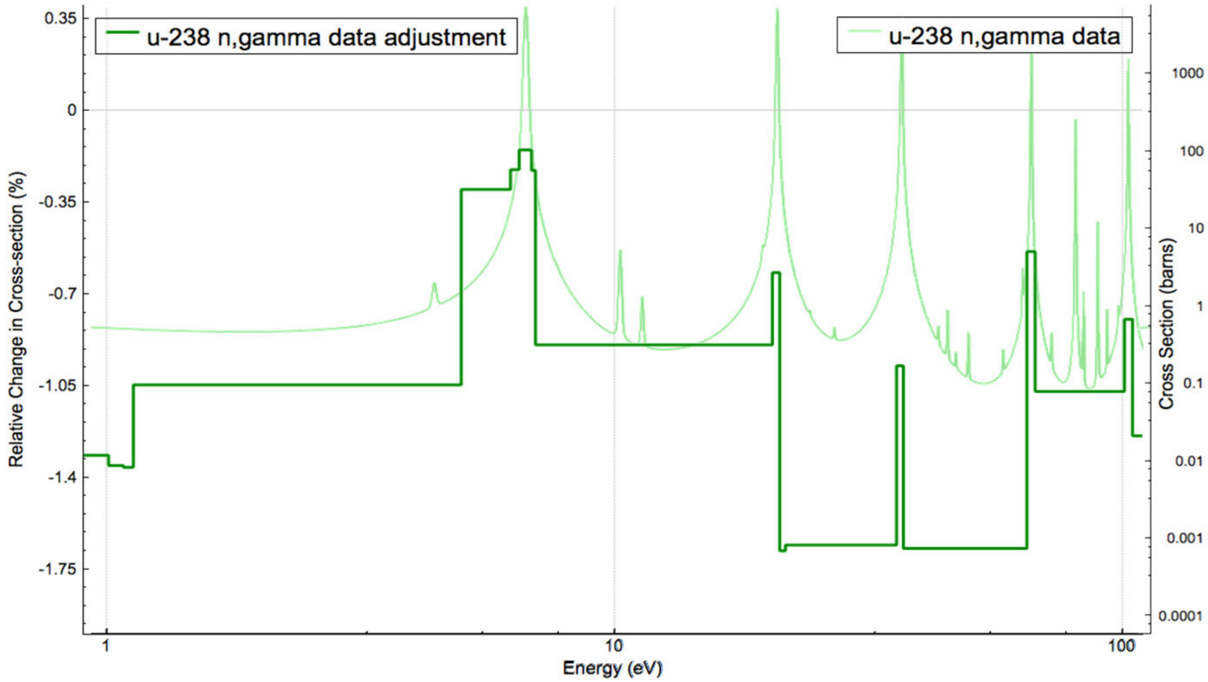
- TSURFER adjusts multigroup (i.e. energy-averaged) cross sections.
- This approach cannot generate usable nuclear data evaluations.



NUCLEAR ENGINEERING

Realistic Cross Section Adjustments?

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



NUCLEAR ENGINEERING

Presentation Outline

- Part 1 – Introduction to Sensitivity Coefficients
- Part 2 – Applications of Sensitivity Analysis
  - Design Optimization
  - Uncertainty Quantification
  - Benchmark Experiment Selection
  - Experimental Data Assimilation
- Part 3 – Current Research

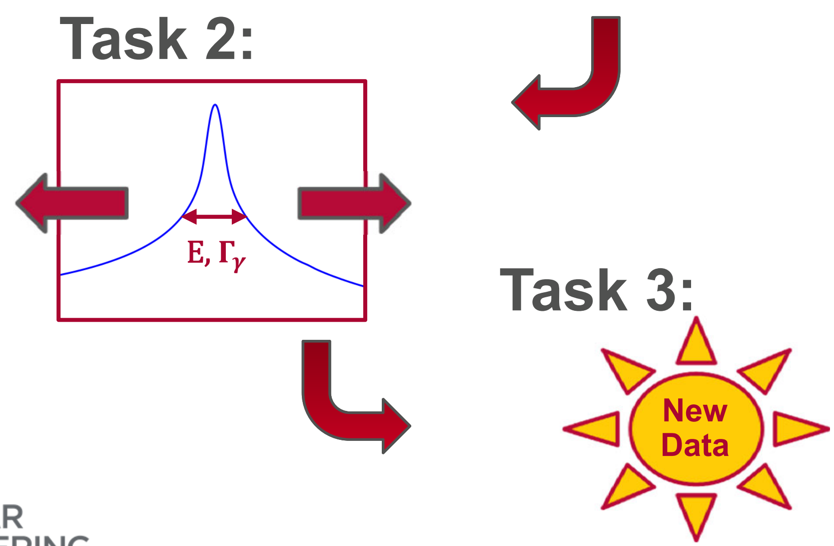
NUCLEAR ENGINEERING

NNSA Consortia on Monitoring, Technology, and Verification: "Improved Calibration of Evaluated Nuclear Resonance Parameters"

- **Task 1:** Develop sensitivity capabilities for evaluated nuclear data.
- **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:

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



NUCLEAR ENGINEERING

LANL Monte Carlo Methods Subcontract:

1. Fission Multiplicity Models in Monte Carlo Simulations

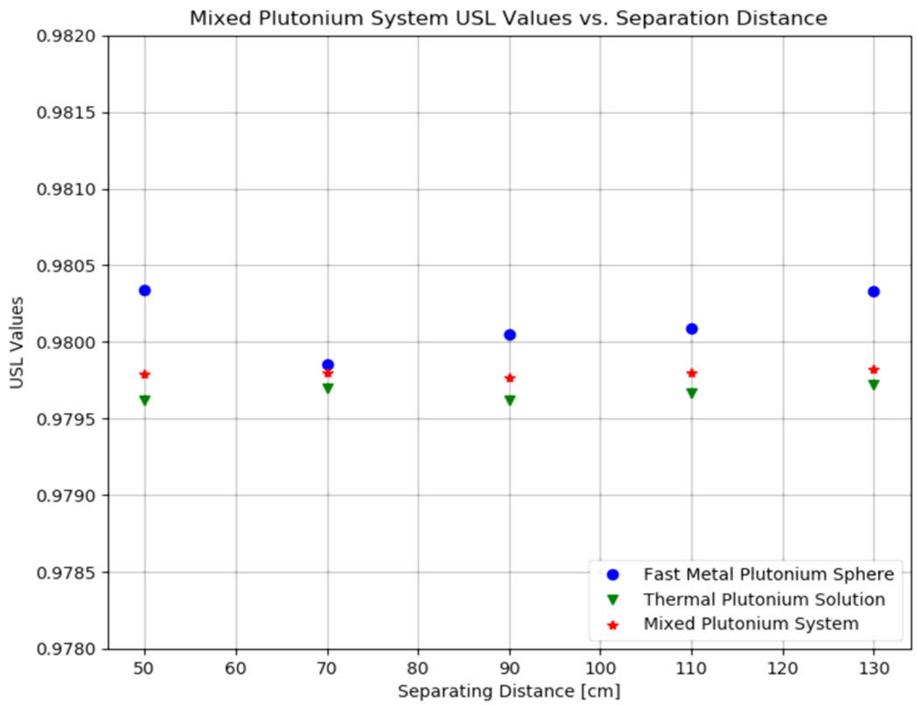
- Goal is to use high fidelity fission multiplicity models in Monte Carlo critical and subcritical simulations.
  - Work is exploring the accuracy of MCNP simulations for subcritical ICSBEP benchmark responses using higher fidelity fission physics models.
  - Work will explore using fission matrices to accelerate near-critical simulations.

LANL Monte Carlo Methods Subcontract:
2. S/U-based Validation for Nuclear Criticality Safety

- Goal is to better understand the use of S/U-based validation in nuclear criticality safety applications.
  - Upper Subcriticality Limit (USL) calculations vary significantly when using sensitivity coefficients for different sub-sections of a system.
  - It is not clear which USL is the most appropriate.

LANL Monte Carlo Methods Subcontract:

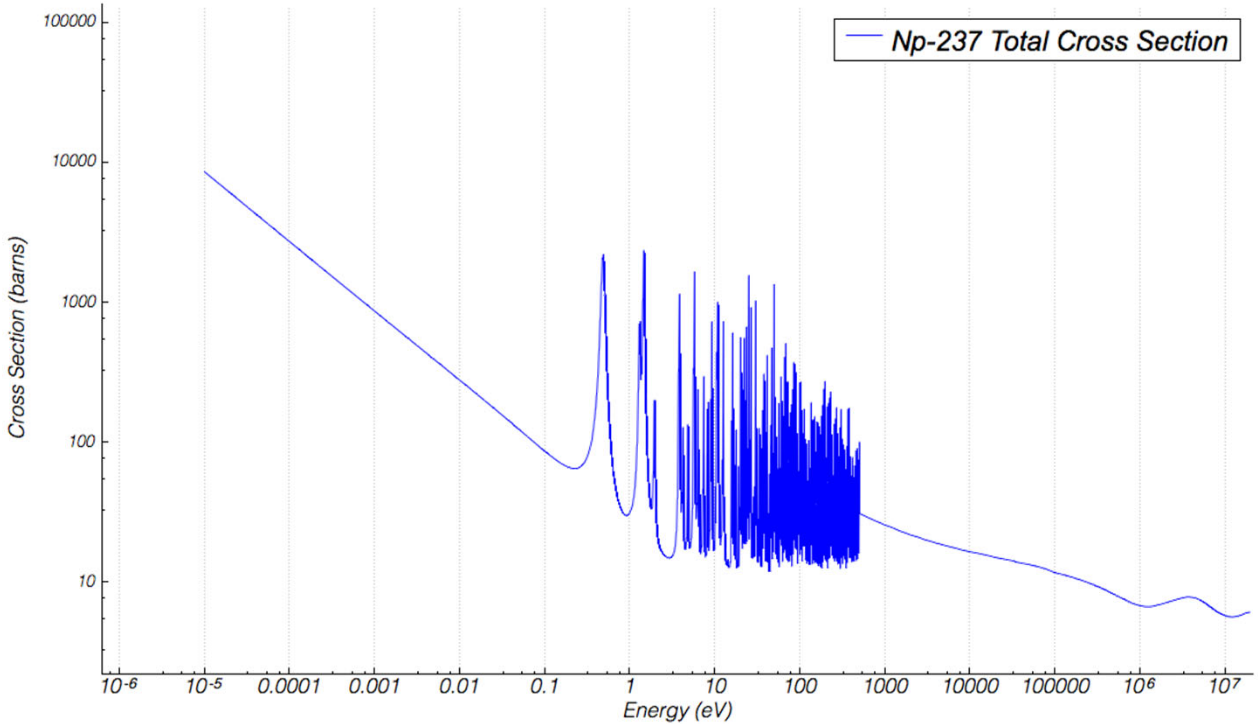
2. S/U-based Validation for Nuclear Criticality Safety



NUCLEAR ENGINEERING

NEUP Grant: Inferring Cross Sections for Short-lived Radioisotopes

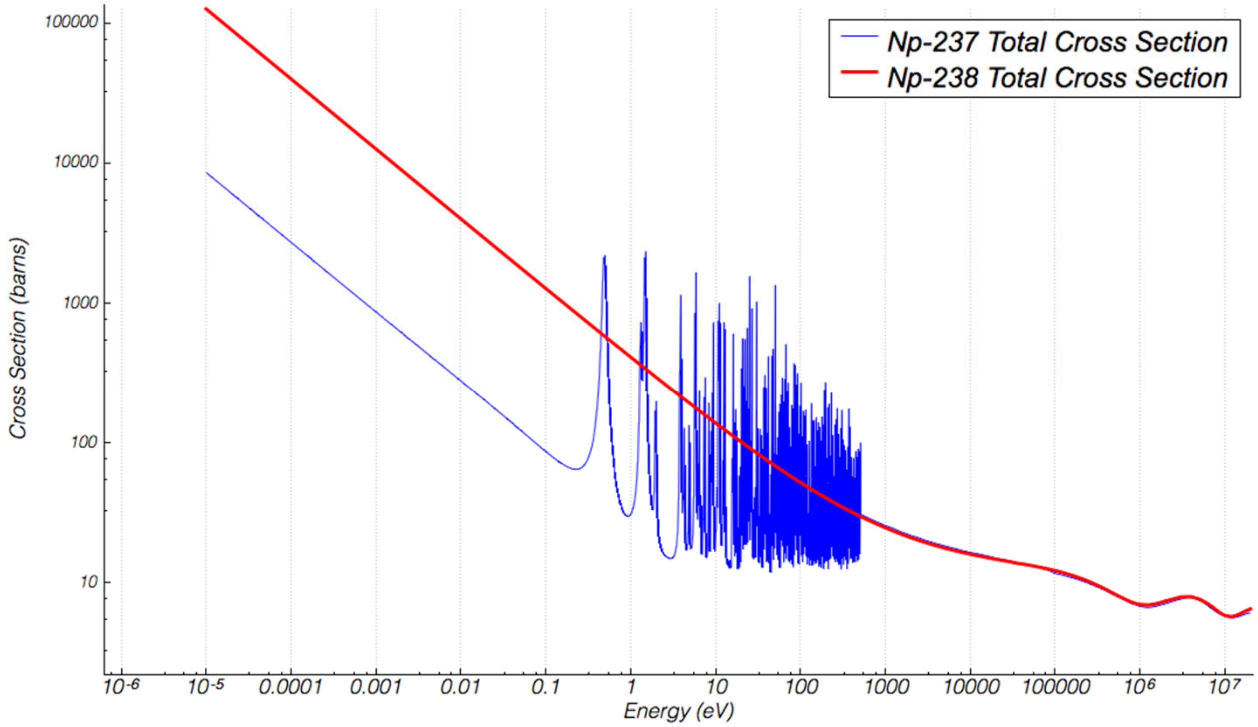
- ^{237}Np is commonly used as the seed material to produce ^{238}Pu.
- Low quality nuclear data for isotopes in the ^{238}Pu activation chain introduces computational bias in models for ^{238}Pu production.



NUCLEAR ENGINEERING

NEUP Grant: Inferring Cross Sections for Short-lived Radioisotopes

- ^{237}Np is commonly used as the seed material to produce ^{238}Pu.
- Low quality nuclear data for isotopes in the ^{238}Pu activation chain introduces computational bias in models for ^{238}Pu production.



NUCLEAR ENGINEERING

NEUP Grant: Inferring Cross Sections for Short-lived Radioisotopes

- Extensive experimental data exists for transcurium irradiation experiments, but current methods cannot assimilate this data.
- Successful assimilation could help infer cross sections for rare or short-lived radioisotopes.

$$S = \frac{d(Isotope\ Number\ Density)/Isotope\ Num.Den.}{d\Sigma_x/\Sigma_x}$$

- A tool performing **sensitivity analysis for the number density of isotopes in depletion and transmutation calculations** is needed for this cross section data calibration.

Questions?

Please contact:

Chris Perfetti
cperfetti@unm.edu

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

– Professor George E. P. Box

NUCLEAR ENGINEERING