Adjoint Sensitivity Analysis and Data Assimilation in a Large-Scale Pu Benchmark

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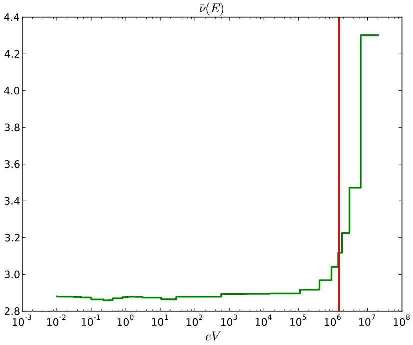
Outline

1. Introduction
   - Pu-239 Data Adjustment
2. Benchmark
   - Experiment
   - Simulation
3. Results
   - Sensitivities
   - Data Assimilation

Introduction: Does ENDF $^{239}\mathrm{Pu}\ \bar{\nu}(E)$ Need Adjustment?



- Recent simulations of a subcritical Pu experiment were discrepant with measurements
- Discrepancy only reduced by $\sim -1.1\%$ adjustment of $\bar{\nu}$. (Miller et. al., 2012)
- ENDF documentation notes poor fits to experimental data for certain energies. (Chadwick et. al. 2006)

Goal: Perform calibration of nuclear data using data assimilation on this subcritical experiment

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Nuclear Data Calibration using DA

Necessary Components

1. Simulate neutron distribution and compute response R for Pu experiment. R corresponds to a detector measurement
2. Sensitivity Analysis - Compute sensitivity of R to each nuclear data parameter $\alpha = (\ldots \sigma_f(E), \bar{\nu}(E), \ldots)$
3. Uncertainty Quantification - Use sensitivities to propagate uncertainty in nuclear data to computed response
4. Data assimilation - combine simulation (response, sensitivities, uncertainties) and experiment to compute "best-estimate values" for nuclear data

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Subcritical Experiment - "BeRP Ball" (Mattingly, J.),*SAND2009-5804*, (2009)

Setup

1. Weapons grade Pu source
2. Gross Neutron Counter (SNAP Detector) counts # neutrons/s
3. ^{3}He proportional counter

SNAP Detector: ^{3}He counter measures

$$n +^3 \mathrm{He} \rightarrow p +^3 H$$

$$R = \int_{V_{counter}} \mathrm{d}r\mathrm{d}E\, \Sigma^{^3\mathrm{He}}_{(n,p)}(r,E)\psi(r,E)$$

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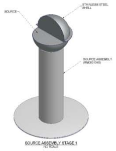
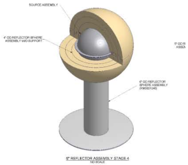
Bare Assembly and Reflected Assembly





- We simulated 2 experiments: Bare Pu sphere and 76.2 mm Reflected
- Reflected assembly is more sensitive to lower energy neutrons and has more chances for fission
- Compute 2 responses (SNAP detector)

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Neutron Distribution (Flux) Computation

Deterministic Time-Independent Transport Equation

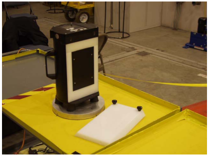
$$\underbrace{\Omega \cdot \nabla\psi(r,E,\Omega) + \Sigma_t(r,E)\psi(r,E,\Omega)}_{\text{streaming\&collision}\equiv \text{L}\psi} =$$

$$\underbrace{\int dE' d\Omega' \Sigma_s(r,E' \to E, \Omega' \to \Omega)\psi(r,E',\Omega')}_{\text{scattering}\equiv \text{S}\psi} +$$

$$\underbrace{\chi(r,E)\int dE' d\Omega' \nu(r,E')\Sigma_f(r,E')\psi(r,E',\Omega')}_{\text{induced fission}\equiv \text{F}\psi} + \underbrace{Q(r,E)}_{\text{spontaneous fission}\equiv \text{Q}}$$

Rewrite in operator form $\to [L - S - F]\,\psi = Q$

Compute Responses and Sensitivity Coefficients



- Bare and Reflected Responses (Detector Count Rates)

$$R = \langle \Sigma^{^3\mathrm{He}}_{(n,p)}, \psi \rangle$$

- First-order Sensitivities

$$S^R_{\alpha_n} \equiv \frac{\partial R}{\partial \alpha_n}$$

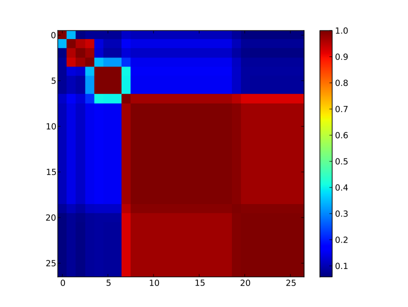
Use 1 Adjoint to compute all $S^R_{\alpha_n}$

- Adjoint quantifies each neutron's important to R
- Computed from: $[L - S - F]^\dagger \psi^\dagger = \Sigma^{^3\mathrm{He}}_{(n,p)}$
- Sensitivities are computed using inner products of operators and ψ, $\psi^\dagger$
- $S^R = (S^R_{\alpha_0}, S^R_{\alpha_1}, \ldots, S^R_{\alpha_n})$
- *Relative* sensitivity coeffients are quoted: $S^R_{\alpha_n} = \frac{\alpha_n}{R}\frac{\partial R}{\partial \alpha_n}$

Uncertainty Quantification

First-order propagation of model parameter errors to responses

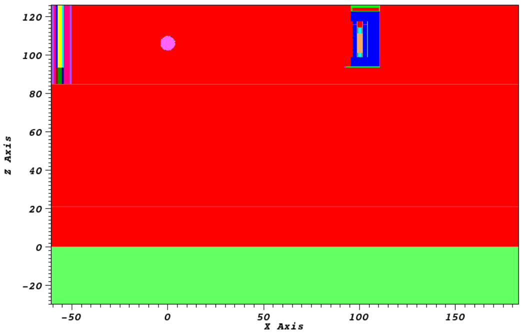
- $C_r = S^R C_\alpha (S^R)^T$ (Error Propagation Formula)
- C_α is nuclear parameter covariance data from ENDF/SCALE6.1



Correlation matrix for $\bar{\nu}(E)$

Simulation Description

- Geometry/Cross sections are generated in SCALE (ENDF/B-VII)
- Spontaneous fission source from SOURCES-4C
- Calculations use 7680 cpus with modified version of ORNL's Denovo.
- 27 groups/1344 angles/P_3/6 million cells



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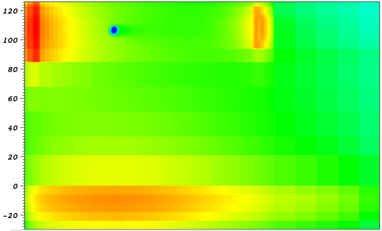
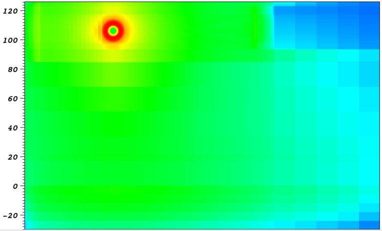
Computation Results

Responses

Assembly	Computed	Measured
Bare	57.786 ± 2.662	57.4 ± 0.4
Reflected	129.521 ± 12.208	116.2 ± 0.6

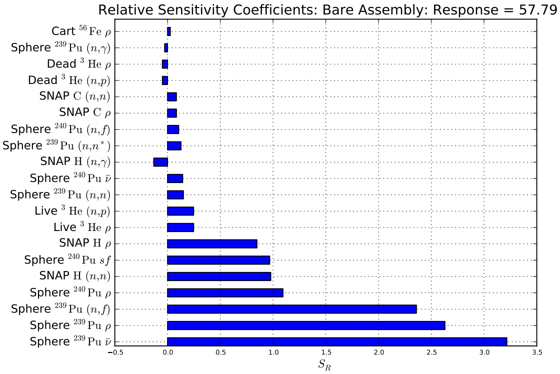
Thermal group (low energy neutrons)





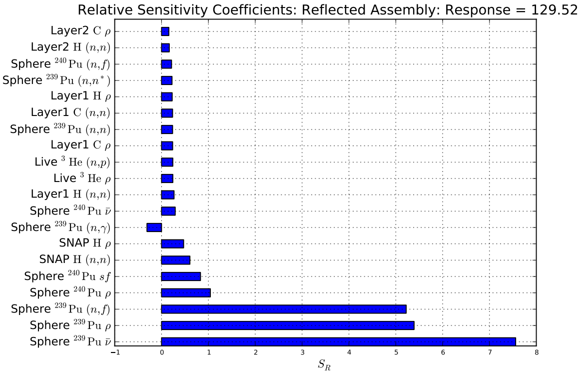
Sensitivity Coefficients: Bare Sphere

Top 20 nuclear data sensitivities - integrated over energy



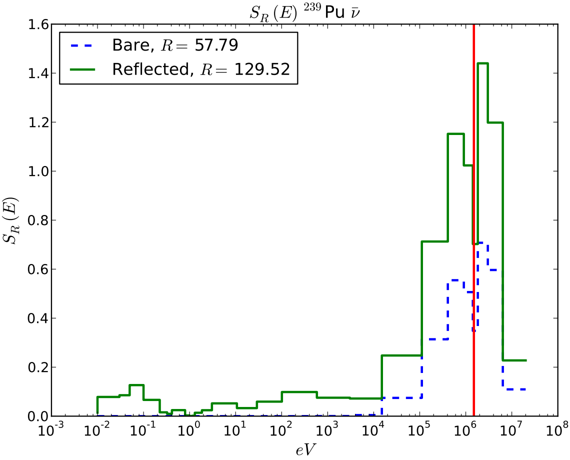
Sensitivity Coefficients: Reflected Sphere

Top 20 nuclear data sensitivities - integrated over energy



Differential Sensitivity Coefficient: ^{239}Pu $\bar{\nu}(E)$

Reflected is more sensitive. Bare is insensitive below 10 KeV.



Data Assimilation

**The methodology is described in:
Cacuci & Ionescu-Bujor, *Nuc. Sci. Eng.* **165** (1), (2010)**

- Based in Bayes' Theorem and Maximum Entropy Principle
- Maximally Objective for Given Data
- Simultaneously calibrates all responses and parameters with sensitivity & uncertainty data.
- For this simple case - Constrained maximization of multivariate Gaussian distribution $e^{-\frac{1}{2}Q(\alpha,r)}$ and linear
- $\alpha = \alpha_0 - C_\alpha (S^R_\alpha)^\dagger \left[C_m + C_r\right]^{-1} (r - R)$

DA: Best-predicted Nuclear Data

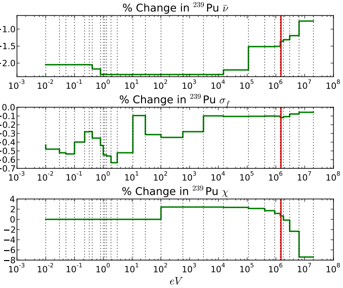


Figure: Adjustments to ^{239}Pu fission data.

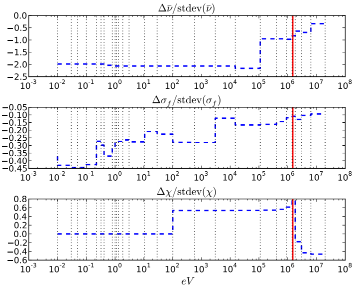


Figure: Adjustments to ^{239}Pu fission data relative to the standard deviation.

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Summary

- This analysis corroborates previous work - $^{239}\mathrm{Pu}$ $\bar{\nu}$ appears to high
- Below roughly 1.5 MeV $\bar{\nu}$ undergoes 1-2 standard deviation adjustment
- This adjustment corresponds to documented discrepancies in evaluated data
- Provides additional information & approach for evaluators (subcritical system with DA)
- Next Step: XSEDE allocation for expanded and refined study (finer energy groups & better convergence verification, additional experiments)

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