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Validation of Nuclear Data Sensitivity Calculations by the MCNP PERT Card

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Introduction and Motivation

- Predictive codes are used to simulate experiments.
- Improving the nuclear data results in more precise/accurate simulations causing higher-fidelity designs and reduced procedural/operational costs.
- Therefore, the improvement of nuclear data is of paramount importance.
- Nuclear data is improved via integral benchmark experiments.
  - Integral benchmark experiments compare simulated and measured quantities to derive recommended changes to improve nuclear data.
- Sensitivity quantifies how much a specific parameter (e.g., multiplication) is changed by perturbation of a contributing parameter (e.g., cross sections).
  - High sensitivity benchmark means high impact benchmark
- There is in no direct tool to estimate the sensitivity of any parameter other than the effective multiplication factor.
- This work validates a method of estimating sensitivities that utilized the MCNP PERT card and tallies.

Mission Relevance

- Sensitivity calculations will be used to create high impact integral benchmark experiments to improve nuclear data.
- Improved nuclear data serves all users, which comprises the entirety of the NNSA.

MTV Impact

- Participation in the MTV Nuclear Engineering Summer School and workshop allowed for the exploration of different areas of interest for graduate studies.
- National laboratory connections allowed for participation in measurement campaigns (like MUSIC) and internships.

Defining Sensitivity

- The Taylor series expansion of some response (R) that is a function of some cross section (σ_x) can be expressed as

$$R(\sigma_x) = R(\sigma_{x,0}) + \left.\frac{dR}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x + \frac{1}{2}\left.\frac{d^2R}{d\sigma_x^2}\right|_{\sigma_{x,0}} (\Delta\sigma_x)^2 + \cdots$$

or more simply

$$R(\sigma_x) = \boxed{R(\sigma_{x,0})} + \boxed{\Delta R_1} + \boxed{\Delta R_2} + \cdots$$

where $\Delta\sigma_x = \sigma_x - \sigma_{x,0}$.

- The relative change in cross section can then be defined as

$$p_x = \frac{\Delta\sigma_x}{\sigma_{x,0}}.$$

- The terms can then be redefined as

$$\boxed{R_0 = R(\sigma_{x,0}),}$$

$$\boxed{\Delta R_1 = \left.\frac{dR}{dp_x}\right|_{p_x=0} p_x = R_1 p_x \rightarrow R_1 = \frac{\Delta R_1}{p_x}\text{, and}}$$

$$\boxed{\Delta R_2 = \left.\frac{d^2R}{dp_x^2}\right|_{p_x=0} p_x^2 = R_2 p_x^2 \rightarrow R_2 = \frac{\Delta R_2}{p_x^2}.}$$

- The first-order relative sensitivity coefficient can then be defined as

$$S_{R,\sigma_x} = \frac{\sigma_x}{R_0}\left.\frac{dR}{d\sigma_x}\right|_{\sigma_{x,0}} = \frac{1}{R_0}\left.\frac{dR}{dp_x}\right|_{p_x=0}.$$

PERT Approach

- The PERT card is limited to reaction cross section perturbations.
- Each energy bin and isotope requires an individual PERT card (run time increase by 5-10%)

Make a copy of the material card that has the isotope of interest and give it its own unique name

↓

Calculate the weight fraction of the isotope of interest for the fictitious material as $W_{fictitious} = (1 + p_x)W_{real}$

↓

Calculate the fictitious materials density as $\rho_{fictitious} = \frac{W_{fictitious}}{W_{real}}\rho_{real}$

↓

The "Method=2" input of the PERT card outputs $\Delta R_1(p_x)$

↓

The sensitivity can the be estimated as $S_{R,\sigma_x} = \frac{1}{R_0}\left.\frac{dR}{dp_x}\right|_{p_x=0} = \frac{R_1}{R_0} = \frac{\Delta R_1(p_x)}{R_0 p_{x,0}}$

Brute Force Approach

- A compact ENDF (ACE) file is the file composed of the cross-section libraries for continuous MCNP calculations
- FRENDY is a nuclear data processing system.
- Each Sensitivity estimate requires three separate runs.

Obtain the ACE file(s) that include the nuclear data of interest

↓

Use FRENDY to perturb the ACE file

↓

Collect the tally response from simulations that utilize the unperturbed and perturbed ACE files

↓

The sensitivity can be estimated using the central-difference theorem $S_{R,\sigma_x} = \frac{1}{R_0}\left.\frac{dR}{dp_x}\right|_{p_x=0} = \frac{R(\sigma_{x,0} + \Delta\sigma_x) + R(\sigma_{x,0} - \Delta\sigma_x)}{2R_0 p_x}$

Results

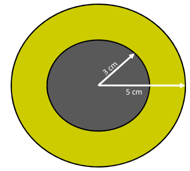

Figure 1. Geometry of the test case.

- 6 cm sphere of plutonium (94% ^{239}Pu, 6% ^{240}Pu)
- 2 cm natural copper reflector
- The response is the track length estimate of cell flux on the inner sphere.

Net Multiplicity = 1.0005

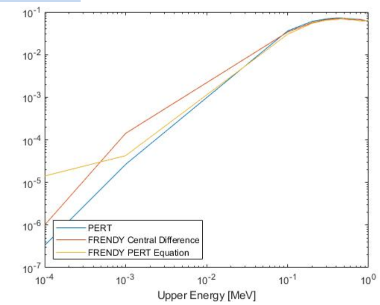

Figure 2. A comparison of the sensitivity estimations.

Conclusion and Future Work

- The agreement of the PERT card and Brute Force results proves the validity of calculating nuclear data sensitivities by use of the MCNP PERT card, especially at higher energies.
- The overall agreement will be easier to understand once an uncertainty analysis is completed.
- In the future,
  - The PERT and Brute Force method will be applied to more complex cases.
  - The validity of the new MCNP sensitivity tool can be compared against current methods.
  - Additionally, work will continue to find ways to calculate the sensitivity of additional parameters.

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