Status of MCNP Sensitivity/Uncertainty Capabilities for Criticality

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September 30, 2013

Abstract

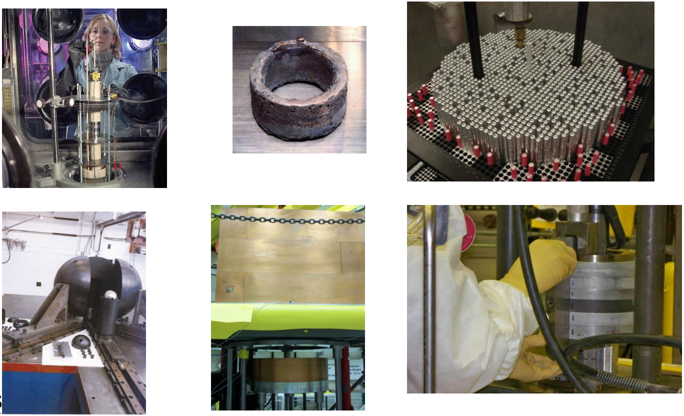
A new capability is being developed in MCNP6 to provide estimates of uncertainties in the effective multiplication *k* because of nuclear cross sections. This has been implemented in a prototype version of MCNP6. The version reads covariance data from the nuclear data libraries, runs a continuous-energy transport calculation to compute sensitivity profiles on the energy grids found in the covariance data, and convolves them to produce estimates of the *k* uncertainty. Results are shown for eight criticality benchmark experiments.

Introduction

- Methodology
- Results
- Future Research and Development

Motivation

- Sensitivity/uncertainty analysis allows us to quantify how well (or poorly) software predicts criticality.



Sensitivity Theory

- The sensitivity coefficient estimates the ratio of the relative change in a response R to the relative change in some system parameter x.

$$S_{R,x} = \frac{\Delta R/R}{\Delta x/x}.$$

- For this work, the response R is the effective multiplication k, and x represents some nuclear data (e.g., cross section, fission ν).
- Sensitivity coefficient estimates the impact of a particular nuclear data on the system criticality.

Sensitivity Methodology

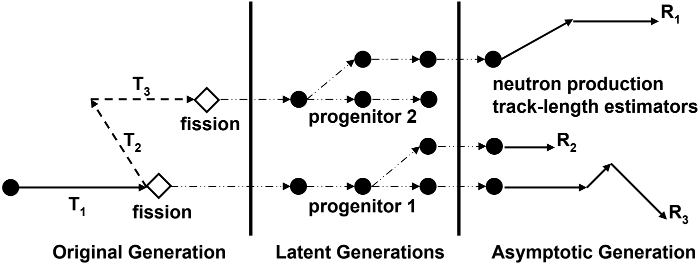
- Derive an integral expression for sensitivity coefficient using linear-perturbation theory:

$$S_{k,x} = -\frac{\langle \psi^\dagger, (\Sigma_x - \mathcal{S}_x - \lambda \mathcal{F}_x)\psi \rangle}{\langle \psi^\dagger, \lambda \mathcal{F} \psi \rangle}.$$

- Must evaluate a ratio of adjoint-weighted integrals.
- Adjoint function computed by Iterated Fission Probability Method.
- No space-energy mesh required.
- One user parameter (to be explained), but default is conservative for almost all problems.

Iterated Fission Probability

- Divide active cycles or generations into “blocks” of some size (default 10).
- First cycle: accumulate scores for forward reaction rates and tag neutrons.
- Follow neutrons through generations, preserving tags.
- Last cycle: multiply forward reaction rates by neutron production of corresponding progeny.



Renormalizing Sensitivities

- For fission and scattering distributions, increases somewhere must be offset by decreases elsewhere, and sensitivities must account for this.
- Assumption is to renormalize by a constant multiplicative factor over entire distribution.

$$\hat{S}_{k,f}(\mu, E, E') = S_{k,f}(\mu, E, E') - f(E' \to E, \mu) \int_0^\infty dE \int_{-1}^{1} d\mu \, S_{k,f}(\mu, E, E').$$

- Total sensitivity (over all outgoing energy and angles) sums to zero.
- Assumes a fine enough incident energy grid structure.

Estimation of Uncertainty

- Apply the "sandwich rule":

$$(\delta k)^2 = \mathbf{SCS}^T.$$

- **S** is a vector of sensitivities.
- **C** is the nuclear data covariance matrix (processed by NJOY).

Covariance Matrix

- Right now, obtained from NJOY and processed into an MCNP readable form.
- Principal eigenvector format used to save space.

$$\mathbf{C} = \mathbf{V}\mathbf{D}\mathbf{V}^T.$$

- **V** is a matrix of principal eigenvectors.
- **D** is a diagonal matrix of corresponding eigenvectors.
- Matrix product reconstructs approximate covariance matrix **C**.
- Unionized energy grid used for each covariance matrix.

Availability

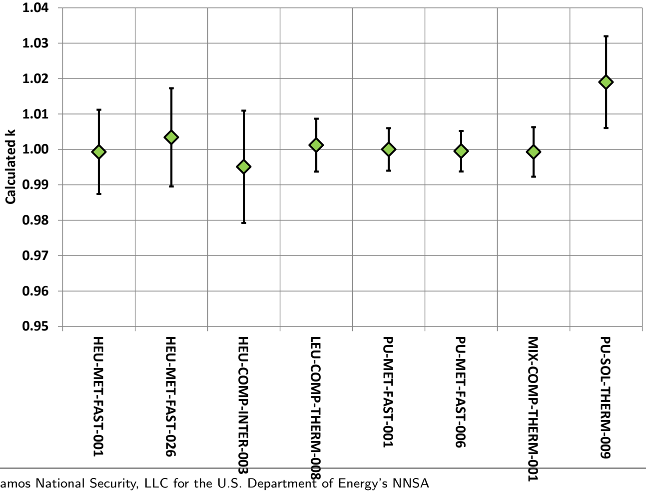
- Sensitivity capability available today in MCNP6.1 from RSICC.
- MCNP/NJOY modifications to compute uncertainties are current research and development, and <u>not</u> currently available.
- DOE/NNSA NCSP plans to fund development of capabilities in MCNP/NJOY through FY 2015.
- Capability will likely be available then in MCNP6.x, but covariance data may take more time to generate.

Results

- Covariance data generated with ENDF/B-VII.1 for ^{1}H , ^{16}O , ^{235}U , ^{238}U , and ^{239}Pu .
- No thermal scattering law covariances included.
- Benchmarks:
    - Bare-HEU Sphere (Lady Godiva)
    - Reflected-HEU Sphere (Flattop)
    - Uranium-Hydride Experiment
    - Light-Water Moderated LEU Lattice
    - Bare-Pu Sphere (Jezebel)
    - Reflected-Pu Sphere (Flattop)
    - Light-Water Moderated MOX Lattice
    - Pu Solution (Light-Water)

Results

- MCNP calculated *k* with nuclear data uncertainty:



Results: Godiva

- Capture, scattering, and fission ν dominant for fast ^{235}U .
- All uncertainties in pcm (1 pcm $= 1 \times 10^{-5}$).

^{235}U	(n,γ)	(n,γ)	873.8
^{235}U	(n,n$'$)	(n,n$'$)	612.4
^{235}U	ν	ν	544.6
^{235}U	(n,n)	(n,n$'$)	-541.8
^{235}U	(n,n)	(n,γ)	341.5
^{235}U	(n,n)	(n,n)	294.1
^{235}U	(n,f)	(n,f)	268.9

Results: Jezebel

- Scattering and fission dominant for fast ^{239}Pu .
- Is fission ν really so much better known for ^{239}Pu over ^{235}U ? (sensitivities very similar)
- Capture (n,γ) quite different too.

^{239}Pu	(n,n′)	(n,n′)	868.8
^{239}Pu	(n,n)	(n,n′)	-865.0
^{239}Pu	(n,n)	(n,n)	455.9
^{239}Pu	(n,f)	(n,f)	331.0
^{239}Pu	χ	χ	173.9
^{239}Pu	ν	ν	81.6
^{239}Pu	(n,n)	(n,f)	-81.4
^{239}Pu	(n,γ)	(n,γ)	72.3
^{239}Pu	(n,n)	(n,γ)	36.1
^{239}Pu	(n,2n)	(n,2n)	10.4

Results: LEU Lattice

- Capture, scattering, and fission ν dominant for thermal ^{235}U .

^{235}U	ν	ν	625.8
^{238}U	(n,γ)	(n,γ)	264.2
^{1}H	(n,γ)	(n,γ)	181.3
^{235}U	(n,f)	(n,f)	144.6
^{235}U	(n,γ)	(n,γ)	131.5
^{235}U	(n,f)	(n,γ)	122.1

Results: MOX Lattice

- Different lattice, but similar interesting trends for fast as thermal ^{239}Pu versus ^{235}U .

^{1}H	(n,n)	(n,n)	317.7
^{239}Pu	(n,γ)	(n,γ)	275.0
^{239}Pu	(n,f)	(n,f)	260.6
^{239}Pu	χ	χ	250.6
^{239}Pu	(n,f)	(n,γ)	222.3
^{238}U	(n,n$'$)	(n,n$'$)	213.9
^{1}H	(n,γ)	(n,γ)	199.6
^{16}O	(n,n)	(n,n)	176.7
^{239}Pu	ν	ν	150.0
^{238}U	(n,n)	(n,n$'$)	-112.9

Results: Uranium Hydride Experiment

- Intermediate spectrum experiment.

^{235}U	(n,γ)	(n,γ)	1327.1
^{238}U	(n,n$'$)	(n,n$'$)	592.9
^{235}U	ν	ν	582.7
^{238}U	(n,n)	(n,n$'$)	-472.6
^{235}U	(n,n)	(n,γ)	320.4
^{235}U	(n,n$'$)	(n,n$'$)	265.8
^{1}H	(n,n)	(n,n)	237.6
^{238}U	(n,n)	(n,n)	213.5
^{235}U	(n,n)	(n,n$'$)	-179.1
^{235}U	(n,f)	(n,f)	160.8
^{235}U	(n,f)	(n,γ)	114.8

Results: Pu Solution

- Outlier (still within 2-σ) in the set of eight benchmarks.

^{1}H	(n,γ)	(n,γ)	1034.0
^{239}Pu	(n,f)	(n,f)	628.4
^{239}Pu	(n,f)	(n,γ)	339.1
^{239}Pu	(n,γ)	(n,γ)	216.0
^{239}Pu	ν	ν	168.9
^{1}H	(n,n)	(n,n)	116.8
^{239}Pu	χ	χ	96.8

Summary

- Continuous-energy *k*-eigenvalue sensitivity capability currently available in MCNP6.1.
- Modifications to NJOY and MCNP for uncertainty propagation are under development.
- Preliminary results show for the small collection of eight benchmarks presented, calculational results are within 2-σ of the experimental result.
- Comparisons between ENDF/B-VII.1 covariances of ^{235}U and ^{239}Pu show (what I think are) inconsistencies.

Future Work

- Continue development of MCNP6/NJOY covariance/uncertainty capability.
- Compare more isotopes, more benchmarks, different datasets.
- Adapt to scattering law (Legendre moments) covariances (see talk tomorrow).

Acknowledgments

- Funding provided by the U.S. DOE/NNSA Nuclear Criticality Safety Program.

Questions?