Importance of Scattering Distributions on Criticality

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Abstract

MCNP6 has the capability to compute sensitivity coefficients for k from scattering distributions as a function of scattering cosine. A new capability has been prototyped, and will hopefully available in a future release, that takes those results and converts them into sensitivities for Legendre scattering moments, which is discussed. Results are shown for a variety of criticality benchmarks for elastic scattering, and it appears that the P_1 elastic scattering Legendre moment (i.e., average scattering cosine $\bar{\mu}$) may indeed have a significant effect in fast, bare and reflected systems with significant leakage. The results also show that higher elastic moments and all inelastic moments are typically not important to criticality

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Introduction

- Methodology
- Derivation
- Results & Observations
- Future Research & Development

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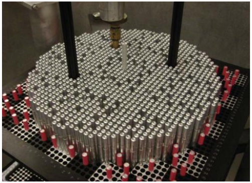
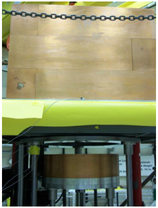
Motivation

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





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Motivation

- Recent work has mostly focused on the effect of nuclear cross sections, fission multiplicity ν, and fission spectrum χ on how they impact criticality and its calculational uncertainty.
- Less attention has been paid to the impact of the kinematics of neutron collisions and their associated uncertainties.
- ENDF format covariances are for Legendre moments, and MCNP must convert its cosine-binned results to match for uncertainty propagation.

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Findings

- The linearly anisotropic (P_1) component of elastic scattering may have a significant effect on k.
- Higher orders of scattering are typically not important, and neither is anisotropy of inelastic scattering.
- For fast systems with significant leakage, core and reflector materials are often significant.
- For thermal systems, scattering distributions matter less.

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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.

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Sensitivity Methodology

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

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

- 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.

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

Legendre Moment Sensitivity – Derivation

- The fractional change in k from a fractional change in distribution f is:

$$\frac{\Delta k}{k} = \int_{-1}^{1} d\mu \, \frac{\Delta f(\mu)}{f(\mu)} \hat{s}_{k,f}(\mu).$$

- Here $\hat{s}_{k,f}(\mu)$ is the sensitivity density in per unit cosine, but MCNP calculates the bin-integrated sensitivity $\hat{S}_{k,f}$.
- Discretize in cosine space, and for cosine bin i, assuming midpoint integration,

$$\hat{S}_{k,f,i+1/2} = \int_{\mu_i}^{\mu_{i+1}} d\mu \, \hat{s}_{k,f}(\mu) = \hat{s}_{k,f,i+1/2} \left(\mu_{i+1} - \mu_i\right).$$

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Legendre Moment Sensitivity – Derivation

- The scattering distribution can be expressed via a series expansion of Legendre moments:

$$f(\mu) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu) f_\ell,$$

- Can find f_ℓ the ℓth Legendre moment by:

$$f_\ell = \int_{-1}^{1} d\mu \, P_\ell(\mu) f(\mu).$$

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Legendre Moment Sensitivity – Derivation

- Let $f(\mu)$ have one of its Legendre moments perturbed by a factor of $1 + p$ with $p \approx 0$.

$$\Delta f(\mu) = \frac{2\ell + 1}{2} P_\ell(\mu) f_\ell p \tag{1}$$

- After a bit of manipulation, a discrete approximation for $\Delta k/k$ may be obtained:

$$\frac{1}{p}\frac{\Delta k}{k} \approx \frac{2\ell + 1}{2} f_\ell \sum_{i=0}^{N-1} (\mu_{i+1} - \mu_i) \frac{P_\ell(\mu_{i+1/2})}{f(\mu_{i+1/2})} \hat{s}_{k,f,i+1/2}.$$

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Legendre Moment Sensitivity – Derivation

$$\frac{1}{p}\frac{\Delta k}{k} \approx \frac{2\ell+1}{2} f_\ell \sum_{i=0}^{N-1} (\mu_{i+1}-\mu_i) \frac{P_\ell(\mu_{i+1/2})}{f(\mu_{i+1/2})} \hat{s}_{k,f,i+1/2}.$$

- Left side is the definition of the senstivity.
- To get in terms of Monte Carlo estimates, replace densities by bin integrated quantities (assume midpoint integration):

$$\hat{S}_{k,f,\ell} = \frac{2\ell+1}{2} f_\ell \sum_{i=0}^{N-1} (\mu_{i+1}-\mu_i) \frac{P_\ell(\mu_{i+1/2})}{F_{i+1/2}} \hat{S}_{k,f,i+1/2}.$$

Legendre Moment Sensitivity – Derivation

- Bin integrated sensitivity $\hat{S}_{k,f,i+1/2}$ estimated by perturbation theory and renormalization relationship.
- Bin integrated scattering probability $F_{i+1/2}$ is the probability that a particle scatters with a cosine between μ_i and μ_{i+1}. This is tallied by finding the ratio of scatters that do to total number of scatters.
- The Legendre moment f_ℓ is found by

$$f_\ell = \sum_{i'=0}^{N-1} F_{i'+1/2} P_\ell(\mu_{i'+1/2}) \left(\mu_{i'+1} - \mu_i'\right) .$$

Comments

- Unfortunately, a discretization of an otherwise continuous method had to be introduced.
- The default of 200 uniform cosine bins is provided, but can be replaced with a custom binning.
- Worked well for verification tests, but **user beware!**
- With Legendre moments, "negative scattering probability" is technically allowed, but not so in Monte Carlo, so Legendre moments may not match data.
- Should be a small effect for well-resolved data using enough Legendre moments to describe PDF in NJOY.
- This capability is **not** in MCNP6.1, but should be in the next release.

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Results

- 22 Benchmarks from the ICSBEP selected to cover a range of spectra, fissile materials, bare/reflected, lattice/solution, etc. (see paper for full list).
- Calculations use ENDF/B-VII.1 data.
- Only free-gas scattering considered, no thermal scattering $S(\alpha, \beta)$ distributions.

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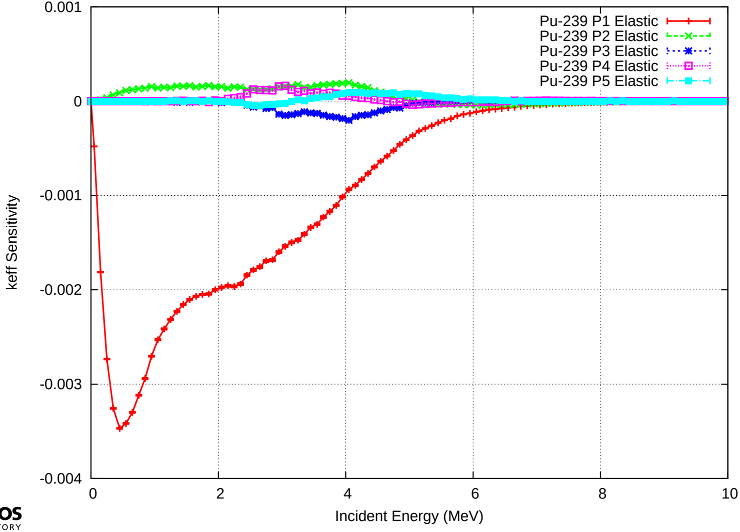
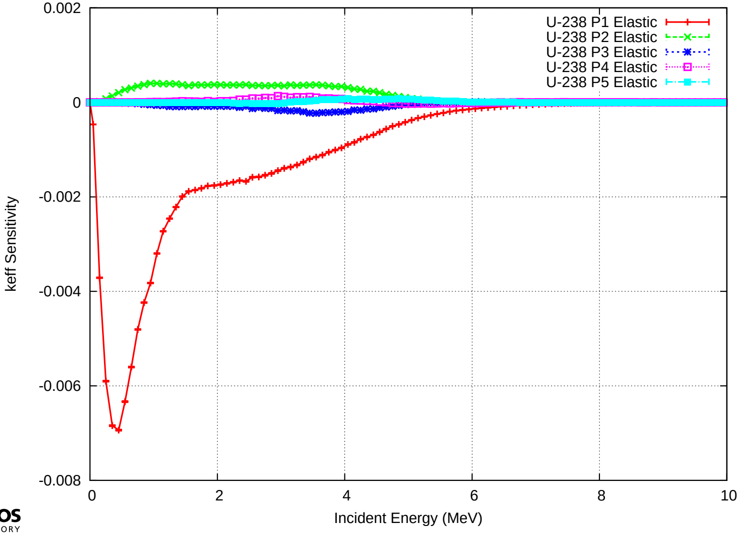
Jezebel ^{239}Pu Elastic Moment Sensitivity



Flattop (HEU) ^{238}U Elastic Moment Sensitivity



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Results: HEU Metal, Bare vs. Reflected

		P_1	P_2	P_3	P_4	P_5
hmf-001	^{235}U	-0.1040	0.0040	0.0000	-0.0002	0.0005
hmf-004	^{1}H	0.0001	0.0000	0.0000	0.0000	0.0000
	^{16}O	-0.0102	0.0038	-0.0003	0.0000	0.0000
	^{235}U	-0.0505	0.0011	-0.0004	-0.0004	0.0015
hmf-028	^{235}U	-0.0388	0.0012	-0.0010	0.0005	0.0002
	^{238}U	-0.1107	0.0159	-0.0047	0.0014	0.0015
hmf-072	^{56}Fe	-0.0172	0.0010	0.0004	0.0002	0.0001
	^{235}U	-0.0084	0.0005	-0.0003	0.0008	-0.0001
hmi-006	C	-0.0126	0.0018	-0.0001	0.0000	0.0000
	^{235}U	-0.0031	0.0011	-0.0006	0.0001	0.0001

Results: Pu Metal, Bare vs. Reflected

		P_1	P_2	P_3	P_4	P_5
pmf-001	^{239}Pu	-0.0896	0.0055	-0.0038	0.0022	0.0013
pmf-002	^{239}Pu	-0.0722	0.0039	-0.0031	0.0022	0.0009
	^{240}Pu	-0.0152	0.0004	-0.0017	0.0015	0.0001
pmf-006	^{238}U	-0.1314	0.0276	-0.0091	0.0027	0.0011
	^{239}Pu	-0.0342	0.0009	-0.0020	0.0021	0.0002
pmf-018	^{9}Be	-0.0417	0.0128	-0.0014	0.0001	0.0000
	^{239}Pu	-0.0512	0.0018	-0.0026	0.0017	0.0009

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Results: ^{233}U and ^{237}Np Metal, Bare vs. Reflected

		P_1	P_2	P_3	P_4	P_5
umf-001	^{233}U	-0.0988	0.0065	-0.0011	-0.0001	0.0013
umf-004	^{182}W	-0.0142	0.0015	0.0003	0.0002	-0.0003
	^{183}W	-0.0068	0.0003	0.0005	-0.0001	-0.0001
	^{184}W	-0.0166	0.0017	0.0004	0.0004	-0.0004
	^{186}W	-0.0177	0.0022	0.0003	0.0005	-0.0005
	^{233}U	-0.0677	0.0030	-0.0010	0.0007	0.0010
smf-008	^{235}U	-0.0818	0.0020	-0.0011	-0.0000	0.0008
	^{237}Np	-0.0031	-0.0000	-0.0004	0.0003	0.00001

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Results: Thermal Lattices

		P_1	P_2	P_3	P_4	P_5
lct-008	^{1}H	0.0000	0.0000	0.0000	0.0000	0.0000
	^{16}O	-0.0014	-0.0001	-0.0001	0.0000	0.0000
	^{235}U	-0.0000	-0.0001	-0.0000	-0.0000	0.0000
	^{238}U	-0.0023	0.0002	-0.0009	0.0002	0.0001
mct-001	^{1}H	0.0003	-0.0000	0.0000	0.0000	0.0000
	^{16}O	-0.0096	0.0017	0.0000	-0.0000	0.0000
	^{238}U	-0.0027	-0.0003	-0.0001	0.0005	0.0001
	^{239}Pu	-0.0004	0.0000	-0.0002	0.0001	-0.0000
uct-002	^{1}H	0.0004	0.0000	0.0000	0.0000	0.0000
	^{16}O	-0.0117	0.0015	-0.0000	-0.0000	0.0000
	^{232}Th	-0.0132	0.0014	-0.0014	0.0011	-0.0001
	^{235}U	-0.0004	-0.0001	0.0001	0.0000	-0.0000

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Results: Thermal Solutions

		P_1	P_2	P_3	P_4	P_5
hst-013	^{1}H	0.0004	0.0000	0.0000	0.0000	0.0000
	^{16}O	-0.0060	0.0012	0.0000	0.0000	-0.0000
	^{235}U	0.0000	0.0000	0.0000	0.0000	0.0000
lst-002	^{1}H	0.0002	0.0000	0.0000	0.0000	0.0000
	^{16}O	-0.0053	0.0004	-0.0000	-0.0000	0.0000
	^{235}U	-0.0000	0.0000	0.0000	0.0000	0.0000
	^{238}U	-0.0004	-0.0003	0.0000	0.0001	0.0000
pst-009	^{1}H	0.0001	0.0000	0.0000	0.0000	0.0000
	^{16}O	-0.0026	0.0001	0.0001	-0.0000	0.0000
	^{239}Pu	-0.0000	0.0000	0.0000	0.0000	0.0000

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Observations

- Elastic scattering distributions tend to have a larger effect in fast systems over thermal systems (about an order of magnitude).
- Isotopes in bare systems or those in reflectors tend to be important.
- Moments higher than P_1 are rarely important.
- P_1 moments appear to have a negative effect (in finite systems) because increasing P_1 means more forward scattering and more leakage.
- Anisotropy in ^{1}H (the best and most common moderator) never appears to matter.

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Elastic vs. Inelastic

- P_1 inelastic scattering distribution sensitivities are typically 1-2 orders of magnitude less than elastic.
- Higher inelastic moments were always insignificant.
- Likely from much smaller cross section and the fact much inelastic scattering is isotropic.

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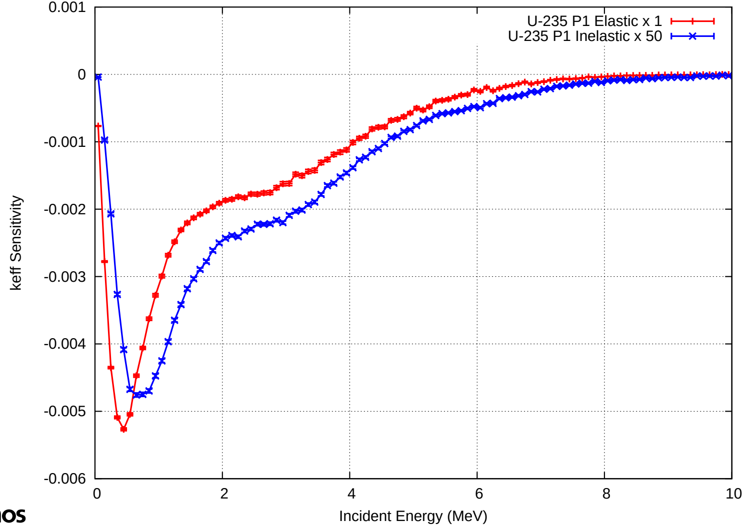
Elastic vs. Inelastic (Godiva, HMF-001)



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Summary & Future Work

- Continuous-energy k-eigenvalue sensitivity capability in MCNP6 has been extended to find sensitivities of Legendre scattering moments – to be released in a future version.
- Several benchmarks studied across ICSBEP parameter space, and consistent trends observed.

- Perform uncertainty quantification for scattering moments.
- Research in way to remove or at least automate appropriate cosine grid.
- Investigate thermal scattering anisotropy.
- Apply to fusion experiments (fixed source) to see if higher moments/inelastic distributions matter.

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Questions?

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