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#### K-Eigenvalue Sensitivities of Secondary Distributions of Continuous-Energy Data

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May 8, 2013



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#### Abstract

MCNP6 has the capability to produce energy-resolved sensitivity profiles for secondary distributions (fission  $\chi$  and scattering laws). Computing both unconstrained and constrained profiles are possible. Verification is performed with analytic test problems and a comparison to TSUNAMI-3D, and the comparisons show MCNP6 calculates correct or consistent results. Continuous-energy calculations are performed for three fast critical experiments: Jezebel, Flattop, and copper-reflected Zeus. The sensitivities to the secondary distributions (integrated over chosen energy ranges) are of similar magnitude to those of many of the cross sections, demonstrating the possibility that integral experiments are useful for assessing the fidelity of these data as well.





# Introduction

- Overview
- Methodology
- Verification
- Critical Experiment Results
- Future Research and Development





- MCNP6 (versions Beta-3 and later) has the ability to compute sensitivity profiles in continuous-energy calculations.
- Results shown for cross sections and fission  $\nu$  in the previous talk.
- The capability may also compute sensitivity profiles for secondary distributions, fission  $\chi$  and scattering laws (this talk).





• Probability density of a neutron emerging with energy E and scattering cosine  $\mu$  given an incident energy E'.

# $f(E,\mu|E')$

- For scattering:  $f(E, \mu | E') = f(E' \rightarrow E, \mu)$ .
- For fission:  $f(E, \mu | E') = \chi(E' \to E)/4\pi$ .





# 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 (secondary distribution).
- 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:

$$\mathcal{S}_{k,x} = rac{\left\langle \psi^{\dagger}, (\lambda \mathcal{F}_x + \mathcal{S}_x - \Sigma_x) \psi 
ight
angle}{\left\langle \psi^{\dagger}, \lambda \mathcal{F} \psi 
ight
angle} .$$

- For secondary distributions (and fission  $\nu$ ),  $\Sigma_x = 0$ .
- For fission  $\chi$  only  $\lambda \mathcal{F}_{x}$  term is non-zero.
- For scattering laws only  $\mathcal{S}_x$  term is non-zero.





# **Physical Meaning and Normalization**

- The sensitivity of a secondary distribution gives the ratio of the relative change in effective multiplication k to a relative increase of the multiplicity of the secondary distribution.
- This is not a physically meaningful question!
- More sensible is to ask about increasing the probability of being emitted at outgoing energy E and direction cosine  $\mu$ .
- Since probability densities must be normalized, an increase somewhere must be offset by decreases elsewhere.





#### Renomalization

• The unnormalized sensitivity  $S_{k,f}$  must be renormalized to find the physically meaningful (normalized or constrained) sensitivity:

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

• MCNP must integrate over finite bins, so this becomes:

$$\hat{S}_{k,f,g,g',n} = S_{k,f,g,g',n} - f_{g,g',n}S_{k,f,g'}.$$

• Here  $f_{g,g',n}$  is averaged over incident energy and integrated over outgoing energy and cosine.





- Show that MCNP can compute secondary distribution sensitivities correctly.
- Two analytic problems (fission  $\chi$  and scattering law).
- Comparison with TSUNAMI-3D (fission  $\chi$  only).





# Analytic Test Case 1

• Infinite-medium, multigroup problem with following data:

g	$\sigma_t$	$\sigma_{c}$	$\sigma_f$	ν	$\chi$	$\sigma_{sg1}$	$\sigma_{sg2}$	$\sigma_{sg3}$
1	2	1/2	0	Ι	5/8	1	1/2	0
2	4	1	0	_	1/4	0	1	2
3	4	1/2	3/2	8/3	1/8	0	0	2

• Analytic solution for k:

$$k = \frac{\nu_3 \sigma_{f3} \sigma_{s23}}{\sigma_{R2} \sigma_{R3}} \left[ \frac{\sigma_{s12}}{\sigma_{R1}} \chi_1 + \chi_2 + \frac{\sigma_{R2}}{\sigma_{s23}} \chi_3 \right].$$

• Take derivatives of  $\chi$  and normalize to compute sensitivities.



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#### Analytic Test Case 1

	$S_{k,x}$						
x	Exact	MCNP6 Adjoint	C/E				
$\chi_1$	+5/12	$+0.4169 \pm 0.09\%$	1.001				
χ2	+1/3	$+0.3334\pm0.07\%$	1.000				
χз	+1/4	$+0.2497\pm0.06\%$	0.999				

	$\hat{S}_{k,x}$						
x	Exact	MCNP6 Adjoint	C/E				
$\chi_1$	-5/24	$-0.2080 \pm 0.12\%$	0.999				
χ2	+1/12	$-0.0834 \pm 0.28\%$	1.001				
χз	+1/8	$+0.1246\pm0.17\%$	0.997				



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# Analytic Test Case 2

• Infinite-medium, multigroup problem with following data:

g	$\sigma_t$	$\sigma_{c}$	$\sigma_f$	ν	$\chi$	$\sigma_{sg1}$	$\sigma_{sg2}$	$\sigma_{sg3}$	$\sigma_{sg4}$
1	3	1	0	-	1	1	1/2	1/4	1/4
2	4	1	0	-	0	0	2	1	0
3	4	2	0	-	0	0	0	1	1
4	6	3	2	12	0	0	0	0	1

• Analytic solution for k:

$$k = \left(\frac{\nu_4 \sigma_{f4} \sigma_{s1}}{\sigma_{R1} \sigma_{R2} \sigma_{R3} \sigma_{R4}}\right) \left[f_{14} \sigma_{R2} \sigma_{R3} + f_{34} \sigma_{s3} \left(f_{13} \sigma_{R2} + f_{12} f_{23} \sigma_{s2}\right)\right].$$

• Take derivatives of f and normalize to compute sensitivities.



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#### **Analytic Test Case 2**

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	$S_{k,x}$						
x	Exact	Adjoint	C/E				
<i>f</i> <sub>11</sub>	+1/2	$+0.504 \pm 1.5\%$	0.995				
f <sub>12</sub>	+1/5	$+0.199 \pm 1.1\%$	1.015				
f <sub>13</sub>	+1/5	$+0.203 \pm 1.1\%$	1.015				
<i>f</i> <sub>14</sub>	+3/5	$+0.598\pm0.4\%$	0.997				

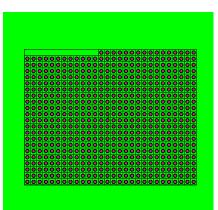
		$\hat{S}_{k,x}$							
	x	Exact	C/E						
	<i>f</i> <sub>11</sub>	-1/4	-0.257	$-0.250\pm0.1\%$	1.001				
	<i>f</i> <sub>12</sub>	-7/40	-0.180	$-0.175\pm0.1\%$	0.999				
~	<i>f</i> <sub>13</sub>	+1/80	+0.013	$+0.012\pm1.4\%$	0.994				
Los Alamos	<i>f</i> <sub>14</sub>	+33/80	+0.405	$+0.413\pm0.1\%$	1.000				





# **MOX Lattice Benchmark**

- Array of mixed-oxide (MOX) fuel pins submerged in water.
- ENDF/B-VII.0 data used, 238-energy bins equivalent to SCALE multigroup library.

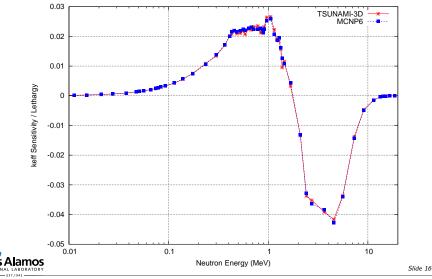




Slide 15



## MOX Lattice: Pu-239 Fission $\chi$



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# **Critical Experiment Results**

- Jezebel
- Flattop (HEU Core)
- Copper-Reflected Zeus





#### **Jezebel**

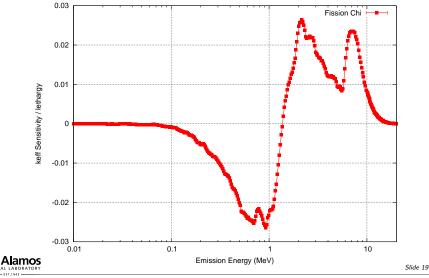
• Plutonium critical experiment at LASL in 1950's:







#### Jezebel: Pu-239 Fission $\chi$

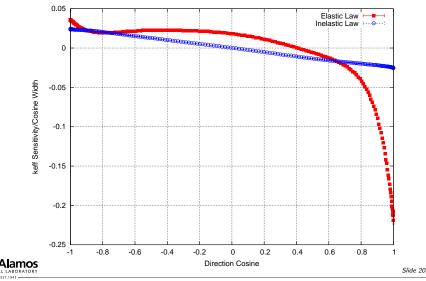


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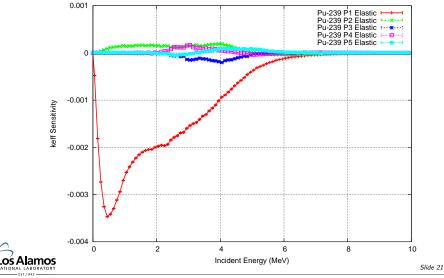
#### Jezebel: Pu-239 Scattering Laws



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#### Jezebel: Pu-239 Elastic Legendre Moments



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# Flattop (HEU Core)

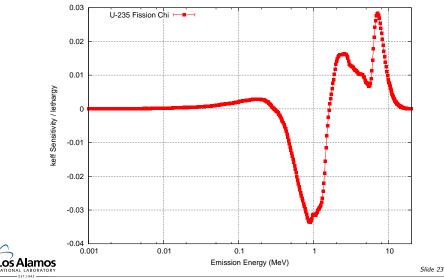
• HEU sphere reflected by natural uranium:







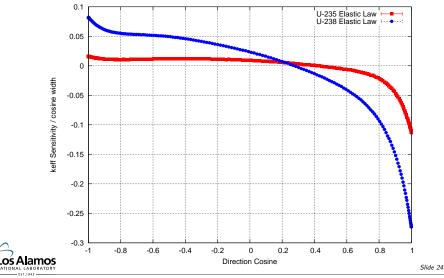
# Flattop: U-235 Fission $\chi$



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# Flattop: U-235/238 Elastic Laws



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#### **Copper-Reflected Zeus**

• HEU plates surrounded by a copper reflector:



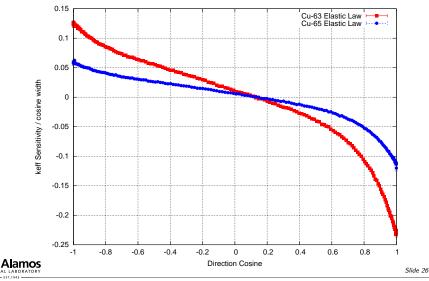


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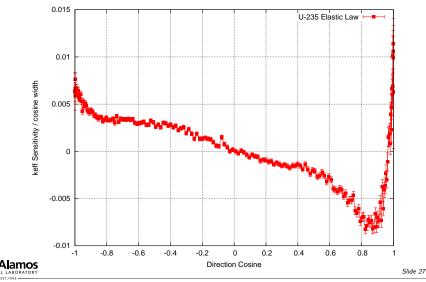
#### Zeus: Cu Elastic Scattering Law Sensitivity



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#### Zeus: U-235 Elastic Scattering Law Sensitivity



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## **Summary and Future Work**

- Continuous-energy *k*-eigenvalue sensitivity capability currently available in MCNP6.
- In addition to cross sections, may compute sensitivities to fission  $\chi$  and scattering laws.
- Verification results show good agreement.
- Results obtained for fast critical experiments.
- Estimate uncertainties with covariance data (effort underway).
- Other responses, fixed source and eigenvalue.





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