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Methodology, Verification, and Performance of the Continuous-Energy Nuclear Data Sensitivity Capability in MCNP6

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May 8, 2013

Abstract

A continuous-energy sensitivity coefficient capability has been introduced into MCNP6. The methods for generating energy-resolved and energy-integrated sensitivity profiles are discussed. Results from the verification exercises that were performed are given, and these show that MCNP6 compares favorably with analytic solutions, direct density perturbations, and comparisons to TSUNAMI-3D and MONK. Run-time and memory requirements are assessed for typical applications, and these are shown to be reasonable with modern computing resources.

Introduction

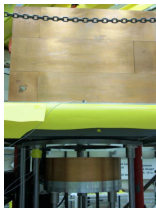
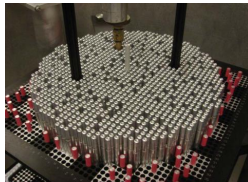
- Overview
- Methodology
- Verification
- Performance
- Future Research and Development

Motivation

- Safe operations involving fissionable material require criticality safety considerations.
- Criticality safety often involves a reliance on computer software (e.g., MCNP, KENO, etc.).
- A computer code is only as good as its nuclear data and validation to benchmarks.
- Question: How can we know if our validation suite covers a specific application?

Motivation

- Answer: Sensitivity analysis tools coupled with engineering judgment.



Development

- Goal: Create a continuous-energy sensitivity tool in MCNP for effective multiplication k .
- Design Philosophy and Goals:
- Use proven adjoint-based methods (linear-perturbation theory) found in SCALE/TSUNAMI.
- Robust design geared toward making it easy for engineers to get the right answer.
- Simple user interface; should be explainable in half-day of an MCNP class.
- Good performance (speed and memory requirements), good parallel scaling (MPI + OpenMP).

Development

- A new method should only be released for production if it has been extensively tested as part of the development process.
- Testing Plan:
- Comparisons with analytic solutions where possible.
- Direct density perturbations.
- Code comparisons with standard calculational benchmarks (TSUNAMI, MONK).
- CPU speed and memory requirement analysis.

Status

- Capability developed intermittently in 2010 and 2011, with completed prototype in Spring 2012.
- First released in MCNP6-Beta3 in Early 2013 (Available now from RSICC).
- Will be included in first production release of MCNP6 (Coming soon!)
- Already being taught with MCNP Criticality Class.

B.C. Kiedrowski, F.B. Brown, "Adjoint-Based k -Eigenvalue Sensitivity Coefficients to Nuclear Data Using Continuous-Energy Monte Carlo," *Nucl. Sci. Engr.*, **174** (3), in publication (2013).

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

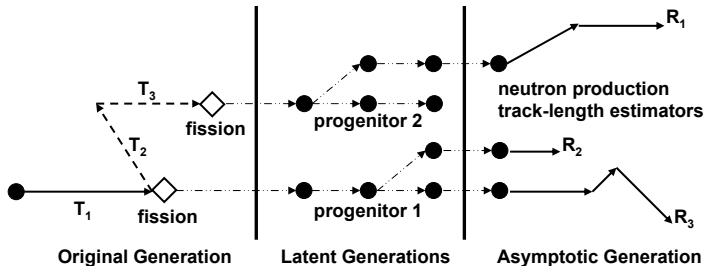
- Derive an integral expression for sensitivity coefficient using linear-perturbation theory:

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

- 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.



Forward Tally Scores

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

- At source emission, add expected-value collision estimator for fission source term.
- For each neutron trajectory, subtract track-length estimator for Σ_x term.
- Following each collision, add analog collision estimator for scattering source term.

Analytic Test Case

- Infinite-medium, multigroup problem with following data:

g	σ_t	σ_c	σ_f	ν	χ	σ_{sg1}	σ_{sg2}	σ_{sg3}
1	2	1/2	0	–	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 to compute sensitivities.

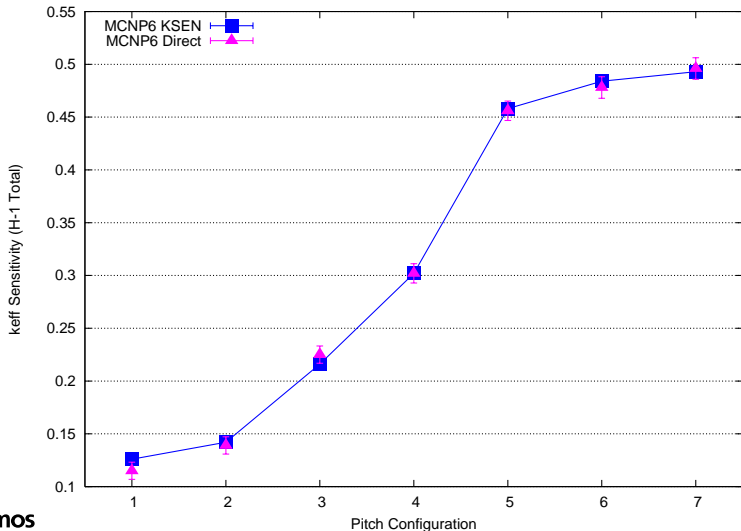
Analytic Test Case Results

x	Exact $S_{k,x}$	MCNP6 $S_{k,x}$	C/E
σ_{c1}	$-5/24$	$-0.20868 \pm 0.10\%$	1.002
σ_{c2}	$-1/4$	$-0.24993 \pm 0.07\%$	0.999
σ_{c3}	$-1/4$	$-0.24985 \pm 0.05\%$	0.999
σ_{s12}	$+5/24$	$+0.20810 \pm 0.16\%$	0.999
σ_{s23}	$+1/4$	$+0.25083 \pm 0.15\%$	1.003
σ_{f3}	$+1/4$	$+0.25045 \pm 0.16\%$	1.002
ν_3	$+1$	$+1.00000 \pm 0.00\%$	1.000

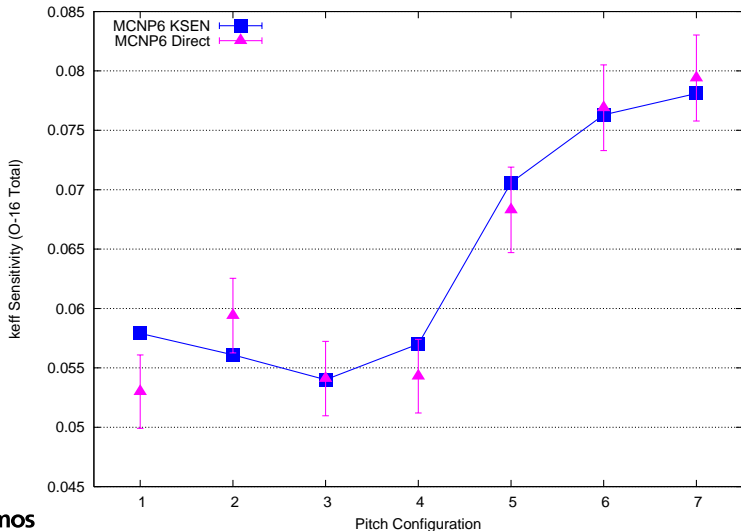
Direct Density Perturbations

- Infinite array of MOX fuel pins, varied pitches, ENDF/B-VII.0 CE data.
- Vary concentrations of H-1, O-16, U-238, and Pu-239 and compute sensitivity coefficients from k obtained from two separate calculations.
- Compare with MCNP6 total cross section sensitivity estimate.

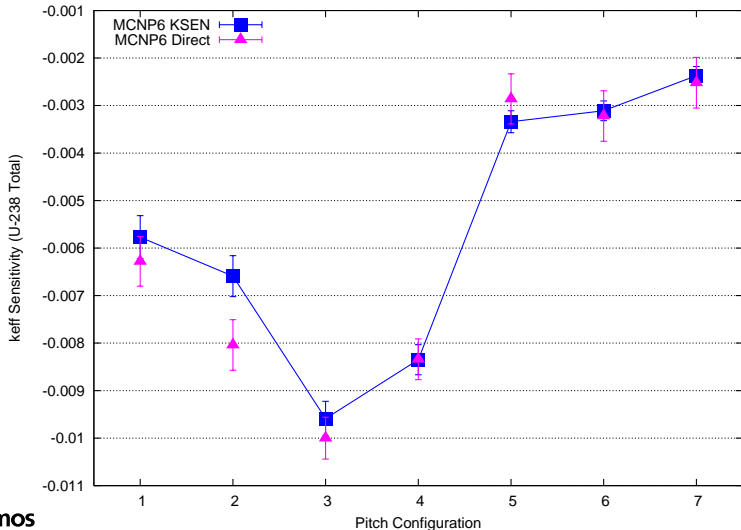
Infinite Pin Array (H-1)



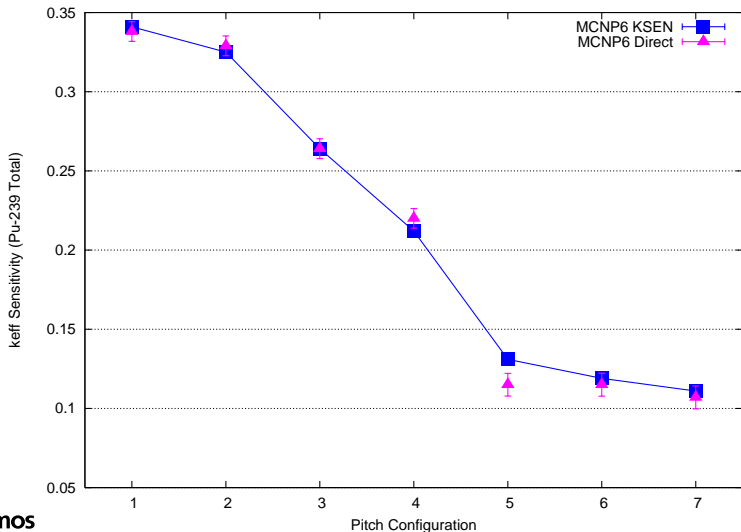
Infinite Pin Array (O-16)



Infinite Pin Array (U-238)



Infinite Pin Array (Pu-239)



Direct Density Results Analysis

- 28 results collected for four different isotopes, seven different pitch configurations covering different levels of moderation.
- 26 out of 28 agree within $2\text{-}\sigma$, which is expected for this sample size.

Software Comparisons

- Results obtained for MCNP6, TSUNAMI-3D (Multigroup Adjoint), and MONK (Continuous-Energy Differential Operator) for two different computational benchmarks.
- Benchmark 1: LEU and IEU spheres with mixtures of UF_4 and Polyethylene.
- Benchmark 2: 3-D MOX lattice benchmark (MCT-001-001).

MCNP-TSUNAMI Comparison: Poly Spheres

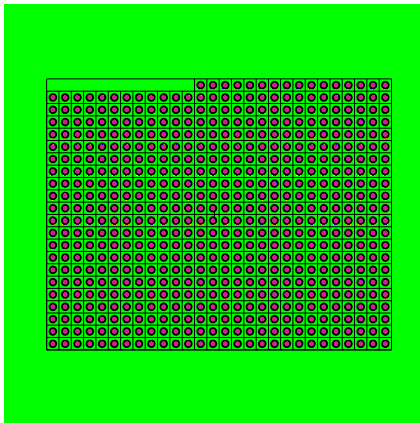
Sphere	Isotope	MCNP6	TSUNAMI-3D	C/E
LEU	^1H	$+2.40 \times 10^{-1}$	$+2.41 \times 10^{-1}$	1.00
	C	$+2.74 \times 10^{-2}$	$+2.77 \times 10^{-2}$	0.99
	^{19}F	$+4.38 \times 10^{-2}$	$+4.56 \times 10^{-2}$	0.96
	^{235}U	$+2.53 \times 10^{-1}$	$+2.53 \times 10^{-1}$	1.00
	^{238}U	-2.01×10^{-1}	-1.95×10^{-1}	1.03
IEU	^1H	$+4.54 \times 10^{-1}$	$+4.55 \times 10^{-1}$	1.00
	C	$+6.54 \times 10^{-2}$	$+6.60 \times 10^{-2}$	0.99
	^{19}F	$+1.18 \times 10^{-1}$	$+1.19 \times 10^{-1}$	0.99
	^{235}U	$+1.30 \times 10^{-1}$	$+1.26 \times 10^{-1}$	1.03
	^{238}U	-1.57×10^{-3}	$+1.35 \times 10^{-3}$	-1.16

MCNP-MONK Comparison: Poly Spheres

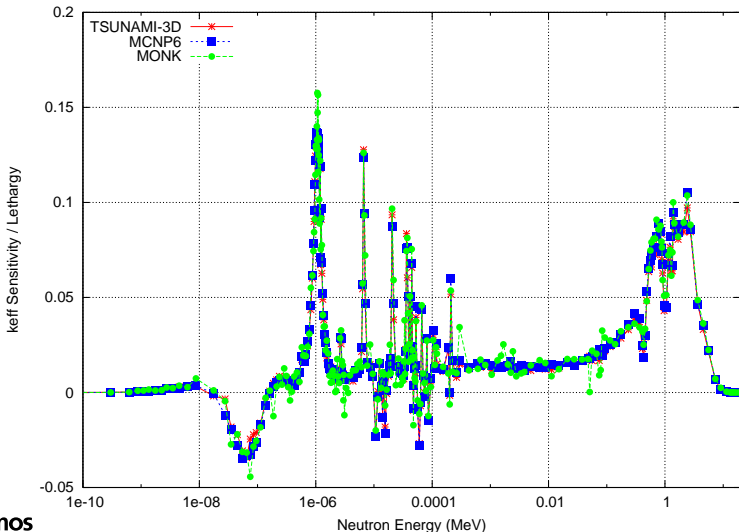
Sphere	Isotope	MCNP6	MONK	C/E
LEU	^1H	$+2.40 \times 10^{-1}$	$+2.45 \times 10^{-1}$	0.98
	C	$+2.74 \times 10^{-2}$	$+2.77 \times 10^{-2}$	0.99
	^{19}F	$+4.38 \times 10^{-2}$	$+4.20 \times 10^{-2}$	1.04
	^{235}U	$+2.53 \times 10^{-1}$	$+2.58 \times 10^{-1}$	0.98
	^{238}U	-2.01×10^{-1}	-2.01×10^{-1}	1.00
IEU	^1H	$+4.54 \times 10^{-1}$	$+4.52 \times 10^{-1}$	1.00
	C	$+6.54 \times 10^{-2}$	$+6.61 \times 10^{-2}$	0.99
	^{19}F	$+1.18 \times 10^{-1}$	$+1.15 \times 10^{-1}$	1.03
	^{235}U	$+1.30 \times 10^{-1}$	$+1.36 \times 10^{-1}$	0.96
	^{238}U	-1.57×10^{-3}	-1.30×10^{-3}	1.21

MOX Lattice Benchmark

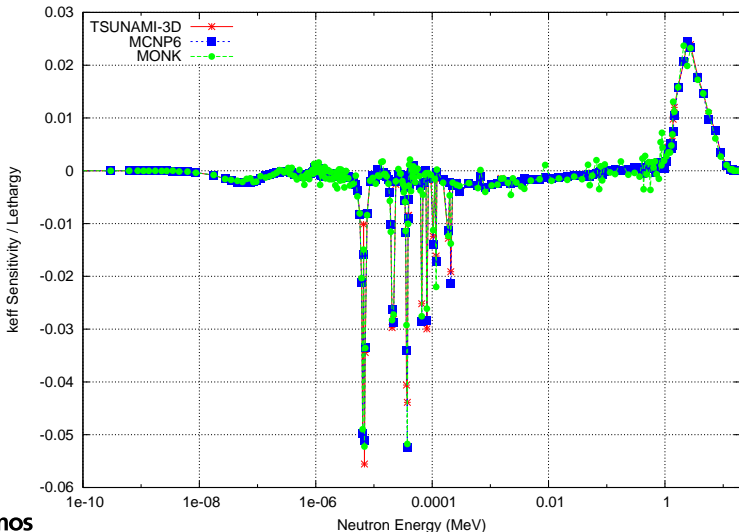
- Array of mixed-oxide (MOX) fuel pins submerged in water.
- ENDF/B-VII.0 data used, 238-energy bins equivalent to SCALE multigroup library.



MOX Lattice: H-1 Elastic



MOX Lattice: U-238 Total



Software Performance

- Even the most accurate, easiest to use method is not useful if it cannot run in a reasonable amount of time or has unreasonable memory requirements.
- Check runtime with polyethylene sphere benchmark.
- Check memory usage with the MOX lattice benchmark.

Runtime Tests

- Use polyethylene sphere benchmark.
- Intel Xeon E5-2670 processors at 2.6 GHz with 32 GB RAM, 16 OpenMP threads.
- For a few dozen sensitivities, 5-10% slowdown (relative to no sensitivities) is observed.
- For several 10,000's (63,335 to be precise), slowdowns of a factor of 3-5 are observed.

	Time (min)	
	Base	Sensitivity
LEU	9.9	41.5
IEU	4.3	14.7

Memory Usage Tests

- The tagging and storing of forward reaction rates can be very costly in memory.
- Since arrays are very sparse, MCNP employs a linked-list approach to store only what information is needed.
- Test is MOX Lattice with 1.64 million sensitivities, batch size of 50,000 neutrons.
- Quad-Core AMD Opteron model 8354 at 2.2 GHz or model 8356 at 2.3 GHz, 16 OpenMP threads.
- Theoretical memory requirement: 615 GB.
- Actual memory requirement: 10 GB (98% savings).

Summary

- Continuous-energy k -eigenvalue sensitivity capability currently available in MCNP6.
- Implementation and software design was done with ease of use in mind.
- Verification results show good agreement.
- Runtime and memory usage requirements appear to be reasonable.

Future Work

- Secondary distributions (next talk).
- Estimate uncertainties with covariance data (effort underway).
- Other responses, fixed source and eigenvalue.

Acknowledgments

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 - James Dryda (AWE)

Questions?
