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Continuous-Energy Sensitivity Coefficient Capability in MCNP6

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INTRODUCTION

Monte Carlo software packages have been used for computing sensitivity coefficients to k_{eff} for uncertainty analysis for several years [1]. To date most implementations, such as those found in TSUNAMI-3D [2], have used multigroup cross section data. This presents several difficulties involving group collapse, self shielding, and the calculation of so-called implicit sensitivity coefficients. Because of these complications, and the desire for higher fidelity with a simpler work flow, there has been a push within the US DOE/NNSA Nuclear Criticality Safety Program to develop continuous-energy sensitivity coefficient capabilities.

Such a capability, based on adjoint methodologies that are employed in TSUNAMI-3D, has been developed in MCNP6 [3] and will be released with the production version. Also included in MCNP6 is a related capability, called KPERT, for adjoint-weighted perturbations from material substitutions, which have been employed for sensitivity coefficient calculations in previous work [4]. While this work does, in theory, allow for more general perturbations, it introduces an approximation in the handling of scattering laws that leads to large and unacceptable deviations in scattering sensitivities. Additionally, the interface is designed with the intent for material substitutions, and using it for sensitivity coefficient calculations may be cumbersome to some users.

For these reasons, a similar capability, called KSEN, that is more accurate and efficient, and easier to use than KPERT for this purpose, has been developed. The details of the Monte Carlo implementation and the associated tallies are discussed. Verification of the capability is performed by comparing results of TSUNAMI-3D and other methods using the OECD/NEA Sensitivity Phase III Benchmarks [5].

MCNP6 KSEN METHOD

The method for calculating sensitivity coefficients in MCNP6 employs the adjoint-based methodology that is used in TSUNAMI-3D. First the equation governing the adjoint-based method is explained, and then the tallies employed in MCNP6 are discussed.

Governing Equation

The sensitivity coefficient of k to nuclear data x^j (x is a cross section, nubar, etc. and j is a specific isotope) may be found by

$$S^j_{k,x} = \frac{\left\langle \psi^\dagger, \mathcal{P}^j_x \psi \right\rangle}{\left\langle \psi^\dagger, \lambda \mathcal{F} \psi \right\rangle}, \tag{1}$$

where ψ is the forward flux and $\psi^\dagger$ is its adjoint, $\lambda = 1/k$, $\mathcal{P}^j_x$ is the perturbation operator for x^j that will be defined, $\mathcal{F}$ is the total fission operator, and the brackets denote integration over all space, angle, and energy variables. The perturbation operator $\mathcal{P}^j_x$ is

$$\mathcal{P}^j_x = -N^j x^j \delta_{xt} + \mathcal{S}^j_x + \lambda \mathcal{F}^j_x, \tag{2}$$

where N^j is the local atomic density of isotope j, δ_{xt} is a Kronecker delta that is one if x is a cross section (e.g., radiative capture) and zero otherwise (e.g., fission χ), $\mathcal{S}^j_x$ is the scattering operator for x^j exclusively, and $\mathcal{F}^j_x$ is the total fission operator for x^j exclusively. Note that if the scattering or fission are not involved in x, then $\mathcal{S}^j_x$ and/or $\mathcal{F}^j_x$ are zero. Otherwise, the modified scattering operator, for example, uses the double-differential scattering cross section for x^j rather than the total double-differential scattering cross section in the regular transport equation.

Tallies and Scoring

As seen from Eqs. (1) and (2), there are adjoint-weighted tallies involving total interactions, scattering, and fission for x^j and one for the adjoint-weighted fission source in the denominator – a total of four, but, in practice, only one is needed because the three tallies in the numerator can be combined and the denominator does not require any extra storage. MCNP6 uses the Iterated Fission Probability methodology [6] to compute adjoint-weighted tallies. Briefly, the method is a forward simulation involving recording contributions to tallies that are to be adjoint weighted and associating neutrons, which are tagged, with them. These neutrons and their progeny are followed through fission generations in a standard Monte Carlo criticality calculation, and then the total population of those neutrons caused by each of the original neutrons is found in some distant generation (usually after ten generations). This total (asymptotic) population is an estimate of the adjoint or importance weight, and is multiplied by the corresponding original contributions to form a score for an adjoint-weighted tally.

The total interaction term is computed by a track-length estimator. For each simulated Monte Carlo track,

$$N^j x^j \delta_{xt} \ell, \tag{3}$$

(ℓ is the length of the track) is subtracted from, because this represents a net loss in neutrons, the original contribution.

At each collision where a non-fission secondary emerges, the reaction z (e.g., elastic scattering) occurs with some isotope i. In theory, the tally that can be scored is the ratio of the double-differential scattering cross section for all x^j for the energy and direction change that occurred to the corresponding total double-differential scattering cross section. For most scattering reactions, however, such as elastic scattering with a stationary target or inelastic level scattering, the double-differential scattering cross section involves a Dirac delta function, and the ratio is one if $x = z$ and $j = i$ and zero otherwise. While other scattering reactions may have ratios between zero and one, often times these are difficult and time consuming to compute in practice, and therefore

$$\delta_{xz} \delta_{ji} \tag{4}$$

is added for each collision (one if $x = z$ and $j = i$ and zero otherwise). On average, both are the same. In other words, MCNP6 uses the analog approach, whereas the other possibility is the expected value approach.

The fission term is calculated for each source emission. Since the fission process is continuous in energy transfer and the direction of emission is isotropic, it makes more sense to perform expected value scoring. For each fission source neutron, the incident and outgoing energies are stored, and for each reaction and isotope for which a sensitivity coefficient is desired,

$$\frac{\chi^j \nu^j \Sigma_f^j \delta_{xf}}{\chi \nu \Sigma_f}, \tag{5}$$

where δ_{xf} is a Kronecker delta for whether x is involved in the fission process, and the term in the denominator is the total $\chi\nu\Sigma_f$ for all isotopes (whether involved in the sensitivity coefficients or not) is added to the accumulator.

The denominator term does not require storing any information that is not already being computed. Simply finding the average of total asymptotic populations of all neutrons gives λ times the adjoint-weighted fission source.

Once the asymptotic populations are known from the forward simulation, they are multiplied by the corresponding contributions for the numerator and divided by the result of the denominator. This gives an estimate for each $S_{k,x}$, which is the tally score. The average of these, for a large number of scores, should converge to the true sensitivity coefficient for a given set of inputs.

It is observed [7] that the memory requirements for this technique can be very high when a large number of sensitivity coefficients (such as those involving a fine energy group) are desired. Having realized this and observing the fact that the arrays for each original neutron tend to be very sparse, the MCNP6 developers employed special handling for such sparse data that only stores what is needed. For many problems, this reduces memory requirements by a factor of 10-100, and also increases parallel scaling because less data must be transferred over the network.

RESULTS

Comparisons are made to the OECD/NEA Phase III Sensitivity benchmarks. The benchmark has three cases, and cases 1 and 3 are presented here. Case 1 is a finite square lattice of MOX fuel pins reflected by water. Case 3 contains two spheres of UF_4 mixed with polyethylene, one with low-enriched (2%) uranium and the other for intermediate-enriched (50%) uranium. All MCNP6 calculations use ENDF/B-VII.0 nuclear data.

MOX Lattice Benchmark

The MOX Lattice Benchmark is based on a specification in the ICSBEP Handbook, MIX-COMP-THERM-001-001 [8]. For this Benchmark case, four approximate models are specified: Cartesian lattice with a detailed 3-D pin representation, Cartesian homogenized, cylindrical homogenized, and an infinite array of MOX pins.

For this summary, only the first of these (the detailed 3-D model) is used. Energy integrated sensitivity coefficients are computed for each isotope in the problem for the following nuclear data: total, n,γ capture, elastic scattering, inelastic scattering (discrete level plus continuum), fission, n,2n, and fission ν. The ten most sensitive nuclear data (except for the totals) are given in Table I. This ranking and the relative magnitudes compare favorably to those found in Ref. [5] .

Table II lists the total and scattering (elastic plus inelastic) sensitivities of all isotopes where the total cross section has a sensitivity greater than 0.001. The agreement with the Benchmark results of the other participants is less clear. Ref. [5] compares S_{k,σ_t} for ^{1}H , ^{238}U , and ^{239}Pu , and S_{k,σ_s} for ^{238}U . The results are obtained from several codes using various different nuclear data libraries. The S_{k,σ_t} largely agree for ^{1}H and ^{239}Pu , and S_{k,σ_s} for ^{238}U is mostly in line with the other participants. The benchmark results for S_{k,σ_t} of ^{238}U show much dispersion, and the MCNP6 predicted results seem low in magnitude comparatively. One thing to note, however, is that the MCNP6 results agree most with those from MONK, which used the differential operator approach with continuous energy, but used JEF-2.2 data, complicating the comparisons. This discrepancy merits more investigation, and it is difficult at the current time to draw firm conclusions.

Table I. Dominant Nuclear Data for MOX Lattice Benchmark

x^j		$S^j_{k,x}$
^{239}Pu	ν	$+0.9248 \pm 0.00\%$
^{1}H	σ_{el}	$+0.4145 \pm 0.27\%$
^{239}Pu	σ_f	$+0.3777 \pm 0.02\%$
^{239}Pu	σ_γ	$-0.2610 \pm 0.02\%$
^{16}O	σ_{el}	$+0.0860 \pm 0.29\%$
^{1}H	σ_γ	$-0.0799 \pm 0.05\%$
^{240}Pu	σ_γ	$-0.0590 \pm 0.04\%$
^{238}U	σ_γ	$-0.0502 \pm 0.04\%$
^{241}Pu	ν	$+0.0283 \pm 0.03\%$

Table II. Significant Total and Scattering Sensitivities of MOX Lattice Benchmark

	S_{k,σ_t}	S_{k,σ_s}
^{1}H	$+0.3346 \pm 0.21\%$	$+0.4145 \pm 0.27\%$
^{16}O	$+0.0854 \pm 0.29\%$	$+0.0873 \pm 0.40\%$
^{52}Ni	$+0.0011 \pm 3.15\%$	$+0.0019 \pm 1.85\%$
^{53}Ni	$-0.0016 \pm 1.61\%$	$+0.0004 \pm 6.47\%$
^{55}Mn	$-0.0016 \pm 2.12\%$	$+0.0006 \pm 6.00\%$
^{56}Fe	$-0.0026 \pm 3.82\%$	$+0.0080 \pm 1.24\%$
^{58}Cr	$-0.0015 \pm 3.56\%$	$+0.0016 \pm 2.72\%$
^{95}Mo	$-0.0013 \pm 0.79\%$	$+0.0002 \pm 5.29\%$
^{235}U	$+0.0026 \pm 0.43\%$	$+0.0001 \pm 10.13\%$
^{238}U	$-0.0099 \pm 1.27\%$	$+0.0224 \pm 0.54\%$
^{239}Pu	$+0.1198 \pm 0.12\%$	$+0.0031 \pm 1.84\%$
^{240}Pu	$-0.0540 \pm 0.06\%$	$+0.0011 \pm 2.15\%$
^{241}Pu	$+0.0075 \pm 0.16\%$	< 0.0001
^{242}Pu	$-0.0020 \pm 0.28\%$	< 0.0001
^{241}Am	$-0.0068 \pm 0.08\%$	< 0.0001

UF_4 in Polyethylene Spheres

Case 3 of the Benchmark are homogeneous mixtures of UF_4 and polyethylene. There are two subcases: one with 2% enriched uranium (LEU subcase), and the other with 50% enriched uranium (IEU subcase). This problem is based on the test problem in Ref. [1].

Like with the previous case, energy-integrated sensitivities to various nuclear data are generated. The sensitivities to the total, scattering, and capture cross sections for both subcases are given in Table III, and appear to be in line with what other benchmark participants calculate.

Table III. Sensitivities for Isotopes in UF_4-Polyethylene Spheres

	LEU	IEU
S_{k,σ_t}		
^{1}H	$+0.2412 \pm 0.79\%$	$+0.4532 \pm 0.16\%$
^{nat}C	$+0.0278 \pm 2.12\%$	$+0.0656 \pm 0.44\%$
^{19}F	$+0.0432 \pm 1.61\%$	$+0.1177 \pm 0.32\%$
^{235}U	$+0.2526 \pm 0.11\%$	$+0.1304 \pm 0.23\%$
^{238}U	$-0.2018 \pm 0.27\%$	$-0.0022 \pm 9.88\%$
S_{k,σ_s}		
^{1}H	$+0.3430 \pm 0.56\%$	$+0.4574 \pm 0.16\%$
^{nat}C	$+0.0285 \pm 2.07\%$	$+0.0659 \pm 0.45\%$
^{19}F	$+0.0484 \pm 1.44\%$	$+0.1195 \pm 0.32\%$
^{235}U	$+0.0004 \pm 18.04\%$	$+0.0273 \pm 0.69\%$
^{238}U	$+0.0416 \pm 1.27\%$	$+0.0409 \pm 0.52\%$
S_{k,σ_γ}		
^{1}H	$-0.1018 \pm 0.04\%$	$-0.0042 \pm 0.04\%$
^{nat}C	$-0.0007 \pm 0.13\%$	$-0.0001 \pm 0.34\%$
^{19}F	$-0.0053 \pm 0.09\%$	$-0.0021 \pm 0.09\%$
^{235}U	$-0.1124 \pm 0.11\%$	$-0.2101 \pm 0.03\%$
^{238}U	$-0.2785 \pm 0.04\%$	$-0.0587 \pm 0.06\%$

Calculations are also done to get energy-resolved sensitivity coefficients. The energy grid used is the same 238-group structure used by TSUNAMI-3D, to better facilitate comparison. Note that the techniques used in MCNP6 are continuous energy, and the results are integrated over each energy grid spacing. Figs. 1 and 2 show energy-resolved sensitivities for ^{1}H scatter and ^{238}U capture for the subcases. Currently, there are no comparison results; however, a feature of the LEU subcase shows scatter and capture roughly mirror each other in the resonance region. This demonstrates that scattering is particularly important for neutrons at ^{238}U resonance energies; this is because scattering increases the probability of resonance escape.

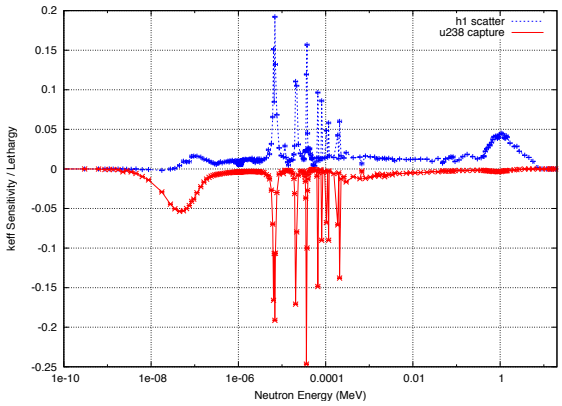

Fig. 1. Energy-resolved sensitivities for the LEU subcase.

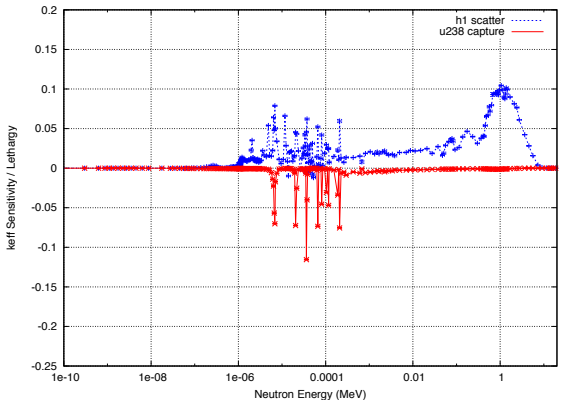

Fig. 2. Energy-resolved sensitivities for the IEU subcase.

CONCLUSIONS

A continuous-energy k sensitivity coefficient capability called KSEN has been implemented into MCNP6. Comparisons have been performed against two of the cases from the OECD/NEA Benchmark Phase III, and the results are generally favorable. Further work will need to be performed to continue validating this capability, however. Future research and development will focus on uncertainty propagation with ENDF covariance data. Another possible application is to apply these techniques to the calculation of temperature coefficients for reactor analysis.

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