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Verification of k-Eigenvalue Sensitivity Coefficient Calculations Using Adjoint-Weighted Perturbation Theory in MCNP

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INTRODUCTION

Using Monte Carlo methods to compute sensitivity coefficients for *k*-eigenvalue with respect to nuclear cross sections is important for applications in criticality safety such as burnup credit. Modifications to MCNP [1] (to be included in MCNP6) allow two flavors of perturbation theory using continuous-energy physics: the differential operator technique [2] and adjoint-weighted perturbation theory [3].

Previously, the only available method for computing sensitivity coefficients in MCNP was the differential operator technique. Misleading results may be produced with this approach [4]. The adjoint-weighted perturbation method appears, from empirical evidence, to typically (albeit not always) produce more reliable answers.

A method for computing sensitivity coefficients from the adjoint-weighted perturbation capability in MCNP6 is presented. Results of calculations are given and compared with equivalent calculations of simple analytic problems, a fine-mesh discrete ordinates calculation in PARTISN [5], and a fine-group calculation from TSUNAMI-3D [6]. The latter illustrates the need for further improvements in the continuous-energy methods.

COMPUTING SENSITIVITY COEFFICIENTS

The sensitivity coefficient for k (the effective multiplication factor) with respect to cross section σ_x is defined as

$$S_{k,\sigma_x} = \frac{\sigma_x}{k}\frac{dk}{d\sigma_x} \approx \frac{\sigma_x}{k}\frac{\Delta k}{\Delta\sigma_x}. \quad (1)$$

Using perturbation theory, it is possible to find a linear estimate of the change in reactivity $\Delta\rho$ times k, the unperturbed eigenvalue:

$$k\Delta\rho = -\frac{\left\langle \psi^\dagger, P\psi \right\rangle}{\left\langle \psi^\dagger, k^{-1}F\psi \right\rangle}. \quad (2)$$

The angular flux is ψ and the corresponding adjoint flux is $\psi^\dagger$. F is the operator for fission, and P is the operator for the perturbation:

$$P = \Delta\Sigma_t - \Delta S - k^{-1}\Delta F. \quad (3)$$

$\Delta\Sigma_t$ is the change (i.e. the defined perturbation) in the total macroscopic cross section, ΔS is the change in the scattering operator, and ΔF is the change in the fission operator.

The change in the cross section can be expressed as the unperturbed cross section times a factor f. Using that and the relationship

$$\Delta k = \frac{k^2\Delta\rho}{1-k\Delta\rho}, \quad (4)$$

Eq. (1) can be rewritten as

$$S_{k,\sigma_x} \approx \frac{1}{f}\frac{k\Delta\rho}{1-k\Delta\rho}. \quad (5)$$

In the limit as f goes to zero, Eq. (5) becomes exact. The parameter f is arbitrary and known, whereas $k\Delta\rho$ must be calculated. Details of calculating this with continuous-energy Monte Carlo using adjoint-weighted perturbation theory are given in [7].

Since $k\Delta\rho$ in Eq. (2) is linear with f, the value of f can be selected arbitrarily and $k\Delta\rho$ can be scaled as needed to converge Eq. (5). Currently, the continuous-energy version of the adjoint-weighted perturbations in MCNP does not account for changes in the scattering laws. Despite this, MCNP is often able to produce reliable perturbation results; however, a problem is illustrated where not accounting for this is likely the cause of discrepancies.

VERIFICATION & RESULTS

The method to compute $k\Delta\rho$ with respect to some perturbation, and, by extension, S_{k,σ_x}, is implemented in MCNP6. The user interface is

similar to the existing differential operator perturbation option that uses the PERT card. The adjoint-weighted perturbation feature uses an analogous KPERT card. The input formats are very similar by design.

For verification, analytic solutions are obtained for homogeneous, two-group, infinite-medium problems. Sensitivity coefficients to capture, fission, and group-to-group scatter cross sections are computed and compared to the corresponding analytic solutions. Next, adjoint-weighted perturbation theory is applied to a 30-group problem involving a sphere with a reflector. The total cross section in the reflector is perturbed and the result of MCNP6 is compared with an equivalent adjoint-weighted calculation in PARTISN. Finally, continuous-energy results are provided for sensitivities and compared with calculations from TSUNAMI-3D.

Analytic, Infinite-Medium Comparisons

Sensitivity coefficients are calculated for a two-group, infinite-medium problem (cross-section data given in Table I) for: the group-1 capture cross section, the group-2 capture cross section, the group-2 fission cross section, and the group 1-to-2 scattering cross section.

Table I. Cross-section data (cm^{-1}) for the two-group infinite-medium problem.

g	Σ_t	Σ_c	Σ_f	ν	χ	Σ_{sg1}	Σ_{sg2}
1	2	1/2	1/2	3/4	1	1/2	1/2
2	3	1	1	9/2	0	0	1

For this infinite-medium problem, the solution for k is

$$k = \frac{\nu\Sigma_{f1}}{\Sigma_{R1}} + \frac{\nu\Sigma_{f2}}{\Sigma_{R2}}\frac{\Sigma_{s12}}{\Sigma_{R1}}, \qquad (6)$$

where the removal cross section is $\Sigma_{Rg} = \Sigma_{tg} - \Sigma_{sgg}$. Analytic solutions for the sensitivity coefficients are found by taking appropriate derivatives of Eq. (6) and inserting them into Eq. (1).

Table II. Comparison of sensitivity coefficients for cross sections from MCNP6 with analytic solutions.

	Exact	**MCNP**	**C/R**
σ_{c1}	-1/3	-0.333323 +/- 0.000135	0.99997
σ_{c2}	-3/8	-0.374922 +/- 0.000195	0.99979
σ_{f2}	3/8	0.375192 +/- 0.000263	1.00051
σ_{s12}	5/12	0.416644 +/- 0.000214	0.99995

The analytic solutions and values computed by MCNP6 are given in Table II. Also provided is C/R, which is the calculated to the reference (or analytic) solution. The results all agree within 0.1% and are within statistical uncertainties.

Multigroup Reflector Density Sensitivity

The next problem [8] is a uranium-oxyfluoride sphere with an aluminum shell and a neutronically infinite water reflector. The sensitivity to the density (or, equivalently, the total cross section) of the reflector is calculated. The 30-group MENDF5 library is used for these calculations.

The sensitivity for the reflector density is computed by MCNP6 as 0.0160498 +/- 0.0004630 (2.9% relative error). For comparison, the result using first-order perturbation theory with PARTISN fluxes is 0.0157639. The two results agree within the 1-sigma confidence band of the MCNP6 result.

This result is within 6% of the direct result computed as a central difference from two independent PARTISN calculations, 0.01516. For comparison, the result computed by the differential operator technique differs by 66%. This is an example where the adjoint-weighted methods are significantly more accurate than the differential operator approach.

Continuous-Energy Comparison

MCNP can obtain results for continuous-energy sensitivity coefficients as well. Results are obtained for a homogeneous sphere containing hydrogen, carbon, fluorine, and low-enriched uranium (see [9]) and compared against those generated by a 238-energy group calculation using TSUNAMI-3D. The calculations are performed with ENDF-VI nuclear data with a light-water $S(\alpha, \beta)$ law.

Table III. Comparison of continuous-energy calculations in MCNP with fine-group calculations in TSNUNAMI-3D.

	TSUNAMI-3D	**MCNP**	**C/R**
Total	3.314×10^{-1}	3.173×10^{-1}	0.957
Capture	-5.081×10^{-1}	-5.019×10^{-1}	0.988
Fission	3.964×10^{-1}	3.978×10^{-1}	1.004
Elastic	4.115×10^{-1}	4.219×10^{-1}	1.025
Inelastic	2.950×10^{-2}	2.198×10^{-2}	0.745

The sensitivity coefficients for each major reaction type are given in Table III. All reactions agree within 5% except for inelastic scatter, which has a C/R of about 0.75. Further analysis shows that when the sensitivities are computed on a per-isotope basis, there is strong agreement for capture and

fission, but poor agreement for both elastic and inelastic scatter. Similar behavior is observed for the differential operator method in [4] except that elastic scatter in hydrogen agrees within 0.1%.

DISCUSSION & CONCLUSIONS

Using adjoint-weighted perturbation theory, MCNP can compute reactivity changes that can be used to calculate sensitivity coefficients of k with respect to some cross sections.

Comparing with analytic solutions and discrete ordinates calculations, it appears MCNP computes multigroup sensitivity coefficients correctly. For continuous-energy problems, there are demonstrated issues in problems where energy or direction transfer via scattering is an important effect. This arises because MCNP currently assumes uniform scattering when calculating the perturbation in the scattering source. Doing this more accurately with continuous-energy scattering laws remains a topic of current research.

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REFERENCES

1. X-5 MONTE CARLO TEAM, "MCNP – A General N-Particle Transport Code, Version 5 – Volume I: Overview and Theory," LA-UR-03-1987, Los Alamos National Laboratory (2003).
2. H. RIEF, "Generalized Monte Carlo Algorithms for Correlated Sampling and a Second-Order Taylor Series Approach," *Ann. Nucl. Energ.*, **11**, 455 (1984).
3. G.I. BELL and S. GLASSTONE, *Nuclear Reactor Theory*, Van Norstrand Reinhold, New York, New York (1970).
4. J.A. FAVORITE, "Eigenvalue Sensitivity Analysis Using the MCNP5 Perturbation Capability," *Proc. Nuclear Criticality Safety Division Topical Mtg.*, Richland, Washington, Sep. 13-17 (2009).
5. R.E. ALCOUFFE et al., "PARTISN: A Time-Dependent, Parallel Neutral Particle Transport Code System," LA-UR-08-7258, Version 5.89, Los Alamos National Laboratory (November 2008).
6. B.T. REARDEN, "TSUNAMI-3D: Control Module for Three-Dimensional Cross-Section Sensitivity and Uncertainty Analysis for Criticality," ORNL/TM-2005/39 Version 6, Oak Ridge National Laboratory (2009).
7. B.C. KIEDROWSKI, F.B. BROWN, and P.P.H. WILSON, "Calculating Kinetics Parameters and Reactivity Changes with Continuous-Energy Monte Carlo," *Proc. PHYSOR 2010*, Pittsburgh, Pennsylvania, May 9-14 (2010).
8. M. PITTS, F. RAHNEMA, and T.G. WILLIAMSON, "Water-Reflected 91-Liter Sphere of Enriched Uranium Oxyfluoride Solution," HEU-SOL-THERM-012 in *Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NSC/DOC(95)03 (2007).
9. B.T. REARDEN, "Perturbation Theory Eigenvalue Sensitivity Analysis with Monte Carlo Techniques," *Nucl. Sci. Eng.*, **146**, 367-382 (2004).