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# Second Order Perturbations of Monte Carlo Criticality Calculations

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## I. Introduction

Perturbation techniques are powerful tools for determining the effects of small changes, or perturbations, to a problem. Perturbations have long been problematic in Monte Carlo calculations because the effects of small changes to the problem are usually masked by the inherent statistical uncertainties.

The recently released MCNP4B<sup>1</sup> Monte Carlo computer code uses the differential operator technique<sup>2,3</sup> to calculate changes in tallies caused by perturbations in density and composition over given energy ranges and reaction types. This technique will allow for precise calculation of the changes in tallies even if the standard deviation of the unperturbed tally is larger than the change. The differential operator is approximated by a second order Taylor series. The implementation of the Taylor series expansion assumes that the coefficients are independent of any perturbed cross-sections. However, if the tally is multiplied by cross-section data this assumption is invalid and incorrect results will be generated.

Of significant interest is the use of perturbations in criticality calculations. Although the criticality source feature for MCNP cannot directly calculate perturbed eigenvalues, a track-length estimate for  $K_{eff}$  can be tallied and the perturbation feature can be applied to this tally. However, since this tally multiplies the flux by the macroscopic fission cross-section, this tally is dependent on perturbed cross-section data and incorrect results will be calculated by the perturbation feature. In order to compute the correct tally, a correction term is needed that will account for the dependence of the Taylor series coefficients on the perturbed cross-section data.

## II. Results

We present here, for the first time, the appropriate first and second order corrections to the MCNP4B track length estimator of  $K_{eff}$  and show how these can be extracted from a combination of standard MCNP4B tallies. Although this paper deals with the track length estimator of  $K_{eff}$ , similar corrections terms can be applied to any perturbed tally with a cross-section multiplier, such as a reaction rate estimator. Thus this paper enables MCNP users to

apply the perturbation technique to criticality and other cross-section dependent problems.

The corrected first order perturbation is given by

$$\Delta c = PERTuc1 + Tally\Delta v \quad (EQ 1)$$

where PERTuc1 is the uncorrected first order perturbation as reported by MCNP, Tally is the unperturbed tally, and  $\Delta v$  is the percent change in the macroscopic cross-section. The corrected second order perturbation is

$$\Delta c = PERTuc2 + PERTuc1\Delta v \quad (EQ 2)$$

where PERTuc2 is the uncorrected second order perturbation as reported by MCNP. Adding equations 1 and 2, the total (first plus second order) corrected perturbation is

$$\Delta c = PERTucT + PERTuc1\Delta v + Tally\Delta v \quad (EQ 3)$$

where PERTucT is the total uncorrected perturbation as reported by MCNP.

All of the variable in equations 1, 2, and 3 can be calculated by MCNP or with a simple hand calculation. The unperturbed tally is normally given in the MCNP output, while the perturbation feature can be used to calculate first order, second order, or total perturbations. The percent change in the macroscopic cross-section is just the percent change in the atom density (the microscopic cross-section is not perturbed by density or composition changes). For a density perturbation the calculation of  $\Delta v$  is simple; it is just the percent change in the density. However, composition perturbations are more complicated. The change in the fraction (either weight or atom) of the isotope plus the corresponding change in the density must be taken into account.

Care must be taken when a perturbed material contains more than one isotope. If only the density is perturbed, equations 9, 10, and 11 will hold. However, if the perturbation is a composition change, the tally must be separated into the contribution of each isotope. These individual perturbations can then be corrected and added to together to calculate the correct total perturbation.

Next, we have, and will present, several examples<sup>4</sup> showing how the perturbation capability can be used to estimate the effect of small perturbations upon criticality. These examples demonstrate that the second order perturbation technique can be used with confidence for criticality calculations, although not to the extent of fixed source problems. This inherent bias is due to the inability of the differential operator technique to calculate perturbed eigenfunctions.

Finally, we have modified the MCNP code so that future versions will automatically calculate the correct perturbed values for the track-length estimates of Keff whenever the problem is perturbed.

#### IV. Summary

The differential operator technique is a powerful method for estimating the change in Monte

Carlo tallies due to small perturbations such as density or composition changes. But if the tallies involve the quantities being perturbed, correction terms are required. We have, for the first time, presented the correction terms and demonstrated how they can be used for MCNP4B. In addition, we have several examples that demonstrate the accuracy of the second order corrected perturbation for criticality calculations. Finally, we have also developed the modification to MCNP to automatically provide the perturbed values of Keff for criticality calculations.

## V. References

- (1) J. Breismeister, Editor, "MCNP -- A General Purpose Monte Carlo N-Particle Transport Code." Los Alamos National Laboratory Report, LA-12625-M (1997).
- (2) G. W. McKinney, "Theory Related to the Differential Operator Perturbation Technique." Los Alamos National Laboratory Memo, X-6:GWM-94-124 (1994).
- (3) G. W. McKinney, "Verification of the Monte Carlo Differential Operator Technique for MCNP." Los Alamos National Laboratory Report, LA-13098 (1996).
- (4) John C. Wagner et al., "MCNP: Criticality Safety Benchmark Problems." Los Alamos National Laboratory Report, LA-12415 (1992).

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