Title: MCNP PERTURBATION CAPABILITY FOR MONTE CARLO CRITICALITY CALCULATIONS

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Submitted to: Sixth International Conference on Nuclear Criticality Safety,
September 20-24, 1999, Palais des Congres,
Versailles, FRANCE
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MCNP PERTURBATION CAPABILITY FOR MONTE CARLO CRITICALITY CALCULATIONS

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Abstract

The differential operator perturbation capability in MCNP4B has been extended to automatically calculate perturbation estimates for the track length estimate of \( k_{\text{eff}} \) in MCNP4B. The additional corrections required in certain cases for MCNP4B are no longer needed. Calculating the effect of small design changes on the criticality of nuclear systems with MCNP is now straightforward.

Introduction

The effect of small design changes on the criticality of nuclear systems is difficult to assess with the Monte Carlo method. Often the change being calculated is masked by the statistical fluctuations of the Monte Carlo method. A new capability has been added to the MCNP4B\(^1\) differential operator perturbation capability\(^2\) to provide an automatic estimate of changes in \( k_{\text{eff}} \) for perturbations in criticality problems.

The differential operator perturbation technique\(^2\) is used in MCNP4B to calculate, in a single run, the effects of perturbations to material compositions or density on track-length or surface estimator tallies. The technique uses a second-order Taylor series expansion and allows the
calculation of perturbations even if the standard deviation of the unperturbed tally is greater than the calculated perturbation. But to simplify the implementation in MCNP4B, it was assumed that the tallies of a problem are independent of the cross sections being perturbed by the perturbations of a problem. The assumption of no cross-section dependence of the perturbed tallies is correct for surface tallies, track length tallies in unperturbed cells, and heating tallies where the heating normalization cancels the correction for cross-section dependency. But for track length tallies multiplied by a cross section, such as reaction rates, the perturbed tally can be strongly dependent upon the perturbed cross section, and the perturbation treatment in MCNP4B is not applicable. Calculation of the criticality eigenvalue, $k_{\text{eff}}$, is in effect a cross-section-dependent tally since it is the track length flux estimator multiplied by the fission $\nu$ and fission cross section. Furthermore, the $k_{\text{eff}}$ calculation is a tally over the entire problem, so perturbations of the fissioning regions anywhere affect the $k_{\text{eff}}$ estimation. Use of the differential operator perturbation method without a cross-section dependency correction caused the predicted value of $k_{\text{eff}}$ to go down in a Godiva criticality assembly even as the density of $^{235}\text{U}$ was increased. Attempts to provide a simple formula for manual correction of cross-section dependent tallies proved difficult, at best. Therefore, the powerful differential operator perturbation method implemented in MCNP4B was of limited use in criticality calculations.

**Theory**

The differential operator perturbation method has been extended to cross-section dependent tallies in MCNP4C. In criticality problems the perturbed value of the track length estimator of $k_{\text{eff}}$ is now automatically output for all perturbations along with the standard deviation. The method is still approximate in that the fundamental eigenvector mode (flux distribution) is assumed unchanged by all perturbations, and the underlying Taylor Series expansion is truncated after two terms. Nonetheless, the improved perturbation capability is sufficient for many applications.

The differential operator perturbation method implemented in MCNP4B assumed that tallies were independent of cross sections. Thus, the method worked well for surface tallies and cell flux tallies, but failed for reaction rate tallies when the reaction rates involved the same cross sections as the perturbed materials of the problem. The track length $k_{\text{eff}}$ estimation is like a reaction rate tally in that it includes the fission cross section. The perturbed part of the tally accumulated along every track length has the form

$$P_{ij}\Delta\nu + \frac{1}{2}(P_{2ij} + P_{ij}^2)\Delta\nu^2 + R_{ij}\Delta\nu + P_{ij}R_{ij}\Delta\nu^2$$

In MCNP4B it was assumed that the fraction of the reaction rate tally involved in the perturbation, $R_{ij} = 0$. That is, it was assumed that the tallies or $k_{\text{eff}}$ estimator is independent of the perturbed cross section, and these terms were not even in the code or its documentation. In MCNP4C the $R_{ij}$ terms have all been derived, documented, incorporated into the code, and tested. MCNP4C now computes cross-section dependent reaction rate tallies and track length $k_{\text{eff}}$ estimates correctly and by default for criticality KCODE calculations.

**Results**

Results for the Godiva critical assembly are illustrated in Table I.
The results in Table I show the effects of perturbations to a nominal Godiva assembly, 94.73 wt% $^{235}$U and 5.27 wt% $^{238}$U with a density of 18.74 gm/cm$^3$ and $k_{\text{eff}} = 0.998063 (.000798)$. The numbers in parenthesis are standard deviations; thus $-30.269 (1.423)$ has a confidence interval of -28.846 to -31.692. All the MCNP4C results were from a single run with two perturbations: a density perturbation where the density of the uranium was increased in steps from 18.74 gm/cm$^3$ to 26.0 gm/cm$^3$; and a composition perturbation where the weight fraction of $^{238}$U was increased from 5.27% to 50%. In the MCNP4C run the perturbed $k_{\text{eff}}$ values were automatically printed out for each perturbation (PERT card) without requiring the user to establish auxiliary tallies. The last “Actual % Change” column required separate, long, MCNP4B calculations to get converged values of $k_{\text{eff}}$ for each of the separate perturbed configurations; these $k_{\text{eff}}$ values were then compared to the $k_{\text{eff}}$ of the nominal case to determine the change.

The density change results for Godiva are illustrated in Fig. 1. The composition change results are illustrated in Fig. 2.

A second example is a hexagonal lattice core of a light water reactor taken from test problem 18 in the MCNP test set. The reactor is illustrated in Figs. 3 and 4. In this problem the density of the fuel is perturbed from 13.75 g/cm$^3$ to 26 g/cm$^3$ in 5 steps. The results are tabulated in Table II. The results are plotted in Fig. 5. The MCNP4C results are from a single run with the density perturbations; the “Actual % Change” column required separate, long, MCNP4B calculations to get converged values of $k_{\text{eff}}$ for each of the separate perturbed configurations. Note that in this problem the discrepancy between the actual and predicted values increases at a greater rate than in the Godiva problem because the underlying eigenfunction is more perturbed in this thermal system than for the Godiva bare fast system.

### Table I

<table>
<thead>
<tr>
<th>Density (g/cm$^3$)</th>
<th>MCNP4C % Change</th>
<th>Actual % Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>20.0</td>
<td>5.282 (.015)</td>
<td>5.499 (.116)</td>
</tr>
<tr>
<td>21.1</td>
<td>9.302 (.028)</td>
<td>9.467 (.111)</td>
</tr>
<tr>
<td>23.5</td>
<td>18.683 (.063)</td>
<td>19.389 (.117)</td>
</tr>
<tr>
<td>26.0</td>
<td>27.110 (.103)</td>
<td>28.256 (.122)</td>
</tr>
<tr>
<td>$^{238}$U wt %</td>
<td>MCNP4C % Change</td>
<td>Actual % Change</td>
</tr>
<tr>
<td>13</td>
<td>-4.233 (.084)</td>
<td>-4.251 (.121)</td>
</tr>
<tr>
<td>26</td>
<td>-12.292 (.357)</td>
<td>-11.749 (.107)</td>
</tr>
<tr>
<td>38</td>
<td>-20.778 (.796)</td>
<td>-19.346 (.104)</td>
</tr>
<tr>
<td>50</td>
<td>-30.269 (1.423)</td>
<td>-28.273 (.101)</td>
</tr>
</tbody>
</table>

### Table II

<table>
<thead>
<tr>
<th>Density (g/cm$^3$)</th>
<th>MCNP4C % Change</th>
<th>Actual % Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>15.5</td>
<td>5.417 (.044)</td>
<td>5.212 (.152)</td>
</tr>
<tr>
<td>17.0</td>
<td>9.128 (.078)</td>
<td>9.307 (.155)</td>
</tr>
<tr>
<td>21.5</td>
<td>18.690 (.201)</td>
<td>19.622 (.164)</td>
</tr>
<tr>
<td>26.0</td>
<td>24.680 (.386)</td>
<td>27.868 (.162)</td>
</tr>
</tbody>
</table>
Summary

Calculation of the effects of material density or composition changes upon the estimate of $k_{eff}$ is now automatic and simple with the extended differential operator perturbation technique of MCNP4C. MCNP4C has been modified to include the rather complex terms required for the perturbation of cross-section dependent tallies. Perturbed values of the track length $k_{eff}$ are printed by default in KCODE calculations. Small perturbations are not masked by the Monte Carlo statistical error. Perturbations up to 5% in $k_{eff}$ are quite accurate. Larger perturbation up to 30% still provide useful information but lose accuracy because the underlying eigenfunction remains unperturbed and the differential operator only includes the first two terms of the Taylor series.

References


FIGURE 1

dashed line: predicted change
solid line: actual change