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One-group MCNP5 Criticality Calculations with Anisotropic Scattering

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INTRODUCTION

One-group Monte Carlo calculations are used often to: (1) verify production codes against known analytical solutions, (2) verify new methods and algorithms that do not involve detailed collision physics, (3) compare Monte Carlo calculation methods with deterministic methods, and (4) as a teaching tool for students. Reference [1] provides a tutorial on setting up and running one-group problems with the *onegxs* utility code and MCNP5 [2].

In this work we demonstrate that MCNP5 calculations for one-group criticality problems agree in all cases with analytical solutions when scattering is either isotropic (P_0) or linearly anisotropic (P_1) with $|\bar{\mu}| \le 1/3$. For P_1 scattering with $|\bar{\mu}| > 1/3$, MCNP5 results can be seriously incorrect. Further, various common schemes for replacing the scattering distribution by a positive distribution that preserves the first moment are not effective in reducing the error.

ANALYTIC CRITICALITY BENCHMARK CALCULATIONS WITH MCNP5

In previous work [3,4], a set of 75 criticality problems that have analytical solutions for the k-effective (or c) eigenvalue problem were identified in the published literature. Of these, 30 problems are 1-group with P_0 scattering, 11 are 1-group with P_1 scattering, 2 are 1-group with P_2 scattering, 26 are 2-group P_0, 4 are 2-group P_1, 1 is 3-group P_0, and 1 is 6-group P_0. The geometry for these problems is necessarily simple, either infinite medium, infinite slabs, infinite cylinders, or spheres, with reflectors in a few problems.

For P_1 problems with $|\bar{\mu}| > 1/3$, the scattering probability density function (PDF) is negative over a portion of the range of μ, [-1,1], and hence is nonphysical. MCNP cannot model such a nonphysical PDF. For the P_2 problems, similar nonphysical negative PDFs are possible, but do not occur in the test problems used. Out of the 75 problems, only 4 involve nonphysical P_1 scattering with $|\bar{\mu}| > 1/3$, three 1-group problems and one 2-group problem.

When the 75 problems are run using MCNP5 (in multigroup mode), the 71 problems with non-negative scattering PDFs give results for k_{eff} that match the exact analytic solutions within statistics. The 4 problems with P_1 scattering and $|\bar{\mu}| > 1/3$ do not match the analytic solutions and show significant errors:

Table I. Comparison of exact results & MCNP5

			k-effective	
Problem		$\bar{\mu}$	**exact**	**MCNP5**
71 different problems		$|\bar{\mu}| < 1/3$	*All 71 match within statistics*	
34	slab	0.4545	1.0000	1.0027
37	cylinder	0.8553	1.0000	1.0620
43	sphere	-0.5998	1.0000	0.9968
71	slab	0.4389	1.0000	1.0021

(std.dev. for all MCNP5 results ≤ 0.0001)

It can be seen that the larger the magnitude of $\bar{\mu}$, the larger the error in the k_{eff} computed by MCNP5. This is a direct result of the nonphysical scattering PDFs. It should be noted that the differences in Table I were previously observed in [4], and there was a cursory investigation of possible fixes for the problems with negative scattering. In the current work, we investigated alternate forms of representing the scattering PDFs while still preserving first moments. These investigations are described next.

INVESTIGATION OF SAMPLING FROM TRUNCATED SCATTERING PDFS

For normal MCNP5 calculations, the ENDF/B-VI or –VII nuclear data typically contain 20 Legendre moments for scattering, enough moments so that the reconstructed PDFs for scattering are physically realizable (non-negative). The Legendre moments are used to construct either equally-probable bins or piecewise linear representations of the PDF. When creating the multigroup datasets for use in running the set of analytic benchmark problems, 1,000 equally probable bins were used to represent the scattering PDFs.

The scattering PDFs for the 4 problems noted in Table I, however, are truncated at P_1, with no attempt to represent a physically realizable non-negative PDF. Over portions of the range, the PDF is negative. MCNP5 cannot deal with negative scattering PDFs. (In principle, Monte Carlo codes could resolve this difficulty by introducing negative weights for particles scattered at these negative values of μ. Negative weights are problematic, however, leading to code complications and to larger variances on results.) Figure 1 illustrates such a nonphysical P_1 scattering PDF with $\bar{\mu} > 1/3$.

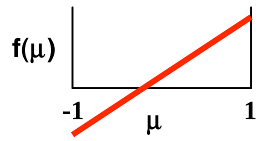

Figure 1. Nonphysical scattering PDF

During the preparation of the multigroup datasets for the MCNP5 calculations, the ad hoc fix applied to the negative portion of the PDFs is to simply set the PDF to zero over that range & renormalize the positive portion of the PDF. This procedure is clearly not correct, since it preserves neither the shape nor the first moment, $\bar{\mu}$.

A more reasonable way to fix the problems with negative scattering PDFs is to choose a different form for the PDF that is positive but preserves the physical information, the first moment $\bar{\mu}$. While there are infinitely many such PDFs, 4 common choices (frequently used in other Monte Carlo codes and even in other parts of MCNP5) are shown in Figure 2.

To determine whether the use of any of these non-negative, moment-preserving PDFs improved the accuracy of MCNP5 results for Problems 34, 37, or 43, MCNP5 was modified to permit any of the forms shown in Figure 2. The problems were then repeated with each of the PDFs, giving the results shown in Table II.

While the MCNP5 results for the set-to-zero fix are particularly bad, the other PDFs do not provide much, if any, improvement. This is somewhat surprising, since conventional wisdom holds that preserving the first moment preserves the essential physical data and should always be a reasonable approach. All of the PDFs (2a) – (2d) properly preserve the first moment (the physical data) and are non-negative, but fail to yield correct results

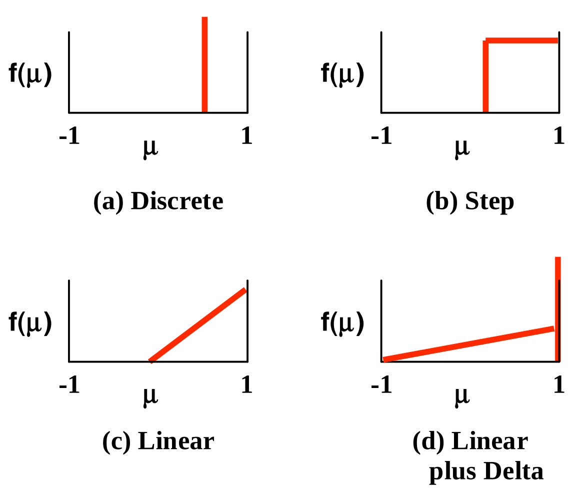

Figure 2. Non-negative scattering PDFs that can preserve $\bar{\mu}$, for $\bar{\mu} > 1/3$

for these problems. As a result, the production version of MCNP5 will not be modified to handle the alternate PDFs shown in Figures 2a, 2c, 2d. Existing code logic in MCNP5 and the default for the *onegxs* setup code support the step model shown in Figure 2b.

Table II. Results for Problems 34, 37, 43 Using Alternate Scattering PDFs

Problem:	**34** $\bar{\mu} = .45$	**37** $\bar{\mu} = .86$	**43** $\bar{\mu} = -.60$
Exact Keff	1.0000	1.0000	1.0000
MCNP5 Keff			
(1) Set-to-zero	1.0027	1.0620	0.9968
(2a) Discrete	0.9959	1.0186	0.9986
(2b) Step	0.9999	1.0197	0.9990
(2c) Linear	1.0017	1.0195	1.0000
(2d) Linear+delta	1.0082	1.0226	0.9995

(std.dev. for all MCNP results ≤ 0.0006)

CONCLUSIONS

The results discussed in this work and in [4] provide convincing verification evidence that MCNP5 yields correct results for all of the analytic k_{eff} benchmark problems that have non-negative scattering PDFs. For problems with scattering PDFs which may become negative over part of the range, such as P_1 scattering with $|\bar{\mu}| > 1/3$, MCNP5 results can differ significantly from the exact benchmark results. These differences are due not to errors in the code, but rather to difficulties with treating negative scattering PDFs without introducing negative weights. It is thus a fundamental limitation on multigroup MCNP5 calculations that the scattering PDFs be restricted to non-negative data. In particular, when performing multigroup MCNP5 calculations using datasets from deterministic codes, comparisons are only valid for the case of P_0 scattering or when the multigroup data are checked to confirm that no negative scattering PDFs are being used in the MCNP5 calculations.

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