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Revised by OSTI
AUG 06 1990

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

LA-UR--90-2514

DE90 014896

TITLE MONTE CARLO NEXT-EVENT ESTIMATES FROM
 THERMAL COLLISIONS

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SUBMITTED TO ANS 1990 Winter Meeting, Washington, DC,
 November 11-15, 1990. Also being submitted
 to Nuclear Science and Engineering.

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MONTE CARLO NEXT-EVENT ESTIMATES FROM THERMAL COLLISIONS

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Introduction

A new approximate method has been developed by Richard E. Prael to allow $S(\alpha, \beta)$ thermal collision contributions to next-event estimators in Monte Carlo calculations. The new technique is generally applicable to next-event estimator contributions from any discrete probability distribution. The method has been incorporated into Version 4 of the production Monte Carlo neutron and photon radiation transport code MCNP.^{1,2}

Thermal Scattering and Next-Event Estimators

The $S(\alpha, \beta)$ scattering model^{3,4,5} is a complete ENDF/B⁶ representation of thermal neutron scattering by molecules and crystalline solids, including Bragg scattering, which is important in the energy range 4 eV down to 10^{-5} eV. Next-event estimators³ include point detectors,^{1,3,7} ring detectors,^{1,7} and other schemes such as DXTRAN.^{1,7} Point and ring detectors, deterministic estimates of the flux at a point in space, are made from source and collision events throughout a Monte Carlo random walk. DXTRAN is an MCNP variance reduction option that uses a next-event estimator to put particles in small regions of space (DXTRAN spheres) where their random walk can be continued.

Until now MCNP has been unable to use next-event estimators in conjunction with $S(\alpha, \beta)$ scattering because the scattering distributions, $p(\mu)$, processed by the NJOY nuclear data code^{8,9} are discrete. The quantity $p(\mu)$ is the value of the probability density function for scattering from the incident random-walk particle direction at a polar angle $\mu = \cos\theta$ exactly toward the next event at a point detector, ring detector, or DXTRAN sphere. The MCNP nuclear data library as processed by NJOY represents the $S(\alpha, \beta)$ scattering data as discrete polar angles, μ , at each collision, and the probability of any of these angles pointing exactly toward the next-event point is infinitesimally small. An exact next-event estimator scheme with discrete angles may be possible; in such a scheme, at each collision the particle would be backed up along its random-walk trajectory to a point where scattering exactly in the direction of the next event would be possible, and then particle weights would be appropriately adjusted. However, this scheme would be horrendously complicated, particularly if the trajectory crossed any geometric boundaries.

Prael's Histogram Method

Prael's new method approximates discrete distributions as histogram functions for next-event estimators. The discrete distributions are still used for the random walk. The next-event estimator histograms follow certain rules to preserve selected properties. Calculation of the $p(\mu)$ values from a histogram distribution rather than from a discrete distribution is relatively straightforward. The histograms are chosen by the following rules:

- The midpoint of the histogram must be centered at the location of the discrete distribution line to preserve the mean.
- Histograms may not overlap.
- Histograms may not exceed the cosine boundaries -1 and +1.
- The width of the histogram cannot exceed $\Delta\mu \leq .1$.

In the cases of incoherent elastic scattering and inelastic scattering, the histogram width is governed only by the first three criterion because line spectra are sometimes a poor representation of the true physical situation. In particular, the NJOY-processed $S(\alpha, \beta)$ angular distribution data represents even isotropic scattering as seven equiprobable lines. If the histogram width is allowed to expand without the fourth constraint in cases where NJOY represents potentially continuous distributions with discrete distributions, the histogram approximation can be a better representation of the physics than is the data used in the random walk. Of course, in any realistic thermal problem there are many collisions, and the representation of incoherent elastic scattering and inelastic scattering with discrete lines by NJOY, even when the distributions are continuous, is an acceptable convenience.

Implementation and Validation

Prael's method has been incorporated as a standard feature of MCNP Version 4. Forty-nine MCNP calculations have been run to test the scheme; the runs took over forty hours of Cray X-MP/48 computer time. The results of these trial runs will be presented. They indicate, often dramatically, that the new approximate method works well. As expected, in those cases where discrete data are used to represent continuous distributions, the new approximate method gives even better results than does the random walk. Figure 1 shows particle flux measured from single collisions at twenty angles relative to an incident thermal neutron direction. The histogram is the random-walk flux tally, the dotted line is the true isotropic flux from the collision, and the circles are the point-detector estimates of the flux.

Summary

Prael has devised an approximate method to allow contributions to next event estimators from discrete probability distributions. The method has been incorporated into MCNP Version 4 to allow detector and DXTRAN estimates from $S(\alpha, \beta)$ thermal collisions. Extensive testing indicates the approximation works well, and when discrete data are used to represent continuous distributions, the approximation works even better than the random walk.

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Figure 1.