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1 Introduction

Much emphasis has been placed on the fact that the explosion in computer power has enabled Monte Carlo transport simulations to be performed that were previously impractical. Much less attention has been given to the idea that simply being able to calculate hundreds of millions, or even billions of particle histories may not ensure an accurate solution if the simulation is limited by nuclear data approximations inherent in the Monte Carlo code.

The purpose of this paper is to describe several such nuclear data approximations that have recently been eliminated (or mitigated) from the MCNP family of codes [1,2] and associated nuclear data libraries. Specific examples described are probability tables in the neutron unresolved resonance region, delayed neutrons from fission, secondary charged particles from neutron collisions, photonuclear physics, table-based charged-particle transport, and improvements in secondary scattering representations. We will also describe remaining nuclear data approximations in MCNP and the prospects for addressing them.

2 Unresolved Resonance Probability Tables

The neutron unresolved resonance range is that energy region between low neutron energies, where cross sections are derived from explicit resonance parameters, and high neutron energies, where cross sections are relatively smooth and are obtained from slowly-varying tabulations. It is an energy region where experimentalists have difficulty resolving individual resonances. Therefore, nuclear data evaluations in ENDF format[3] often provide statistical information in this energy range, including average level spacings and average neutron, radiative, fission, and competitive widths. As examples, the unresolved resonance range in ENDF/B-VI extends from 2.65 to 100 keV for ^{184}W, from 2.25 to 25 keV for ^{235}U, and from 10 to 149 keV for ^{238}U.

Versions of MCNP up through and including 4B did not take full advantage of the unresolved resonance data provided by evaluators. Instead, smoothly-varying average cross sections were used in the unresolved range. As a result, any neutron self-shielding effects in this energy range were unaccounted for. Better utilizations of unresolved data have been known and demonstrated for some time [4,5], and in MCNP Version 4C the probability table treatment was incorporated [6].

In this model, a processing code (NJOY [7]) is used to generate ladders of resonances that obey the chi-square distributions for widths and Wigner distribution for spacing. Cross sections are sampled from the ladders at randomly selected energies and accumulated into probability tables until reasonable statistics are obtained. MCNP then samples the cross sections from these probability tables when a neutron is in the unresolved region. A data library for MCNP including probability tables for 27 isotopes has been generated and distributed [8].

Calculations for a variety of uranium and plutonium criticality benchmarks have been performed with and without the probability-table treatment [9]. Small but significant reactivity changes are seen for plutonium and ^{233}U systems with intermediate spectra. More importantly, substantial reactivity increases can be obtained for systems with large amounts of ^{238}U and intermediate spectra when the probability-table method is used.

3 Delayed Neutrons from Fission

A small but important fraction of the neutrons emitted in fission events are delayed neutrons, emitted as a result of fission-product decay at times much later than prompt fission neutrons. MCNP users have always been able to specify whether or not to include delayed fission neutrons by using either total nubar (prompt plus delayed) or prompt nubar only. However, in versions of MCNP up through and including 4B, all fission neutrons (whether prompt or delayed) were produced instantaneously and with an energy sampled from the spectra specified for prompt fission neutrons.

For many applications this is adequate. However, it is another example of a data approximation that is unnecessary. Therefore, Version 4C of MCNP allows delayed fission neutrons to be sampled (either analog or biased) from time and energy spectra as specified in nuclear data evaluations. There are two impacts. One is that the delayed neutron spectra are softer than the prompt spectra. The second is that experiments measuring neutron decay after a pulsed source can now be modeled with MCNP because the delay in neutron emission following fission is properly accounted for. A library based on ENDF/B-VI including detailed delayed fission neutron data for 20 isotopes has been prepared and is part of the MCNP 4C data distribution package.

Ref. 10 describes the impact of sampling delayed neutron energy spectra on reactivity calculations. As expected, most of the reactivity impacts are very small, although changes of 0.1-0.2% in k_{eff} were observed. Overall, using the delayed neutron spectra produced small positive reactivity changes for most fast and intermediate HEU systems and small negative changes for some systems in which a significant fraction of the fissions occurs in ^{238}U.

4 Neutron-Induced Charged Particles

All versions to date of MCNP assume that charged particles produced by neutron collisions are deposited locally. This assumption has been eliminated, however, in the MCNPX code. In MCNPX, neutron induced charged particles (isotopes of hydrogen and helium) are sampled and banked for subsequent transport at the option of the user.

This capability was enabled by utilization of changes in the ENDF6 format that allowed evaluators to fully specify charged-particle reaction products. In particular, Chadwick and Young at Los Alamos have produced over 40 neutron evaluations to 150 MeV in ENDF6 format [11]. In these evaluations, they include production cross sections and energy-angle correlated spectra for secondary light particles. The format of MCNP neutron data was modified to include secondary charged-particle data, and NJOY was updated to process evaluated data into this new format. Implementation in MCNPX is described in [12]. A library based upon Los Alamos evaluations including neutron-induced charged particle data for 41 isotopes has been prepared and is part of the MCNPX 2.1.5 distribution.

One additional aspect warrants mention. Whereas previous MCNP neutron transport had assumed that the energies of all secondary charged particles would be deposited locally, users of MCNPX are now given flexibility to decide whether to transport some or all of the light charged particles. This required expansion of the MCNP heating (energy deposition) values to include not only the total, but also the partial contributions due to each secondary charged particle. In MCNPX if a particular charged particle is being transported, its contribution to the heating is subtracted from the total. After production, of course, the energy of the charged particle itself may be deposited elsewhere in the geometry as a result of transport.

5 Photonuclear Physics

MCNP through Version 4C and MCNPX through Version 2.1.5 account for only photoatomic processes; photonuclear physics is completely ignored. This limitation will be removed in MCNP 4D and MCNPX 2.2.

Substantial work to produce complete nuclear data evaluations for incident photons, including multiplicities and spectra of secondary particles, has enabled this work. A library based upon Los Alamos evaluations for 12 isotopes has been processed with NJOY and will be distributed with the code versions mentioned in the last paragraph. The Los Alamos evaluations are part of an international collaboration organized by the IAEA [13].

The photonuclear physics implementation is complete and consistent with existing photoatomic physics and other code features. Secondary neutrons and photons may be created in MCNP from a photonuclear collision; in addition, light charged particles may be created in MCNPX. The implementation includes the ability to bias photonuclear events. Complete documentation, including validation examples, is available in [14].

6 Charged-Particle Tables

Until recently, the only possibility in MCNP for charged-particle transport (other than for electrons) was by using the multigroup Boltzmann-Fokker-Planck option. MCNPX also has featured continuous-energy light charged-particle transport by use of various physics models, primarily intranuclear cascade for energies below 150 MeV.

Recently, complete nuclear data evaluations have been prepared for incident protons and a table-based continuous-energy transport capability has been included in MCNPX 2.2. Evaluations have been completed for 42 isotopes [11], processed by NJOY, and a library for MCNPX based on these data will be distributed with Version 2.2.

The implementation of table-based proton transport in MCNPX relies on the data tables to describe nuclear reactions and large-angle scattering. Non-table-based continuous slowing down and multiple scattering models are used for small-angle scattering. The implementation is described more fully in [15]. Results of benchmark calculations using table-based proton transport in MCNPX have been reported in [16-18]. The capability will be generalized in the future to include table-based transport for additional light charged particles.

7 Secondary Scattering Distributions

Angular distributions of secondary particles have traditionally been represented in the MCNP family of codes by using 32 equally-probable cosine bins. This representation has the advantages of being compact and very easy to sample. Stimulated initially by the highly forward-peaked nature of proton scattering distributions, a new, more rigorous angular distribution representation has been implemented in MCNP 4C and in MCNPX 2.1.5.

The new representation features a tabulation of the probability density function (pdf) as a function of the cosine of the scattering angle. Interpolation of the pdf between cosines may be either histogram or linear-linear. The new tabulated angular distribution allows more accurate representations of original evaluated distributions in both high-probability and low-probability regimes. NJOY now processes angular distribution data for certain reactions for all incident particles into the new representation.

ENDF6 format also has featured various formalisms to describe correlated secondary energy-angle spectra. The MCNP family of codes samples from many such representations. In connection with the discussion in the previous paragraphs, we have recently added a correlated representation that presents data as tabulated angular distributions that are a function of tabulated energy distributions. This capability exists in MCNP 4C and in MCNPX 2.1.5. Libraries described in Sections 4-6 all include the new secondary scattering representations described here.

8 Remaining Approximations

Many challenges remain in terms of eliminating nuclear data approximations in the MCNP family of codes. Among those that might be addressed in the relatively near future are:

- The number of fission neutrons is always sampled as one of the nearest integers to $\nu(E)$
- Neutron F6 heating (energy deposition) tallies are the same whether or not secondary photons are transported
- There is no consideration of delayed photon production from fission

Other approximations that are much more challenging include:

- The type of reaction responsible for the creation of various secondary particles at a single nuclear collision is not correlated
- Each secondary particle from a collision is sampled independently
- The treatment of temperature effects is limited in its range of validity

9 Summary

In summary, several physics improvements have been made recently to the MCNP family of codes by eliminating or mitigating previous nuclear-data assumptions. These physics improvements complement other capability improvements resulting from the explosion in computing power. Together, they enlarge the suite of applications that can be performed with Monte Carlo and allow improved fidelity and accuracy of all simulations.

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