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# NEW PROBABILITY TABLE TREATMENT IN MCNP FOR UNRESOLVED RESONANCES


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## ABSTRACT


**An upgrade for MCNP has been implemented to sample the neutron cross sections in the unresolved resonance range using probability tables. These probability tables are generated with the cross section processor code NJOY, by using the evaluated statistical information about the resonances to calculate cumulative probability distribution functions for the microscopic total cross section. The elastic, fission, and radiative capture cross sections are also tabulated as the average values of each of these partials conditional upon the value of the total. This paper summarizes how the probability tables are utilized in this MCNP upgrade and compares this treatment with the approximate "smooth" treatment for some example problems.**


## 1. INTRODUCTION

The resonances in the unresolved energy range have been treated by replacing the statistical resonance information with average smooth cross sections for versions of MCNP[1] up through and including Version 4B. This approximation means that any self-shielding effects in the unresolved region are not currently modeled by MCNP. An upgrade has been implemented to sample the neutron cross sections in the unresolved resonance range using probability tables. These probability tables are generated with the cross section processor code NJOY,[2] by using the evaluated statistical information about the unresolved resonances for a particular isotope to calculate cumulative probability distribution functions for the isotope's microscopic total cross section. The elastic, fission, and radiative capture cross sections are also tabulated as the average values of each of these partials conditional upon the value of the total. These tables are created on a grid of incident neutron energies across the unresolved energy range with typically 20 probabilities in each table.

The utilization of probability tables is not a new idea in Monte Carlo applications. A code[3] to calculate such tables for Monte Carlo fast reactor applications was utilized in the early 70's. Temperature difference Monte Carlo calculations[4] and a summary of the VIM Monte Carlo code[5] that uses probability tables are pertinent early references. Sampling the cross section in the random walk from the probability tables is a valid physics approximation if the average energy loss at a collision is much greater than the average width of a resonance; i.e., if the narrow resonance approximation[6] is valid. Then the detail in the resonance structure following a collision is statistically independent of the magnitude of the cross sections prior to the collision.

Section 2 of this paper briefly describes the contents of the probability tables and how MCNP has been upgraded to utilize such data. In Section 3 we describe three sample problems and provide MCNP results with and without the probability table treatment. A summary of the work is provided in Section 4.

## 2. MCNP UNRESOLVED RESONANCE TREATMENT WITH PROBABILITY TABLES

Nuclear data evaluations commonly provide unresolved resonance data to bridge the energy range between low neutron energies (where cross sections are obtained explicitly from resolved resonance parameters) and higher neutron energies (where cross sections are relatively smooth and are obtained from slowly-varying tabulations). Evaluations in ENDF format[7] include data such as average level spacings and average neutron, radiative, fission, and competitive widths in the unresolved region. All such data can be a function of incident neutron energy.

NJOY is used to process evaluated ENDF unresolved data into a probability table form that is convenient for MCNP. The PURR module of NJOY generates "ladders" of resonances that obey the chi-square distributions for widths and Wigner distribution for spacing as specified by the ENDF data. Cross sections are sampled from the ladders at randomly selected energies and accumulated into probability tables until reasonable statistics are obtained. NJOY has recently been upgraded to preserve correlation between various temperatures in the probability tables.

Shown in Table 1 is a sample probability table for ENDF/B-V Rev. 2 $^{239}$Pu at an incident neutron energy of 430 eV and at a temperature of 300 degrees Kelvin. This specific table has twenty probabilities and corresponding cross sections. Twenty probability values are typically sufficient, although the MCNP upgrade is written to allow any number of probability values. Since the cross section changes relatively slowly with probability for probabilities less than about 0.8, it is usually not necessary to have a fine grid over this lower range of probabilities. This probability range represents the low cross sections between resonances. The probabilities above about 0.8 describe the resonances, where the corresponding cross sections in Table 1 change much more rapidly with probability.

The values from Table 1 are shown graphically in Figure 1, where we plot the cross-section distributions as a function of probability. The total, elastic, fission, and capture cross sections have been shown. For comparison purposes, the "smooth" cross-section values at 430 eV are: total - 25.1 b; elastic - 11.8 b; fission - 8.89 b; and capture - 4.38 b.

Sampling a cross section from such a table is straightforward since it simply involves selecting a random number and obtaining the partial cross sections from the "row" where the random number is less than the probability in the table, but greater than the preceding probability. The upgrade in MCNP obtains the total as the sum of the three partials, rather than using the total directly from the table, to avoid any possible roundoff problems. If other partial cross sections are possible in the unresolved region, such as inelastic scattering or other absorption reactions, these are separately added to this total by MCNP during the random walk by using their smooth values. The "capture" column in the probability tables represents the radiative capture reaction.

Two probability tables will actually be involved when sampling the cross sections, where the incident neutron energy in the random walk lies between the two adjacent energies of the corresponding probability tables. The same random number is used to obtain the elastic, fission, and radiative capture cross sections from each table with linear-linear or log-log interpolation between the two tables to determine these three partial cross sections at the incident energy of interest.

Although the actual sampling of the cross sections from the probability tables is fairly straightforward, retaining correlation along flight paths is a requirement that can lead to complications. This requirement dictates that once a cross section is sampled for an isotope along a flight path (from collision to collision or from collision to leakage) that same cross section must be used for all random walk pseudo-particles along the flight path. Importance splitting or splitting from using weight windows are examples where information needs to be banked so that the cross sections used for the parent pseudo-particle along the flight path can be retained for the other pseudo-particles. This is accomplished in the MCNP upgrade by banking the sampled cross section information when the neutron is in the unresolved energy range. The random number used to sample the cross sections is also banked so that correlation can be retained if there is a cross section set being used along the flight path for the same isotope, but at a different temperature.

**Table 1. Probability table for $^{239}$Pu at an incident neutron energy of 430 eV and a temperature of 300 degrees Kelvin [based on ENDF/B-V, Rev. 2]**

| | cumulative probability | total | elastic | fission | capture |
|---|---|---|---|---|---|
| 1 | 0.00717 | 0.8067E+01 | 0.6145E+01 | 0.1220E+01 | 0.7018E+00 |
| 2 | 0.07133 | 0.9996E+01 | 0.8752E+01 | 0.9580E+00 | 0.2861E+00 |
| 3 | 0.34225 | 0.1166E+02 | 0.9970E+01 | 0.1405E+01 | 0.2863E+00 |
| 4 | 0.53333 | 0.1387E+02 | 0.1053E+02 | 0.2738E+01 | 0.6087E+00 |
| 5 | 0.64767 | 0.1664E+02 | 0.1076E+02 | 0.4663E+01 | 0.1218E+01 |
| 6 | 0.72067 | 0.2004E+02 | 0.1086E+02 | 0.7148E+01 | 0.2030E+01 |
| 7 | 0.77967 | 0.2408E+02 | 0.1123E+02 | 0.9497E+01 | 0.3352E+01 |
| 8 | 0.82000 | 0.2895E+02 | 0.1162E+02 | 0.1222E+02 | 0.5102E+01 |
| 9 | 0.85467 | 0.3481E+02 | 0.1218E+02 | 0.1630E+02 | 0.6329E+01 |
| 10 | 0.88833 | 0.4206E+02 | 0.1252E+02 | 0.2033E+02 | 0.9215E+01 |
| 11 | 0.91342 | 0.5036E+02 | 0.1386E+02 | 0.2378E+02 | 0.1272E+02 |
| 12 | 0.93617 | 0.6042E+02 | 0.1501E+02 | 0.2906E+02 | 0.1635E+02 |
| 13 | 0.95200 | 0.7228E+02 | 0.1652E+02 | 0.3567E+02 | 0.2008E+02 |
| 14 | 0.96642 | 0.8747E+02 | 0.2035E+02 | 0.4176E+02 | 0.2536E+02 |
| 15 | 0.97850 | 0.1054E+03 | 0.2452E+02 | 0.4657E+02 | 0.3435E+02 |
| 16 | 0.98667 | 0.1267E+03 | 0.2775E+02 | 0.6243E+02 | 0.3649E+02 |
| 17 | 0.99092 | 0.1526E+03 | 0.3403E+02 | 0.7385E+02 | 0.4471E+02 |
| 18 | 0.99467 | 0.1835E+03 | 0.4693E+02 | 0.8406E+02 | 0.5252E+02 |
| 19 | 0.99750 | 0.2200E+03 | 0.6376E+02 | 0.8705E+02 | 0.6918E+02 |
| 20 | 1.00000 | 0.2866E+03 | 0.1027E+03 | 0.7617E+02 | 0.1078E+03 |

Other aspects involved in the simulation of the individual histories of the random walk also require appropriate correlation. These include: production of secondary photons in coupled (neutron, photon) problems consistent with the neutron reaction cross sections that were sampled; tallies involving cross sections; and point detector tallies. Accommodations have been made in the upgrade of MCNP to include all such correlations when unresolved probability tables are used.

An additional column of nuclear heat deposition numbers is included in the probability tables. These heating numbers are not shown in Table 1. For the initial testing, we have just used the "smooth" heating numbers for the entire column, but detailed heating numbers as a function of probability can be utilized if that additional precision in the calculation of nuclear heat deposition is required.

The implementation of the probability tables in MCNP allows for the tables to contain the actual cross sections as shown in Table 1, or optionally, the tables can contain factors. If factors are used, they are sampled in the same manner as described above for cross sections. Then, these factors are multiplied by the "smooth" tabulated cross sections at the incident neutron energy to obtain the cross sections to be used during the random walk. The use of factors involves more on-line computation in the random walk, but may occasionally be a useful option for some cross section evaluations -- for example, for an evaluation that includes structure in the "smooth" cross sections on a finer energy scale than that for which the unresolved parameters are provided.

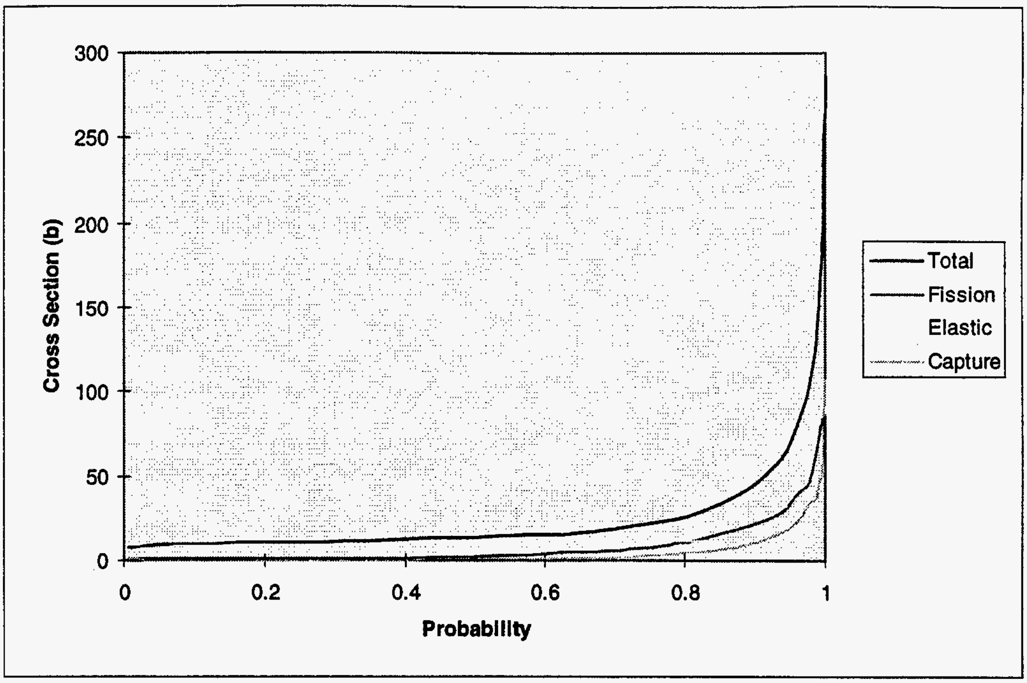


**Fig. 1. Chart of cross sections as a function of cumulative probability for $^{239}$Pu at 430 eV.**

## 3. RESULTS

Several sample MCNP problems have been created to test NJOY generation of probability table data and the subsequent implementation in MCNP. Results from three of these problems are presented in this section. These problems are somewhat contrived, in that we have attempted to design problems that emphasize the unresolved-region effects. As a result, the magnitude of the apparent differences between a probability table treatment and a "smooth" treatment is certainly greater here than would be expected for most realistic transport problems.

### 3.1 TRANSPORT OF NEUTRONS IN THE UNRESOLVED ENERGY RANGE THROUGH A SHIELD OF $^{238}$U

Depleted uranium is sometimes used to rapidly attenuate gamma-rays. In such applications, it may also be important to quantify the attenuation of neutrons. In this test problem, we have a 70 cm thick $^{238}$U shield. There is a 1/E neutron source normally incident on the shield between 10 keV and 300 keV. We calculate the neutron flux emerging from the shield. Two calculations are performed; one with the usual "smooth" treatment of the unresolved cross sections and the other with the upgraded probability table treatment of the unresolved cross sections.

The ENDF/B-V cross section set 92238.50c has "smooth" cross sections in the unresolved resonance region, which extends from 4 keV to 149 keV. An alternate cross section set, 92238.48c, was generated to be identical to 92238.50c except that 36 probability tables were included to describe the cross section distributions in the unresolved energy range.

Shown in Table 2 is the neutron flux emerging from the $^{238}$U shield for some broad energy groups. The total neutron flux with the probability table treatment is a factor of 3.18 greater than that with the "smooth" treatment. The major contribution to the total flux is from the 10 keV to 50 keV energy bin where the flux in this bin calculated with the more precise probability table treatment is a factor of 3.31 greater than that with the "smooth" treatment. This example clearly illustrates that self-shielding effects in the unresolved region can be significant for thick materials.

**Table 2. Energy dependent neutron flux emerging from the 70-cm $^{238}U$ shield with probability tables compared to "smooth"**

| Upper Energy(MeV) | Neutron Flux($n/cm^2/s$) Probability Tables | Smooth | Flux Ratio: Prob Table/Smooth |
|---|---|---|---|
| 1.0000E-03 | 1.26837E+04 0.1781[a] | 1.12345E+04 0.3045[a] | 1.13 |
| 4.0000E-03 | 9.84824E+05 0.2076 | 5.40045E+05 0.1566 | 1.82 |
| 1.0000E-02 | 1.86177E+06 0.0201 | 1.00405E+05 0.0654 | 1.85 |
| 5.0000E-02 | 8.65171E+06 0.0095 | 2.61510E+06 0.0151 | 3.31 |
| 1.5000E-01 | 7.13573E+05 0.0334 | 4.92229E+05 0.0425 | 1.45 |
| 3.0000E-01 | 8.72611E+04 0.1172 | 7.16865E+04 0.1391 | 1.22 |
| 3.0000E+01 | 7.70899E+04 0.1408 | 6.86573E+04 0.1746 | 1.12 |
| total | 1.23889E+07 0.0187 | 3.89936E+06 0.0270 | 3.18 |

a) Relative statistical uncertainties in the MCNP calculation.

The $^{238}U$ density used in the calculations to obtain Table 2 was 18.9 g/cm$^3$. The contribution to the flux in the 300 keV to 30 MeV energy bin is from the small number of sub-threshold fissions. The flux incident upon the shield was arbitrarily set to $1.0 \times 10^{12}$ (n/cm$^2$/s) so the calculated flux attenuation was $1.24 \times 10^{-5}$ for the probability table treatment and $3.90 \times 10^{-6}$ for the "smooth". The tissue dose rate at the incident surface was $1.31 \times 10^{10}$ mrem/hr, which decreased by a factor of $2.54 \times 10^{-6}$ for the probability table treatment and a factor of $1.05 \times 10^{-6}$ for the "smooth." There is less change in the dose rate (factor of 2.42) due to the improved unresolved cross-section treatment than in the flux (factor of 3.18) because the flux to dose conversion factors are higher at the higher energies so that the spectrum above 150 keV becomes relatively more important for the dose rates compared to the flux.

## 3.2 TRANSPORT OF NEUTRONS IN THE UNRESOLVED RANGE THROUGH $^{239}Pu$

Although $^{239}Pu$ is not used as a shield material, its high fission rate in the unresolved energy range provides another interesting example of the difference in attenuation rates between a probability table treatment and the traditional "smooth" treatment. The ENDF/B-V.2 cross section set 94239.55c has "smooth" cross sections in the unresolved resonance region of $^{239}Pu$ from 300 eV to 25 keV. An alternate MCNP cross section set, 94239.58c, was generated with the identical data except that 94 probability tables were included to describe the cross sections in this unresolved energy range.

In this test problem, neutrons are normally incident (1 neutron/cm$^2$/sec) upon a material of pure $^{239}Pu$ having an atom density of 0.01 atoms/b-cm. The monoenergetic source energy of 391 eV is within the unresolved energy range. We calculate the flux on the far side of a 20 cm thick slab using both the smooth treatment (94239.55c) and the treatment with the probability tables (94239.58c). We suppress all secondary fission neutrons by using the MCNP "nonu" option. Results are as follows:

Total flux with probability tables = 0.1572 (0.30%) (n/cm$^2$/s)

Total flux with smooth = 0.0231 (0.69%) (n/cm$^2$/s).

Hence, the use of probability tables leads to a significant change in the emerging flux, and in the direction one would expect; i.e., when the lower cross sections are sampled from the probability tables with small random numbers, the neutron flight paths are much longer and those flight paths penetrate the shield more easily.

When there is only a very small amount of material for the neutrons to penetrate, the number of collisions should be about the same for the smooth as for a probability table treatment. For such a case, the probability table treatment gives:

$$\text{Number of source neutrons suffering a collision} = \int_0^1 \{1 - e^{-N\sigma(\xi)x}\}\, d\xi \cong \int_0^1 N\sigma(\xi)x\, d\xi = Nx\,\sigma_{smooth}$$

where N is the atom density, x is the slab thickness, $\xi$ is a random number, and $\sigma(\xi)$ is the total cross section from the probability table.

To test this supposition, we repeated the above calculations after reducing the atom density by a factor of 1000. The number of collisions from 1,000,000 source neutrons was 4,619 for the probability table treatment and 4,640 for the smooth. These results differ by less than the statistical uncertainties. This demonstrates that the probability tables have been generated by NJOY in such a way as to correctly preserve the average (infinitely-dilute) cross sections.

A calculation was also made using the original atom density but changing the source energy of 391 eV (which is near the bottom of the unresolved region) to a source energy of 20 keV (which is near the top of the unresolved region). The fluxes obtained (again using the "nonu" option to suppress all secondary fission neutrons) were:

Total flux with probability tables = 0.3161 (0.21%) ($n/cm^2/s$)

Total flux with smooth = 0.3089 (0.21%) ($n/cm^2/s$).

There is not as much attenuation near the top of the unresolved region and more overlap of the resonances. More overlap of the resonances indicates that the actual cross sections are becoming more and more smooth. This is confirmed by these results. The flux obtained with probability tables is only 2% greater than that obtained with the smooth for a neutron source energy near the top of the unresolved region, while it was a factor of 6.8 greater for a neutron source energy near the bottom of the unresolved region.

## 3.3 EIGENVALUE CALCULATION USING PROBABILITY TABLES

Although the emphasis in this paper is on shielding applications, one criticality problem will be summarized. An eigenvalue calculation was made for an infinite medium of homogeneous material with the composition chosen to emphasize the unresolved energy range. The composition utilized in atom percent was: 8.9286% $^{239}Pu$ ; 89.2857% $^{238}U$; and 1.7857% hydrogen. The $^{239}Pu$ and $^{238}U$ cross section sets with probability tables that were utilized in the previous examples were also utilized here. The eigenvalues obtained from the probability table and smooth treatments were:

k with probability tables = 1.51068 (0.00129)

k with smooth = 1.49337 (0.00165)

Delta k = 0.01731 (0.0021),

where the numbers in brackets are the one standard deviation statistical uncertainties. Approximately 32% of the fissions with $^{239}Pu$ were in the unresolved energy range of $^{238}U$. Decreased capture in the $^{238}U$ in the unresolved region as a result of the probability table treatment leads to a larger eigenvalue in this problem.

## 4. SUMMARY

MCNP has been upgraded to include a probability table treatment for neutron cross sections in the unresolved resonance region. This allows the code to correctly account for neutron self-shielding effects in the unresolved region. These effects have not previously been accounted for in MCNP, because the code utilized smooth (i.e., infinitely-dilute) cross sections in the unresolved range.

The upgrade has been performed on MCNP Version 4B. The modified code has been tested on various computer platforms (PC, UNIX, CRAY) using probability tables generated from ENDF data by the NJOY processing code. Sample results have been included here. This capability will be included in the next publicly-released version of MCNP.

## REFERENCES

1. J. F. Briesmeister, Editor, " MCNP - A General Monte Carlo N-Particle Transport Code, Version 4B," LA-12625-M, Los Alamos National Laboratory (March 1997).

2. R. E. MacFarlane and D. W. Muir, "The NJOY Nuclear Data Processing System, Version 91," LA-12740-M, Los Alamos National Laboratory (October 1994).

3. J. M. Otter, R. C. Lewis, and L. B. Levitt, "UBR, A Code to Calculate Unresolved Resonance Cross Section Probability Tables," AI-AEC-13024 (July 1972).

4. R. E. Prael, "Application of the Probability Table Method to Monte Carlo Temperature Difference Calculations," Trans. Am. Nuc. Soc., 17, p. 261 (November 1973).

5. R. N. Blomquist, R. M. Lell, and E. M. Gelbard, "VIM - A Continuous Energy Monte Carlo Code at ANL," Proceedings of a Seminar-Workshop, A Review of the Theory and Application of Monte Carlo Methods, April 21-23, 1980, Oak Ridge, Tennessee, ORNL/RSIC-44.

6. G. I. Bell and S. Glasstone, Nuclear Reactor Theory, Van Nostrand Reinhold Company, New York, 1970.

7. V. McLane, C. L. Dunford, and P. F. Rose, Editors, "ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6," BNL-NCS-44945, Revised, Brookhaven National Laboratory (November 1995).

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