*May 29, 2002* PHYSOR2002 Paper # A0107

Nuclear Science and Technology Division (94)

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Submitted to the
International Conference on the New Frontiers of Nuclear Technology:
Reactor Physics, Safety and High-Performance Computing
October 7–10, 2002,
Sheraton Walker Hill Hotel,
Seoul, Korea

Organized and Sponsored by
Korean Nuclear Society, ANS — Reactor Physics Division
Co-sponsored by
ANS — M&CD and RPSD, Atomic Energy Society of Japan,
Brazilian Association for Nuclear Energy, Canadian Nuclear Society
European Nuclear Society, OECD/Nuclear Energy Agency



*Managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy.

# CALCULATING PROBABILITY TABLES FOR THE UNRESOLVED-RESONANCE REGION USING MONTE CARLO METHODS

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## ABSTRACT

A new module, PURM (**P**robability tables for the **U**nresolved **R**egion using **M**onte Carlo), has been developed for the AMPX-2000 cross-section processing system. PURM uses a Monte Carlo approach to calculate probability tables on an evaluator-defined energy grid in the unresolved-resonance region. For each probability table, PURM samples a Wigner spacing distribution for pairs of resonances surrounding the reference energy (i.e., energy specified in the cross-section evaluation). The resonance distribution is sampled for each spin sequence (i.e., $\ell$-J pair), and PURM uses the $\Delta_3$-statistics test to determine the number of resonances to sample for each spin sequence. For each resonance, PURM samples the resonance widths from a Chi-square distribution for a specified number of degrees of freedom. Once the resonance parameters are sampled, PURM calculates the total, capture, fission and scatter cross sections at the reference energy using the single-level Breit-Wigner formalism with appropriate treatment for temperature effects. Probability tables have been calculated and compared with NJOY. The probability tables and cross-section values that are calculated by PURM and NJOY are in agreement, and the verification studies with NJOY establish the computational capability for generating probability tables using the new AMPX module PURM.

## 1. INTRODUCTION

In the United States, the Evaluated Nuclear Data File (ENDF) system [1] is the repository for evaluated cross-section data. The AMPX-2000 code system [2], which is maintained at the Oak Ridge National Laboratory (ORNL), is used to process ENDF evaluations and generate continuous-energy (pointwise) and multigroup cross-section libraries. For resonance isotopes in neutron cross-section evaluations, the unresolved-resonance region (URR) is an energy region in which the experimental resolution is inadequate for determining the resonance parameters of individual resonances. Energy-averaged unresolved-resonance parameters are typically provided for the URR, and the resonance parameters are averages of resolved-resonance parameters over specific energy intervals; however, the values of the parameters vary as a function of the different energy intervals. Because of the statistical nature of the unresolved-resonance parameters,

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probability tables can be used to provide cross-section probability distribution functions for energy ranges at specific temperatures within the URR.

Different approaches have been used to generate probability tables for an isotope of interest. The conventional or historical approach is to generate continuous-energy cross-section data from a "ladder" of resonances and determine contributions to a probability table based on the point data. This process is then repeated over additional ladders of resonances until the desired number of ladders is processed. The ladder approach, which is described by Levitt [3], is the basis for the probability-table method in NJOY [4].

A new and different procedure relative to the "ladder" approach is used in the AMPX cross-section processing system that has been developed at ORNL. A new AMPX module, PURM has been developed to calculate probability tables in the URR using Monte Carlo (MC) procedures. The motivation for the probability-table development is twofold. **(1)** At ORNL, work is in progress to develop a continuous-energy version of the radiation transport code KENO V.a [5]. In order to support the development efforts for the pointwise version of KENO, a probability table treatment capability is needed for the URR, and the PURM module has been developed to provide probability tables for use in the pointwise version of KENO V.a. **(2)** Prior to the development of AMPX-2000, NJOY was the only production-level cross-section processing system that could be used to provide cross-section libraries based on ENDF/B data through Version VI. Consequently, radiation transport analyses have been limited to a single cross-section processing capability for generating libraries based on ENDF/B-VI data. AMPX-2000 is an independent cross-section processing system that can be used to provide continuous-energy or multigroup cross-section libraries based on ENDF/B data through Version VI for nuclear applications. As part of the AMPX-2000 development, an independent capability to generate probability tables for the URR has been developed. The objective of this work is to demonstrate the capability for calculating probability tables using PURM.

## 2. METHODOLOGY

The objective of the probability-table method is to calculate a distribution function for the cross-section values in a specific energy range within the URR. The approach is in direct contrast with the procedures of the resolved-resonance region (RRR) in which the neutron cross section is obtained at a specific energy using the appropriate resonance formula. The cross-section distribution function is characterized by having a mean value that is equivalent to the infinite-dilution cross-section value for the energy range of interest.

### 1. Resonance-parameter Sampling

PURM uses a MC procedure to calculate probability tables on the evaluator-defined energy grid in the unresolved region. The MC procedure used in PURM is based on the methodology of the code URR [6] that was developed at ORNL in the late 1980s. As opposed to generating a ladder of resonances, PURM determines pairs of resonances or levels surrounding the reference energy or energies for each table. Note that the reference energies are provided in the unresolved-resonance data of the ENDF/B evaluation. As in the ladder approach, the level spacings are sampled from a Wigner distribution:

$$f(x) = W(x) = \frac{\pi}{2} x\, e^{-\frac{\pi}{4}x^2} , \qquad (1)$$

where $x$ is the ratio of the level spacing to the mean level spacing provided in the ENDF data. The resonance and mean level spacing are denoted as $D_{\ell,J}$ and $< D_{\ell,J} >$, respectively, for relative neutron-nucleus angular momentum, $\ell$, and resonance spin, $J$. The spacing distribution in Eq. (1) is a probability density function (PDF) that is normalized to 1. In order to sample the level spacing for a specific $\ell$-$J$ series of resonances (i.e., $D_{\ell J}$), the PDF is converted to a cumulative distribution function (CDF) by integrating Equation (1) from 0 to $x$. The value of $x$ is obtained by setting the CDF equal to a random number, $R$, between 0 and 1. After solving for $x$, the resonance spacing is calculated as the product of $x$ and $< D_{\ell,J} >$.

Once the spacing is sampled from the Wigner distribution, the position, $x'$, of the reference energy in the spacing is selected from a uniform distribution (i.e., $x' = R\, D_{\ell,J}$). The positions of the first and second resonances relative to the reference energy, $E_0$, are obtained by the following expressions:

$$E_{\lambda=1} = E_0 + x' , \qquad (2)$$

and

$$E_{\lambda=2} = E_0 + x' - D_{\ell,J} . \qquad (3)$$

The first pair of resonances that are located above and below the reference energy is determined by Eqs. (2) and (3), respectively. For the remaining pairs of resonances to be processed, the resonance spacings are sampled from the Wigner distribution, and the location of the resonances are determined using a procedure that is analogous to the steps for the first pair of resonances. Although the procedure for sampling the resonance spacing is straightforward, the code must determine the appropriate number of pairs of resonances to sample. To estimate the number of resonances to sample, PURM uses the $\Delta_3$-statistics test which is described in Section 2.2.

Once the distribution of energy levels is sampled, the resonance widths must be sampled for each resonance. In the unresolved region, the ENDF data provide average widths for reference energies in the URR. The distribution function for the resonance widths follows a Chi-square distribution with a designated number of degrees of freedom, $\nu$:

$$P_\nu(y) = \frac{\nu}{2G(\nu/2)} (\nu y/2)^{\frac{\nu}{2}-1} e^{-\nu y/2} , \qquad (4)$$

where $y$ is the ratio of the resonance width for a particular channel (i.e., $\Gamma_{\lambda c}$) to the mean channel width for a given energy range (i.e., $<\Gamma_{\lambda c}>$ ). The different channels, $c$, that are considered are fission, capture and scattering. In Eq. (4), the quantity $G(\nu/2)$ is the mathematical gamma function. For the neutron width, $\nu$ is typically equal to 1, and Equation (4) has the form of the Porter-Thomas distribution law of the neutron width.[7, 8] Fission is regarded as a few-channel process, and two or three degrees of freedom ($\nu$ = 2 or 3) are typically assumed for the fission width distribution.

Regarding neutron capture, there are a large number of capture channels that are available, and the number of degrees of freedom is assumed to approach infinity ($\nu \rightarrow \infty$), and the Chi-square distribution becomes a Dirac-delta function centered at $\Gamma_{\lambda\gamma} = <\Gamma>$. As noted previously, the ENDF data provide the average resonance widths along with the number of degrees of freedom for the corresponding Chi-square distribution. During the MC simulation, PURM obtains the widths for each resonance by sampling the Chi-square distribution with the corresponding number of degrees of freedom.

The sampled widths and spacings are used to calculate cross sections in the URR using the single-level Breit-Wigner (SLBW) formulae. PURM has the capability to calculate temperature-dependent cross sections in the unresolved region. The sampled resonance parameters are used in conjunction with the SLBW formulae to calculate temperature-dependent cross sections for scattering, capture, fission and total. The SLBW formulae [6] are well documented and not presented in this paper. Note that the temperature dependence of the cross sections are obtained using the symmetric and antisymmetric-line-shape functions (i.e., $\psi$ and $\chi$, respectively) that are documented in most reactor theory textbooks.

## 2. Dyson and Mehta $\Delta_3$-Statistics Test

One of the essential tasks for constructing the resonance distribution for a given spin sequence (i.e., $\ell$-$J$ pair) is the determination of the appropriate number of pairs of resonances to process. A useful tool for evaluating the distribution of resonances is the $\Delta_3$-statistics test that was developed by Dyson and Mehta [7, 9]. PURM uses the $\Delta_3$-test to determine the appropriate number of pairs of resonances to process for each spin sequence.

The $\Delta_3$-test provides a measure of the mean-square deviation between the number of observed energy levels within an energy interval from $E_i$ to $E_f$ [9]:

$$\Delta_3 = Min(a,b)\left[\frac{1}{2L}\int_{E_i}^{E_f}(N(E) - aE - b)^2 dE\right], \qquad (5)$$

where $2L$ is the total number of resonances and $N(E)$ is the observed cumulative number of resonances as a function of energy. In Eq. (5), $a$ and $b$ are the slope and constant, respectively, for a linear fit to the observed cumulative number of resonances as a function of energy.

The numerical procedures that are provided in Ref. 7 for calculating $\Delta_3$ for a spin sequence are used in PURM to evaluate the expression in Eq. (5). For the sampled distribution of resonances for each spin sequence, PURM calculates a $\Delta_3$ value and the linear fit for the cumulative number of levels (i.e., $N(E) = aE + b$ ). The Dyson and Mehta $\Delta_3$-test also predicts that the theoretical average value for $\Delta_3$ is given by the following expression:

$$<\Delta_3> = \frac{1}{\pi^2}[\ln(n) - 0.0687], \qquad (6)$$

where $n$ is the number of energy levels observed in the interval from $E_i$ to $E_f$. The variance of $<\Delta_3>$ is $1.169/\pi^4$.

The objective of the $\Delta_3$-test is to determine a resonance spacing distribution that provides a $\Delta_3$ value that is in agreement with $<\Delta_3>$. In addition to the comparison between the calculated and theoretical values for $\Delta_3$, the linear fit for the cumulative number of levels should agree with the observed number of levels in the sampled distribution.

There is a two-part convergence problem for the implementation of the $\Delta_3$-statistics test. One part involves the linear fit for $N(E)$ as a function of energy, and the second part involves the convergence of the $\Delta_3$ values. In other words, reasonable $\Delta_3$ values (i.e., within 2 standard deviations of theoretical value) may be obtained for a sampled distribution; however, the cumulative number of resonances that is predicted by the linear fit may not correspond to the observed number of resonances for the distribution. In contrast, an acceptable linear fit for the cumulative number of resonances may be obtained for a sampled distribution, but the $\Delta_3$ value for the sampled distribution may disagree with the theoretical value by more than two standard deviations. The $\Delta_3$ test is extremely sensitive to the location of each level in the distribution.

Regarding implementation of the $\Delta_3$ test, PURM determines the number of levels to sample for each spin state based on a linear fit for the cumulative number of observed levels. In other words, PURM samples a Wigner distribution to obtain a distribution of resonances using some initial value for the pairs of resonances to sample about the reference energy. The linear fit for the cumulative number of levels is compared with the observed number of levels in the sampled distribution. The number of pairs of resonances to sample is incremented until the observed number of levels in the sampled distribution is predicted to within 0.1% by the linear fit for $N(E)$. The $\Delta_3$ value is also calculated for the sampled distribution; however, PURM currently does not attempt to find a resonance distribution that has a $\Delta_3$ value within two standard deviations of the theoretical value as well as an acceptable linear fit for the cumulative number of levels. Extensive CPU times would be required to seek convergence for both the $\Delta_3$ value and an acceptable fit for the cumulative number of levels. PURM searches for the distribution that provides an acceptable linear fit for the cumulative number of levels. Based on calculational experience, accurate cross-section values can be obtained by seeking convergence for the cumulative number of levels.

## 3. Monte Carlo Simulation

Because the URR is an energy region where the parameters are averages of resolved-resonance parameters over an evaluator-defined energy region within the URR, MC procedures can be used to calculate the average cross sections within the URR. Since random variables are used in the sampling procedures for the resonance parameters, different resonance parameters and cross sections can be obtained from different random number sequences. However, the MC simulation of the problem can estimate the desired cross-section quantity by observing the behavior of a large number of individual histories.* The exact solution can be approximated if a sufficiently large number of histories are processed. This concept is often referred to as "The Law of Large Numbers."

For the purposes of discussion, a single history or $i^{th}$ estimate of a cross-section quantity is denoted as $\sigma_{cI}$, where $c$ denotes either total, capture, fission or scatter. For each history, pairs of resonances are randomly sampled for each $\ell$-$J$ spin sequence, and the number of resonances is determined using

*A history denotes a single calculation or estimate of the total cross-section at an energy $E$ from the sampled resonances and corresponding widths. Note that the capture, fission and scatter cross sections are also calculated as part of a single history.

the $\Delta_3$-statistics test. For each resonance, the partial widths are sampled from a Chi-square distribution as defined by Eq. (4). The resonances and corresponding widths are sampled for each $\ell$-$J$ spin sequence. The $i^{th}$ estimates for the capture, fission and scatter cross sections are obtained using the SLBW formulae and summing the contribution from all $\ell$ and $J$ states. The $i^{th}$ estimate for the total is obtained by summing the capture, fission and scatter cross section. The process is repeated for each history until $n$ histories have been processed. The MC estimate of the mean cross-section value is given by the following expression with the reaction identifier, $c$, implied in the expression:

$$\bar{\sigma}_j = \frac{1}{n} \sum_{i=1}^{n} \sigma_i \ . \tag{7}$$

Note that the definition of $j$ will be provided shortly. The value of $\bar{\sigma}_j$ will approach the true mean as $n$ approaches $\infty$. The variance of $\bar{\sigma}_j$ is estimated with the following expression:

$$V^2_{\bar{\sigma}_j} = \frac{1}{n(n-1)} \sum_{i=1}^{n} ( \sigma_i - \bar{\sigma}_j )^2 \ . \tag{8}$$

In Eq. (7), the value of $\bar{\sigma}_j$ is obtained from $n$ estimates of the mean value. Let the quantity defined by Eq. (7) constitute a "batch" estimate of the mean value. Using the batch terminology, the $j^{th}$-batch estimate for the mean value is denoted with the subscript $j$ in Eq. (7). If a different set or batch of $n$ random samples is taken, a different mean cross-section value would be calculated. Based on the Central Limit Theorem [8], if $N$ batch estimates for $\bar{\sigma}_j$ are obtained, the distribution of $\bar{\sigma}_j$ will approach a normal distribution as $N$ increases. The Central Limit Theorem implies that the statistical nature of the distribution of $\bar{\sigma}_j$ is independent of the actual distribution of the individual samples (i.e., $\sigma_i$). If $N$ batches are processed, the "grand mean" is calculated by averaging over all the batches:

$$\bar{\sigma} = \frac{1}{N} \sum_{j=1}^{N} \bar{\sigma}_j \ . \tag{9}$$

The variance is calculated with the following expression:

$$V^2_{\bar{\sigma}} = \frac{1}{N(N-1)} \sum_{j=1}^{N} ( \bar{\sigma}_j - \bar{\sigma} )^2 \ . \tag{10}$$

In PURM, the mean value for the total, capture, fission and scatter cross sections is obtained using Eq. (9) based on $N$ batch estimates of each reaction.

Each probability table is constructed using monotonically increasing band limits (i.e., $B_1 < B_2 < ... < B_k < ... < B_K < B_{K+1}$) that are based on the total cross section. If $K$ cross-section bands are defined, $K$+1 band limits are required to define the table. The band limits increase in value with a corresponding increase in band number. As a result, the lower cross-section band value for the first band is the minimum band value for the table, and the upper cross-section band value for the last band is the maximum band value for the table. Because the table construction is based on the total cross section, the average total cross-section value in each band should also increase monotonically with increasing band number. Note that the band averages for the corresponding partial reaction cross sections are conditional averages that correspond to the average total cross section for the

band. Consequently, the band-average cross-section values for capture, fission and scatter will not necessarily increase monotonically.

In PURM, there are three options to determine the band values for each table. For the first option, the user can specify the band values for each table, and for the remaining two options, PURM can construct each table with either equal- or nonequal-probable cross-section bands. If nonequal-probable cross-section bands are used, the total cross-section band values are calculated with the following expression:

$$B_k = B_{\min}\left( \frac{B_{\max}}{B_{\min}} \right)^{\frac{k-2}{K-2}} ; \; k = 2,3,.....,K , \tag{11}$$

where $B_{min}$ is the lower bound for the second band, and $B_{max}$ is the lower bound for the last band (i.e., $B_K$). The values of $B_{min}$ and $B_{max}$ can be specified by the user or determined by the code. If the user does not specify the values of $B_{min}$ and $B_{max}$, PURM estimates these values. Once the values of $B_{min}$ and $B_{max}$ are established, PURM uses Eq. (11) to construct the cross-section band limits for each probability table. Note that $B_1$ and $B_{K+1}$ are not determined prior to the calculation of a probability table. The values of $B_1$ and $B_{K+1}$ represent the absolute minimum and maximum cross-section values of the MC simulation. As a result, the absolute minimum and maximum cross-section values are determined during the calculation of each probability table. The value of $B_1$ must be $\geq 0$ and $< B_2$, and the value of $B_{K+1}$ can be any value that is greater than $B_K$.

Once the cross-section band limits are established for a table, PURM performs a MC simulation for each table using a specified number of iterations or histories for a specified number of batches. For a single history in PURM, the procedures of Section 2.1 and 2.2 are used to sample the resonance parameters for the reference energy point in the URR. Subsequently, the SLBW formulae are used to calculate the scatter, capture, fission and total cross sections at the reference energy. As noted previously, the calculation of the total cross section and corresponding partial reactions at the reference energy constitute a single history.

For each history in a batch, the calculated total cross-section value is compared with the cross-section band limits for the table. The total cross-section is added to the appropriate cross-section band (i.e., $k^{th}$ band) within the probability table. In addition, a counter assigned to the band is advanced by unity. The corresponding band values for the scatter, capture and fission cross sections are also added to the appropriate registers for the $k^{th}$ band. Note that the band selection for the partial reactions is based on the value of the total cross section. At the completion of the number of histories for the batch, the average value for the total cross section for the $k^{th}$ band (i.e., $\bar{\sigma}_{l,k}$) is calculated by dividing the cumulative sum for the band by the number of tallies within the band. The corresponding average band values for the scatter, capture and fission cross sections are calculated in a similar manner to the total cross section. The batch estimate for the probability for each band is obtained by dividing the number of tallies for the band by the number of histories in a batch. Once the initial batch is completed, the next batch is processed using the same procedure for each history in a batch. The calculation for a table is complete when all of the batches have been processed.

Due to the nature of the calculational procedures, PURM provides a mechanism for monitoring the convergence of the cross-section calculation. During the MC calculation for a table, PURM stores

a "running" average (i.e., by batch processed) of the total, capture, fission and scatter cross section for the entire probability table. PURM has the capability to plot the cross-section calculation by batches run. Also, PURM provides histogram frequency plots for each calculation for a reaction and performs a test for normality (i.e., Chi-square test) for the MC calculation for each reaction.

Using the MC approach with the Dyson and Mehta $\Delta_3$-test to calculate probability tables in the URR provides distinct advantages relative to the conventional ladder approach. The $\Delta_3$-test provides a statistical procedure to determine the number of resonances to sample in the probability calculation. In addition, the MC procedures coupled with the statistical checks (i.e., cross-section calculation plot by batches processed, frequency distribution plot, chi-square test for normality of sampled distribution) allows the user to determine if the cross-section calculation is converged. In contrast, the conventional ladder approach does not have a mechanism for determining whether a sufficient number of ladders have been processed to ensure convergence. As with any method, there are advantages and disadvantages. For the MC approach, the CPU times can be longer relative to the ladder approach; however, the total number of histories that are needed for a probability table calculation are relatively low when compared with a MC radiation transport calculation (e.g., deep-penetration shielding problem, eigenvalue calculations, etc.). For a MC radiation transport calculation, millions of histories may be needed to solve the transport problem. In contrast, the number of histories needed to calculate a probability table will be on the order of a few thousand (e.g., 10,000). A comparison of the CPU time for the ladder approach relative to the MC approach is provided in the next section.

## 3. RESULTS

PURM has been used to calculate probability tables for ENDF/B-6 $^{235}$U (MAT = 9228). Results are provided to demonstrate the capabilities of PURM. In addition, comparisons are made with the NJOY99.14 module PURR to verify the calculational results obtained with PURM. All calculations were performed on a DEC Alpha XP1000 workstation.

For ENDF/B-6 $^{235}$U, the URR extends from 2.25 keV to 25 keV, and the evaluation has 14 reference energies in the unresolved region. PURM was used to calculate 14 probability tables that correspond to the reference energies in the evaluation. Each probability table was calculated at 300 K using 200 batches with 50 histories per batch for a total of 10,000 histories per table. As noted previously, the total number of histories is relatively low compared with typical MC radiation transport calculations (e.g., deep-penetration shielding problems, eigenvalue calculations, etc.). Fortunately, probability-table calculations do not have the complexities that are associated with radiation transport problems (e.g., complex geometry, particle streaming, etc.). As a result, a probability table calculation is generally a well-behaved problem. Therefore, a relatively large number of histories is not required to obtain acceptable statistics in a probability-table calculation.

The PURM results for the probability table at 2.25 keV are presented in Table I. For $^{235}$U, the probability tables were calculated with 5 nonequal probable cross-section bands. The probability and standard deviation associated with each band are also provided in Table I. Moreover, the average cross-section values and standard deviations for the total, capture, fission and scatter cross-sections are provided for each band within the probability table. PURM also provides the average cross-section values for each table, and the average values (in barns) for total, capture, fission and scatter are 19.68 ± 0.04, 2.04 ± 0.01, 5.70 ± 0.02 and 11.94 ± 0.01, respectively. Note that the

average cross-section values for the table represent the infinite dilution values for $^{235}$U at 2.25 keV and 300 K.

Table I. Probability-table for $^{235}$U at 2.25 keV and 300 K

| Band | Limits[a] | Probability[b] | Total[a, b] | Capture[a, b] | Fission[a, b] | Scatter[a, b] |
|---|---|---|---|---|---|---|
| 1 | 11.86 | 0.197 (0.004) | 14.78 (0.02) | 0.82 (0.01) | 2.53 (0.02) | 11.43 (0.01) |
| 2 | 16.01 | 0.383 (0.005) | 17.79 (0.01) | 1.54 (0.01) | 4.49 (0.02) | 11.76 (0.01) |
| 3 | 19.75 | 0.281 (0.005) | 21.75 (0.03) | 2.52 (0.02) | 7.14 (0.03) | 12.10 (0.02) |
| 4 | 24.38 | 0.114 (0.003) | 26.54 (0.05) | 3.86 (0.05) | 10.00 (0.08) | 12.68 (0.04) |
| 5 | 30.08 | 0.025 (0.002) | 32.83 (0.18) | 5.64 (0.15) | 13.62 (0.19) | 13.55 (0.11) |
| | 56.28 | | | | | |

[a] Cross-section values are in barns

[b] Quantities in parentheses represent 1 standard deviation

For each probability-table calculation, PURM provides the results of the $\Delta_3$-statistics. The number of levels that is predicted from the $\Delta_3$-statistics test is provided in Table II for the $^{235}$U calculation at 2.25 keV. In Table II, the observed number of levels, which is obtained by iteration, is provided for each $\ell$-$J$ spin sequence. Based on the $\Delta_3$-statistics test, the predicted number of levels, $N(E)$, is also provided for comparison. The value for $N(E)$ is obtained by performing the $\Delta_3$-statistics analysis for the observed number of levels and corresponding spacing distribution. As shown in Table II, the predicted values are within 0.01% of the observed number of levels in the MC calculation.

Table II. Predicted number of levels from $\Delta_3$-statistics for $^{235}$U at 2.25 keV and 300 K

| $\ell$ | $J$ | Observed no. of levels | $N(E)$ | $a$ | $b$ |
|---|---|---|---|---|---|
| 0 | 3. | 727 | 727.01 | 1.02 | $-1.93 \times 10^3$ |
| 0 | 4. | 895 | 895.05 | 1.28 | $-2.43 \times 10^3$ |
| 1 | 2. | 538 | 537.94 | 0.76 | $-1.44 \times 10^3$ |
| 1 | 3. | 717 | 717.03 | 1.02 | $-1.94 \times 10^3$ |
| 1 | 4. | 889 | 889.03 | 1.26 | $-2.39 \times 10^3$ |
| 1 | 5. | 997 | 997.0 | 1.41 | $-2.68 \times 10^3$ |

In order to compare the calculated probability tables between the NJOY module PURR and the AMPX-2000 module PURM, NJOY99.64 was used to calculate probability tables for $^{235}$U at 300 K. For the NJOY calculations, NJOY was instructed to generate tables with 5 cross-section bands using 4 ladders of resonances. Subsequently, the cross-section bands that were generated by NJOY were specified in the PURM input file, and PURM was used to re-calculate the probability tables with the cross-section bands from NJOY. By using the same cross-section bands, a more accurate comparison can be made between the cross-section calculation procedures of both codes. Note that PURM can accept user-defined cross-section bands or determine the values of the cross-section bands using Eq. (11). In addition, PURM has the capability to determine equiprobable cross-section bands for a user-specified number of bands. The probabilities that are obtained with PURM and NJOY at 2.25 keV are plotted as a function of the cross-section bands in Figure 1. Based on the results in Figure 1, the PURM-calculated probabilities agree with the NJOY values. Similar agreement is obtained for the NJOY and PURM average band values for the total, capture, fission and scatter cross sections. Note that similar results are also obtained for the remaining 13 probability-table calculations for $^{235}$U.

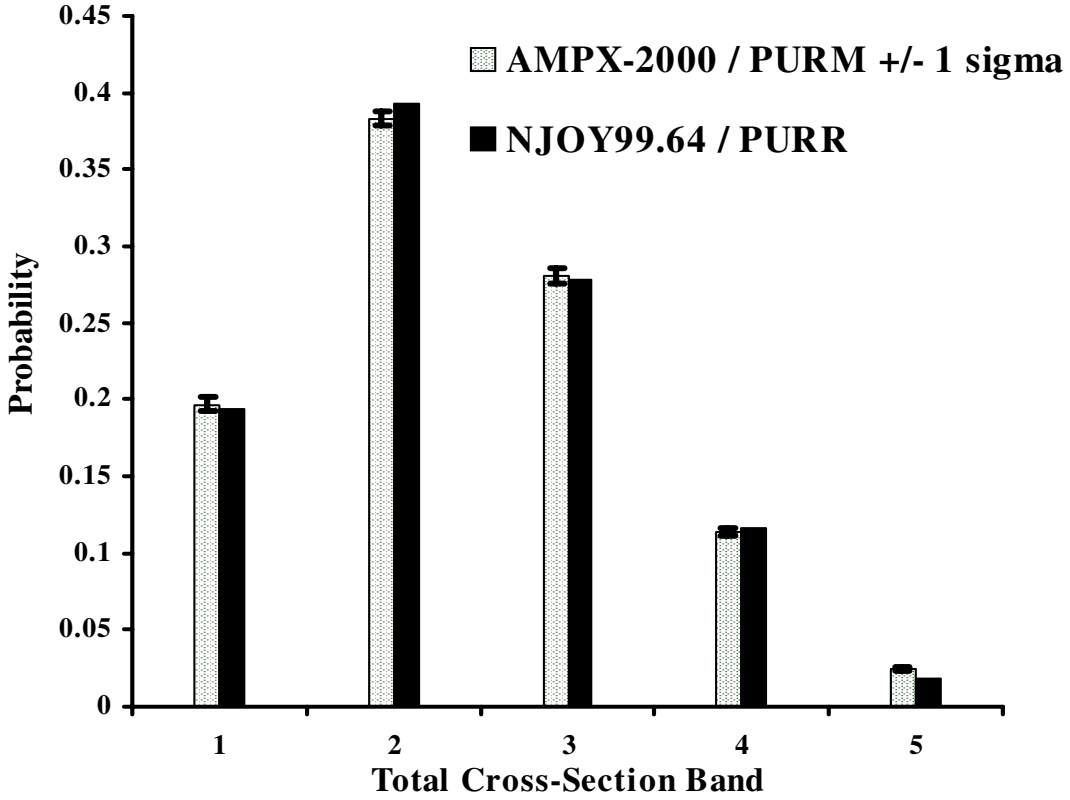


Figure 1. Probability-table comparison between PURM and NJOY for $^{235}$U at 2.25 keV and 300 K

With regard to CPU times, the time required for the NJOY calculation (i.e., for 14 different probability-tables) is 33.6 seconds. In contrast, the time required to calculate the 14 different probability tables using PURM with 10,000 histories is 35.68 minutes. Although the computational times for NJOY are much faster for the $^{235}$U case, the two computational approaches are vastly different, and the longer CPU times for PURM are attributed to the number of histories processed, as well as the implementation of the iterative $\Delta_3$-statistics test for determining the number of resonances to sample for each $\ell$,J-spin sequence. Note that NJOY does not use the $\Delta_3$-statistics test to evaluate the distribution of resonances sampled from a Wigner distribution. Consequently, NJOY does not have a mechanism for assessing the adequacy of the sampled resonance distribution. In addition, acceptable probability tables may be calculated with PURM using far fewer histories; thereby, reducing the CPU time for each table.

A brief parametric study has been performed to investigate the CPU time variation as a function of the number of histories used in the MC calculation. For the 10,000 history case, PURM requires 2.62 minutes of CPU time to calculate a single probability table. For the $^{235}$U case at 2.25 keV and 300 K, the PURM calculation was repeated with histories of 5000, 2500, 1200 and 600. In addition, the quality of results for the probability table was also investigated following each calculation. The different CPU times are presented in Table III as a function of the number of histories processed. Based on the results in Table III, the CPU time per probability table decreases in a linear fashion as the number of histories is decreased. In Figure 2, the probability-table results for the 2.25 keV case are presented for the different number of histories used in the MC calculation.

Based on the results in Figure 2, acceptable probability tables can be obtained with significantly fewer histories relative to the 10,000 history case. Additional parametric studies should be performed to investigate the quality of results obtained by decreasing the number of histories. Based on the verification studies with NJOY, the probability tables as calculated by PURM are suitable for use in nuclear applications. In addition, AMPX-2000 provides an independent approach for calculating probability tables for the URR.

Table III. CPU times as a function of histories processed with PURM for $^{235}$U at 2.25 keV and 300 K

| Number of histories | CPU time for single probability-table calculation |
|---|---|
| 10,000 | 2.62 minutes (157.2 sec) |
| 5,000 | 1.32 minutes ( 79.2 sec) |
| 2,500 | 0.68 minutes ( 40.8 sec) |
| 1,200 | 0.34 minutes ( 20.4 sec) |
| 600 | 0.18 minutes ( 10.8 sec) |

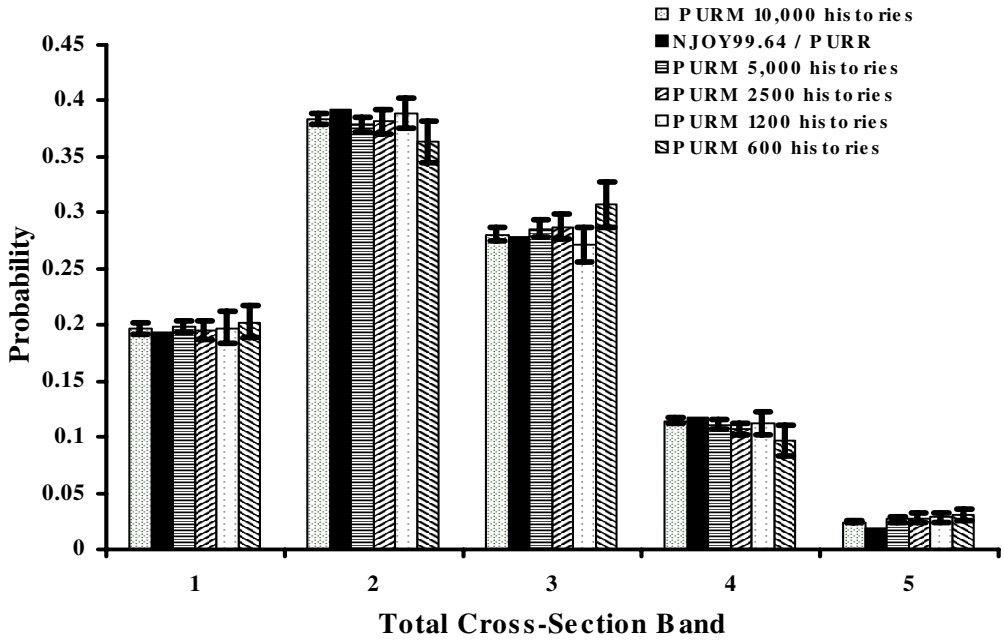


Figure 2. Probability-table results for ENDF/B-VI $^{235}$U ( 2.25 keV and 300 K) with PURM using different number histories in Monte Carlo calculation

## CONCLUSIONS

Prior to the development of AMPX-2000 at ORNL, the NJOY code system was the only complete software package that could be used to process data for all versions of ENDF/B through Version VI. AMPX-2000 has the capability to provide continuous-energy and multigroup cross-section libraries based on ENDF/B data through Version VI for a wide variety of nuclear applications. PURM, which is a Monte Carlo module in AMPX, has been developed to provide probability tables in the URR in order to support development activities for a future version of KENO V.a that will

use continuous-energy cross-section libraries. The libraries that are produced by AMPX are independent from the NJOY cross-section processing system.

PURM uses MC procedures to sample the resonance spacings and widths in the URR. Once the resonance parameters are sampled, the total, capture, fission and scatter cross sections are calculated at the reference energy using the single-level Breit-Wigner formalism with appropriate treatment for temperature effects. The cross-section calculation constitutes a single iteration or history. For the cross-section calculation and corresponding probability-table calculation, a user-specified number of batches with a corresponding number of histories per batch is processed. For each history, the total, capture, fission and scatter cross sections are calculated at the reference energy, and the corresponding contribution to the probability table is determined for each history. After completing the specified number of histories for a batch, a batch estimate for the probability for each cross-section band within a table is obtained by dividing the number of tallies for the band by the total number of histories processed. Additional batches are processed until the user-specified number of batches are complete. Due to the statistical nature of the MC procedures, PURM provides a mechanism for monitoring the convergence of the cross-section calculation. For each reaction, a plot of the calculated cross section is provided by batches run. In addition, PURM provides a frequency distribution plot and Chi-square test for normality for each cross-section calculation.

In an effort to demonstrate the new procedures, probability tables have been calculated for ENDF/B-6 $^{235}$U using PURM and NJOY. The probability tables and corresponding cross-section values obtained with both codes are in agreement. As a result, the verification studies establish the computational capability for generating probability tables using the new AMPX module PURM.

## ACKNOWLEDGMENTS

The work presented in this paper was sponsored by the United States Nuclear Regulatory Commission.

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