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A Study of the Required Fidelity for the Representation of Angular Distributions of Elastic Scattering in the Resolved Resonance Region for Nuclear Criticality Safety Applications[1]

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Abstract – *Angular distributions of elastic scattering in the resolved resonance region can be reconstructed from the resonance parameters directly, or they can be provided in a point-wise manner with respect to incident neutron energy in nuclear data files. This study investigates the required fidelity in energy for the accurate representation of the angular distributions of elastic scattering in the resolved resonance region with respect to the performance in neutron transport calculations for nuclear criticality safety applications. A dense energy grid such as that used to represent angle integrated cross sections in the resolved resonance region, is not necessary for representation of angular distributions. A reduction in the number of points in energy on the order 5–10× (a 5–10× reduction of storage) gives the same results in a wide variety of neutron transport problems simulated.*

I. INTRODUCTION

The evaluated nuclear data file (ENDF) [1] format allows the evaluator to specify that the evaluation in the resolved resonance region (RRR) is suitable for angular distribution of elastic scattering to be reconstructed directly from the evaluated resonance parameters in File 2. Until now, this option has rarely been used. Instead, the angular distribution of elastic scattering has been provided in tabulated and/or Legendre order as a function of the incident particle energy in File 4. One reason to provide a point-wise evaluation of the angular distribution of elastic scattering is that until recently, nuclear data processing codes could not run the calculations needed to reconstruct the full differential cross section from the resonance parameters according to the Blatt and Biedenharn formalism [2] for all types of the R-Matrix theory used to describe the RRR. This capability was recently added to the prerelease of the NJOY [3] processing code.

The NJOY methodology to process angular distribution of elastic scattering requires that the coefficients of expansion of the Legendre moments of angular distribution be reconstructed on the same energy grid as that constructed by the RECONR module. This ensures that the maximum error resulting from linear interpolation between adjacent energy points and the true angle-integrated cross section is less than a user-defined value, usually set to 0.1% relative error. Recent research indicates that such high fidelity in energy when representing coefficients of expansion for the Legendre moments of the angular distribution of elastic scattering is not necessary for neutron transport calculations being used for practical applications. The reconstructed angular distributions are applicable strictly at zero-Kelvin temperature. Doppler-broadening of the scattering moments is an approximation. A consistent implementation in Monte Carlo (MC) codes would be to use a library at zero-Kelvin and then sample the speed and direction of the target atom within the MC code. No known standard MC code is currently capable of doing this, so it is reasonable to thin the angular distributions to follow the broad trends. The actual number of points in energy necessary to preserve highly accurate results in neutron transport calculations is the subject of the present investigation.

While the methodology used in NJOY to reconstruct the angular distributions of elastic scattering from the evaluated parameters of the RRR is conservative in terms of preserving the correct physics, it is not conservative on computer memory. To accommodate for nuclear data processing codes that have not yet implemented the Blatt and Biedenharn formalism calculation methodology for double differential cross section, the authors, as evaluators, recommend providing the coefficients of expansion in the Legendre moments of the angular distribution in a point-wise manner in File 4 with the explicit message in File 1. Resonance parameters are suitable for reconstructing the angular distributions of elastic scattering, but when such a capability is not available, a point-wise evaluation has been provided in File 4. To provide an ENDF file of reasonable size for users who do not have the Blatt and Biedenharn capability in their processing code, a study of techniques has been

conducted to reduce the number of points in energy necessary to (1) represent angular distributions in the RRR, and (2) maintain a highly accurate representation of the physics of the RRR in the neutron transport calculations.

Section III presents the techniques studied to reduce the number of points in energy to represent the angular distribution of elastic scattering. The tests to determine the performance of processed nuclear data files with different fidelity angular distributions in neutron transport problems are discussed in Section IV. Both successful and unsuccessful techniques for reducing the size of the point-wise file are presented. Detailed examples are presented showing how the proposed methodology is applied to the RRR evaluation of three isotopes: ^{16}O, ^{63}Cu and ^{65}Cu.

II. BACKGROUND

A neutron at a given incident energy scatters into solid angle dΩ. The preferred ENDF format method to represent and store angular distributions for elastic and inelastic scattering is the coefficients of Legendre polynomials. The definition of the coefficients, α_l, is,

$$\alpha_l(E) = \frac{2\pi}{\sigma_s(E)} \int_{-1}^{+1} \sigma_s(E,\mu) P_l(\mu) d\mu \,, \qquad (1)$$

where, $\sigma_s(E)$ is the angle integrated scattering cross section. The physical interpretation of the first two Legendre polynomials, $P_1(\mu) = \mu$ and $P_2(\mu) = (3\mu^2-1)/2$, is straightforward. The first Legendre coefficient, $\alpha_1(E)$, is often the primary determining factor of the amount of forward scattering. It determines whether more neutrons will scatter in the forward direction relative to their direction of motion, or if they will back scatter to return to their original location. The second Legendre coefficient, $\alpha_2(E)$, indicates whether the scattering distribution of the isotope is enhanced in the forward/backward direction ($\alpha_2 > 0$) or in the orthogonal direction ($\alpha_2 < 0$).

III. METHODOLOGY

A careful study was performed to determine how to reduce the number of energy points necessary to represent the angular distributions of elastic scattering in terms of the Legendre coefficients. The goal was to find the minimum number of energy points necessary to represent the angular distributions while maintaining the high-fidelity physical representation of the resonance phenomena present in the angular distributions. The study's success was measured by comparing performance of the evaluation with the reduced number of energy points in the angular distribution against the full fidelity representation in continuous-energy radiation transport codes. A progressive series of reductions was proposed based on physics and mathematics, and a comprehensive testing system has been established.

The first step in reducing the number of energy points in the point-wise representation was to successively relax the linear interpolation criteria. Originally, in the full fidelity representation, points are selected on 0.1% linear interpolation criteria. Therefore, at no point in the continuous function between any two consecutive points in the point-wise representation should the relative error exceed 0.1% when compared to the linear interpolation. The resulting reduction in the number of energy points is presented in Table I. A mathematical smoothing algorithm was applied to each reduced set of energy points that smoothed expansion in the coefficients.

TABLE I. Number of Energy Points vs Linear Interpolation Criteria Used to Generate the Energy Grid.

Interpolation Criteria		0.1%	10%	100%
^{16}O		15 601	6 342	2 327
	Smoothed	4 151	1 590	633
^{63}Cu		83 467	16 673	11 440
	Smoothed	10 373	8 568	7 078
^{65}Cu		65 922	14 119	10 341
	Smoothed	7 943	6 805	5 758

For such a significant reduction in the number of energy points, the visual effect on the coefficients of the Legendre expansion is nearly insignificant. Figure 1 presents a segment of the first coefficient of expansion of the angular distribution for ^{63}Cu in the RRR. Figure 2 shows a similar comparison for ^{16}O. Two reductions in the number of energy points are plotted, and the difference between the lines is minimal.

To further reduce the numbers of energy points in the representation of the angular distributions, two successive physical approximations were made. The first approximation eliminated all resonances with associated orbital-angular momentum larger than zero. This is based on the understanding that the structure of the angular distributions of elastic scattering through the Blatt and Biedenharn formalism is dominated by the strong s-wave (orbital angular momentum equal to zero) resonances. Therefore, eliminating all higher orbital angular momentum resonances provides a systematic, physical way to reduce the number of energy points necessary to model major resonance features of angular distributions. Furthermore, all the smallest s-wave resonances can be eliminated if it is necessary to reduce the number of energy points even more dramatically. All the combinations and their final number of energy points for ^{63}Cu and ^{65}Cu are presented in Table II.

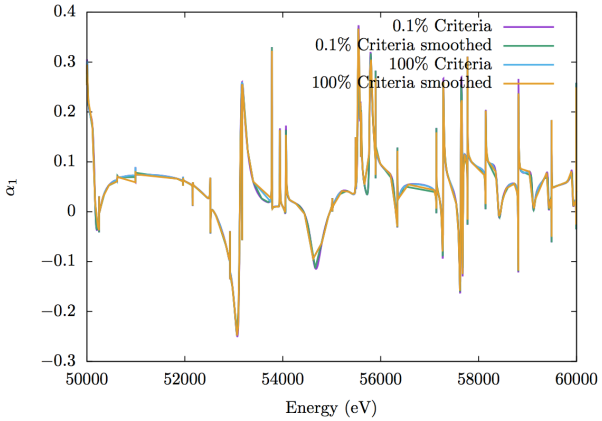

Fig. 1. Coefficient of first moment in Legendre expansion of angular distribution of elastic scattering for ^{63}Cu in RRR for the 0.1% and the 100% relative error in the linear interpolation criteria, with smoothed versions.

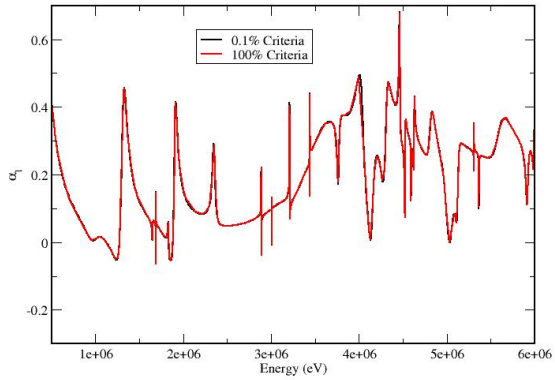

Fig. 2. Coefficient of first moment in Legendre expansion of angular distribution of elastic scattering for ^{16}O in RRR for the 0.1% and the 100% relative error in the energy range 500 keV and 6 MeV.

The angular distribution files with the reduced number of energy points were first subjected to a series-specific MC neutron transport problem to test performance of the angular distribution reconstruction in neutron transport compared to results for nuclear data files processed with the NJOY angular distribution reconstruction capability. The second stage of testing was performed using sets of International Criticality Safety Benchmark Evaluation Project (ICSBEP) [4] benchmark models with significant sensitivities to the isotopes of interest. The goal of this stage was to analyze performance of the processed nuclear data files in real applications.

TABLE II. Number of Energy Points vs Physical Approximation Used to Generate the Reduced Energy Grid

	^{63}Cu		^{65}Cu	
Interpolation criteria	10%	100%	10%	100%
Eliminated p-waves	8624	5409	6080	4089
Eliminated p-waves (smoothed)	3543	2711	2245	1769
Eliminated p-wave Reduced s-waves	5366	2756	3417	1850
Eliminated p-wave Reduced s-waves (smoothed)	2442	1762	1555	1151

Two dedicated computational exercises were devised with the geometry and neutron physics best suited to expose the impact of the angular distributions on neutron transport physics. One problem had a fixed-source, and the other was an eigenvalue-type problem. The fixed source problem consisted of a unidirectional point source of neutrons aimed at a dense sphere of the material of interest. The neutron source was mono-energetic, with energy selected as one of the test parameters. A wide detector was modeled on the other side of the target sphere, and tallies were taken in 50 energy bins and 10 different angular bins. The density of the target material was also varied as one of the test parameters to control the average number of scattering events and to govern how much the neutron slowed down before reaching the detector. This ensured that the angular distribution of elastic scattering was tested from the upper end of the resolved resonance region all the way to thermal energies.

In the second specific test problem, a sphere with a radius of 10 cm centered at the origin was filled with one of the isotopes of interest (^{16}O, ^{63}Cu or ^{65}Cu) up to r = 7 cm. The remainder of the sphere was filled with ^{235}U in a homogenous mixture with ^{1}H. The U/H ratio was decreased until the energy of the average lethargy of neutrons causing fission was down in the resolved resonance region of the evaluation for the isotope of interest. The neutron current tallied in 50 energy bins and 10 cosine bins was recorded on the reflector/fuel boundary. The asymmetric geometry of this computational experiment tested the back scattering of the target isotopes in the resolved resonance region.

The collective set of ICSBEP benchmarks used as a final test of the performance of the reduced angular distributions for ^{16}O is presented in Table III using the short-hand ICSBEP nomenclature. The ICSBEP benchmarks used to test performance of the reduced angular distributions of ^{63}Cu and ^{65}Cu are given in Table IV.

TABLE III. Collection of ICSBEP Benchmarks Used to Test Performance of the Reduced Angular Distribution of Elastic Scattering for ^{16}O.

Benchmark Number	ICSBEP Benchmark Name
1	LMT-15-15
2	LMT-15-16
3	ZED-2

TABLE IV. Collection of ICSBEP Benchmarks Used to Test Performance of the Reduced Angular Distribution of Elastic Scattering for ^{63}Cu and ^{65}Cu.

Benchmark Number	ICSBEP Benchmark Name
1	HMF-72-01
2	HMF-72-03
3	HMF-73-01
4	HMF-84-06
5	HMF-84-18
6	HMF-85-01
7	HMF-85-02
8	HMF-85-04
9	HMI-06-01
10	HMI-06-02
11	HMI-06-03
12	HMI-06-04
13	IMF-20-01
14	IMF-20-02
15	IMF-20-03
16	IMF-20-04
17	IMF-20-05
18	IMF-20-06
19	IMF-20-07
20	IMF-20-08
21	IMF-20-09
22	IMF-22-01
23	IMF-22-05
24	IMF-22-06
25	IMF-22-07
26	IMI-01-02
27	IMI-01-03
28	IMI-01-04
29	PMF-4001

IV. RESULTS

Figure 3 presents the difference between the calculated tally results for two different cases. The Full Angular Distributions case indicates that the nuclear data file for ^{16}O was processed by NJOY with the angular distributions of elastic scattering calculated directly from the resonance parameters. In the Reduced Angular Distributions case, the processed file had the number of energy points necessary to represent the coefficients of the Legendre moments of expansion as a function of energy reduced to 6342 (10 % error).

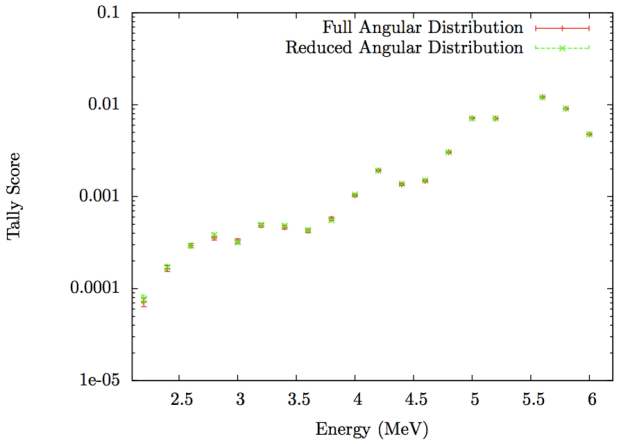

Fig. 3. Tally results for calculated neutron current across one face of a cube model filled with ^{16}O binned versus energy.

In Figure 3, the example compares the effect of reducing the number of points in energy used to represent the coefficient of expansion in the Legendre moments of the angular distribution of elastic scattering of ^{16}O. Figure 3 suggests that thinning the angular distributions has no effect on this integral test. Multiple variations of this configuration were tested using different ^{16}O densities and sources, and all with the same conclusion as this example: without the elimination of isolated resonances, the angular distributions can be thinned to 10% relative error in the linear interpolation without a demonstrable effect in neutron transport calculations.

From the set of two devised neutron transport test problems, it became evident that out of the proposed methodologies, only the mathematical reduction in the number of energy points necessary to represent the high fidelity angular distributions is viable. This also corresponds with the proposed distributions with the least reduction in the number of energy points. Table V provides an example of the deteriorating performance of the reduced angular distributions in transport calculations. Table V presents the tally scores for neutrons with energies between 31.8 keV and 55.7 keV for the 0.6–0.7 cosine bin with a fixed-source energy of 300 keV (end of RRR for ^{63}Cu) and a target density corresponding to an average of 10 scattering events.

Table V. Tally Scores for Neutrons with Energies between 31.8 keV and 55.7 keV for 0.6–0.7 Cosine Bin for the Fixed-Source Type Test Problem Using ^{63}Cu

Angular Distribution File	Tally Score	Number of Energy Points
0.1% criteria	1.227 +/-0.01	83 467
10% criteria	1.230 +/-0.01	16 673
100% criteria	1.212 +/-0.01	11 440
10% criteria eliminated p-waves	1.195 +/-0.01	8 624
10% criteria eliminated p-waves Reduced s-waves	1.247 +/-0.01	5 366

Table V shows results obtained by varying the two input parameters for the fixed-source test problem and the eigenvalue test problem. The results clearly show that once the smaller resonances are eliminated from the angular distribution files, performance of the evaluation in the neutron transport calculations begins to decline.

The comprehensive set of ICSBEP benchmarks for the two copper isotopes confirmed what was seen in the test problems. Figure 4 supports the findings shown in Figure 3 except for ICSBEP benchmarks sensitive to the two isotopes of copper for various reductions in the number of energy points in the representation of the angular distribution of elastic scattering.

V. CONCLUSIONS

A study was made of the different methodologies to reduce the number of energy points required to communicate angular distributions of elastic scattering in the RRR. Several approaches were considered, ranging from mathematical smoothing algorithms to physically intuitive manipulations of resonance parameters.

A testing routine was established with a set of specifically devised neutron transport problems of both the eigenvalue and the fixed-source types, as well as a more general set of criticality safety benchmarks. Both types of testing were compared to the performance of the nuclear data files processed with the full fidelity model. Both types of testing showed the same general trend: mathematical smoothing of the angular distribution function is successful, while manipulations of resonance parameters based on physical intuition do not lead to consistent results in neutron transport calculations.

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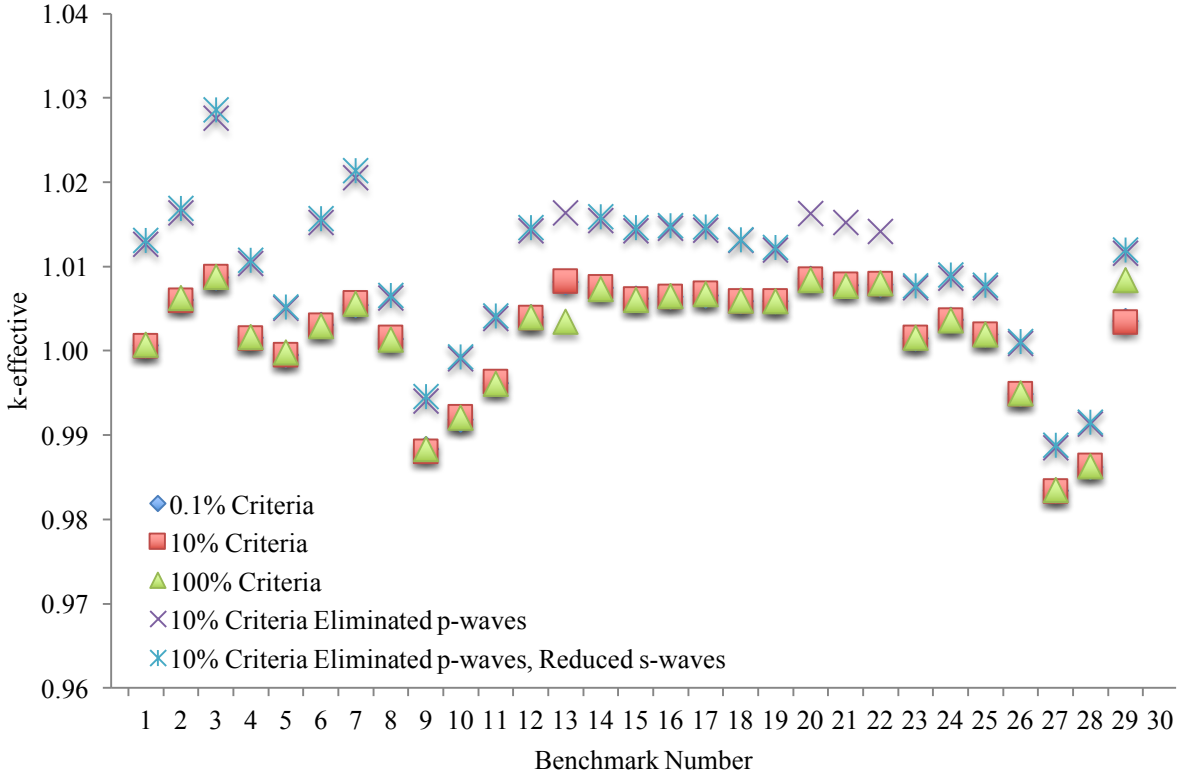

Fig. 4. k_{eff} results for the set of 29 benchmarks described in Table IV for four different reductions of the number of energy points used to describe the angular distributions of elastic scattering for the two isotopes of copper. (The stochastic uncertainty on the calculations is below 10 pcm, which is smaller than the size of the markers.)