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PHYSOR 2016 - Unifying Theory and Experiments in the 21st Century
Sun Valley Resort, Sun Valley, Idaho, USA, May 1 - 5, 2016, on CD-ROM (2016)

ON-THE-FLY DOPPLER BROADENING OF UNRESOLVED RESONANCE REGION CROSS SECTIONS VIA PROBABILITY BAND INTERPOLATION

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ABSTRACT

In this work we present a scheme for computing temperature-dependent unresolved resonance region cross sections in Monte Carlo neutron transport simulations. This approach relies on the generation of equiprobable cross section magnitude bands on an energy-temperature mesh. The bands are then interpolated in energy and temperature to obtain a cross section value. This is in contrast to the typical procedure of pre-generating probability tables at all temperatures present in the simulation. As part of this work, a flexible probability table generation capability is integrated into the continuous-energy neutron transport code OpenMC [1]. Both single-level and multi-level Breit-Wigner formalisms are supported, as is modeling of the resonance structure of competitive reactions. A user-specified cross section band tolerance is enabled with batch statistics. Probability tables are generated for all 268 ENDF/B-VII.1 [2] isotopes that have an unresolved resonance region evaluation. Integral benchmark simulations of the Big Ten critical assembly show that, for a system that is sensitive to the unresolved resonance region, a temperature interval of $\sim$200 K around 293.6 K is sufficient to reproduce the k_{eff} value that is obtained with probability tables generated exactly at room temperature. A finer mesh of < 50 K is required to reproduce some cross section values at the common target relative difference of 0.1%.

Key Words: **unresolved resonance region, Doppler broadening, probability tables, cross sections, Monte Carlo**

1. INTRODUCTION

At intermediate neutron energies, between the highly-structured cross sections of the resolved resonance region and the relatively smooth cross sections of the fast energy region, many isotopes have resonances which are so tightly spaced in energy that they are unresolvable with current experimental techniques [3]. The energies over which this phenomenon is observed comprise the unresolved resonance region (URR). The upper and lower energies of the URR vary from isotope to isotope with heavier nuclei typically exhibiting unresolved resonance structure at lower energies and over narrower energy intervals.

While the precise structure of cross sections in the URR is unknown, sometimes by orders of magnitude, energy-averaged cross section values are available. However, it is generally not advisable to use these averaged cross sections in transport simulations, especially for systems with an appreciable flux at URR energies. Energy self-shielding effects are effectively neglected when resonance structure is not taken into account. Without resonance structure, there are no flux depressions at resonance energies and reaction rates are over-predicted. The result is usually an under-prediction of k_{eff} due to increased URR absorption and increased scattering to energies below the URR where the capture-to-fission ratio is typically higher.

Further, because of the structure in URR cross sections, Doppler broadening effects are also observed. Therefore, high-fidelity simulations of fast reactor systems demand methods for modeling temperature-dependent resonance structure in the URR. In Sec. 2 we describe the mostly widely used method for generating temperature-dependent, structured URR cross sections, and how it has been adapted in this work to compute these cross sections on-the-fly, instead of as a pre-processing step. The results of integral benchmark simulations are presented in Sec. 3. Additional results and analysis to be included in the full paper are listed in Sec. 4.

2. PROBABILITY TABLES AND ON-THE-FLY DOPPLER BROADENING

The most common way of incorporating URR cross section resonance structure into Monte Carlo neutron transport simulations is with the probability table method [4]. The method, which relies on randomly sampling cross section magnitudes, has been implemented in many established nuclear data processing codes such as NJOY [5] and CALENDF [6] for pre-generating data to be used in particle transport codes (e.g MCNP [7], TRIPOLI [8]). Details of various probability table generation implementations are documented elsewhere [9–11]. In Sec. 2.1 we describe the adapted implementation, which is the focus of this work, for on-the-fly calculations of temperature-dependent cross sections. The results of both differential cross section and integral benchmark testing are given in Sec. 2.2

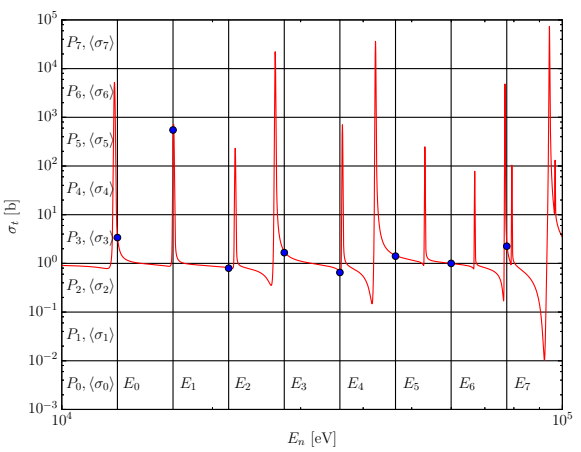
2.1. Implementation

Though precise cross section values in the URR are unknown, average resonance parameters can be deduced through a combined examination of the parameters of resolved resonances and fitting of gross structure in the unresolved region. These parameters are provided in ENDF-6 format [12] nuclear data evaluations. Additionally, theoretical statistical distributions of URR resonance parameters are well-known. For example, the distance in energy between adjacent resonances is described by the Wigner distribution for level spacings. Partial reaction widths can be obtained by sampling a χ^2_x-distribution with a number of degrees of freedom that depends on the reaction, x. An ensemble of URR resonances can be randomly generated by sampling these resonance parameter distributions.

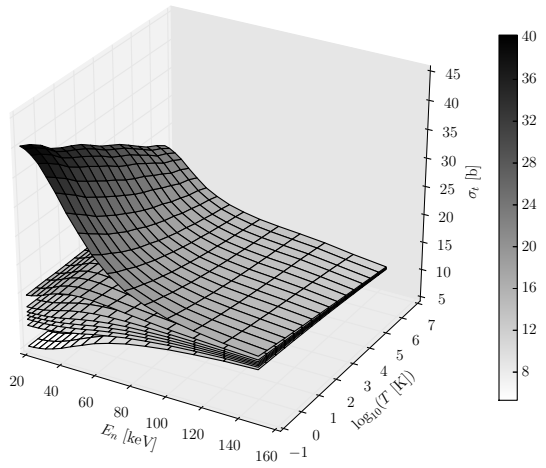
For a single temperature, T, the probability table method proceeds by first establishing a grid in both the incident neutron energy, E_n, and total cross section magnitude, σ_t, variables. Then, one realization of URR resonances is generated and cross section values are calculated. Though any formalism can be used, a summation over single-level Breit-Wigner (SLBW) resonances is the standard prescribed by the ENDF-6 format. A schematic showing an $E_n - \sigma_t$ mesh imposed on one realization of URR cross sections is displayed in Fig. 1a. At each energy, the band containing the cross section magnitude is recorded, as is the value itself. The tallied values are indicated with circular markers in the schematic. In addition, reaction cross section values conditional on the band of the total cross section magnitude are recorded. After many independent realizations of cross section structure are tallied, at each energy, the probability of having a total cross section in a given band is simply the number of realizations that fall within that band divided by the total number of realizations. The mean total cross section magnitude for each band can also be determined by dividing the sum of cross section magnitudes that fall within a band by the number of times that the magnitude is within that band. Mean reaction cross sections that are conditional on the band of the total cross section can be computed in an analogous manner. Transport codes can then sample these probability-cross section pairs each time that a cross section value is needed in order to capture the effects of URR resonance structure.

Probability table method implementations typically require that this process be repeated for each temperature that is present in the model of the system being simulated. For models with continuous or highly-detailed temperature distributions, this would result in a massive increase in probability table data memory requirements. In order to mitigate this problem, an on-the-fly method for calculating temperature-dependent cross section values directly from resonance parameters at each event within the simulation was investigated [13]. This approach is very memory efficient because it relies only on temperature-

independent average resonance parameters. With respect to simulation runtime for simple criticality calculations, [1] though, it can be quite inefficient due to the sampling of resonance parameters and calculation of cross sections at each event. For this reason, we develop an interpolation scheme which allows for the calculation of cross sections at all intermediate points on a coarse temperature grid. Consistent interpolation is enabled through the generation of equiprobable cross section magnitude surfaces on $E_n - \sigma_t$ meshes. A schematic illustrating these surfaces can be found in Fig. 1b. In the transport simulation a surface is randomly sampled and interpolation[2] is performed in both the E_n and T variables.

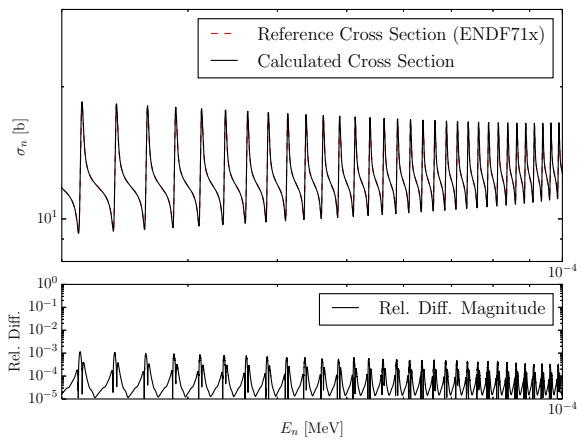


(a) URR realization with an $E_n - \sigma_t$ mesh

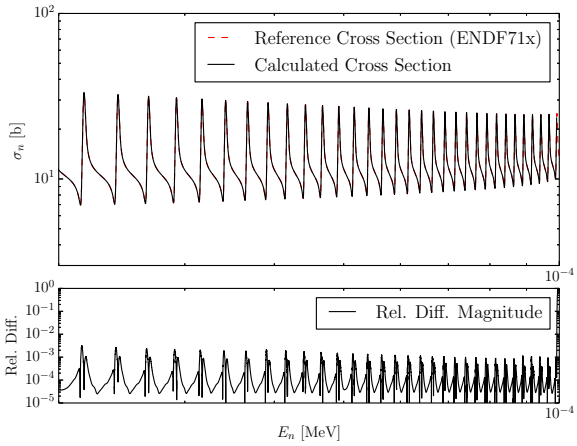


(b) Equiprobable cross section surfaces

Figure 1: Probability table schematics



(a) ^{239}U elastic scattering cross sections



(b) ^{243}Pu elastic scattering cross section

Figure 2: Code-to-code comparison of SLBW cross section calculations

[1] In transient fast reactor analysis simulations with multiphysics feedback, the runtime penalty will not be severe due to other overhead associated with detailed tallies, communication between physics packages, etc.

[2] Thus far, linear-linear and log-log interpolation have been explored.

2.2. Testing

In order to test the implementation of the probability table generation capability, code-to-code comparisons with NJOY are performed. SLBW cross sections computed with both codes, using the same set of resonance parameters are shown in Figs. 2a and 2b.

Table I: Code-to-code comparison of Big Ten k_{eff} eigenvalues

Probability Tables	k_{eff}	1σ
NJOY99.393 (ENDF71x ACE Library)	1.00467	0.00010
OpenMC Implementation	1.00466	0.00010

The results of k_{eff} calculations using the room temperature improved Big Ten integral benchmark model are given in Table I. Excellent agreement is observed between eigenvalues computed using the probability tables generated with the two codes.

3. RESULTS

With the satisfactory performance of the probability table generation capability demonstrated in the results of the testing described in Sec. 2.2, we now seek to investigate the extent to which interpolation of equiprobable cross section magnitude bands to intermediate temperatures is able to reproduce results obtained with cross section data that is generated exactly at those intermediate temperatures. The results of integral benchmark simulations are given in Sec. 3.1.

3.1. Integral Benchmarks

The results of k_{eff} eigenvalue simulations of the improved Big Ten critical assembly model are shown in Table II. Each simulation is performed with probability table data generated at a different room temperature-bounding interval. These results indicate that integral tallies are reproducible with a fairly wide temperature interpolation interval. Interpolation to the Big Ten model temperature of 293.6 K using data generated at bounding temperatures of 200 K and 400 K gives a k_{eff} value that is statistically indistinguishable from the exact 293.6 K result at a relatively tight 1σ uncertainty of 10 pcm. It is expected that intervals even wider than this 200 K will produce acceptable results for the smoother cross sections encountered at elevated model temperatures.

Table II: Big Ten k_{eff} eigenvalues for varying temperature interpolation intervals

ΔT [K]	k_{eff}	1σ
0	1.00466	0.00010
100	1.00463	0.00010
200	1.00468	0.00010
400	1.00533	0.00010

4. FUTURE WORK

In addition to the material presented in this summary, the full paper will contain:

- Expanded integral benchmark analyses including reaction rate spectra
- Comparisons of interpolated and directly-calculated differential cross sections
- Discussion of temperature correlation effects which are accounted for in this methodology
- Comments on competitive reaction resonance structure and the use of a multi-level resonance formalisms, as related to temperature effects
- Recommendations for the generation of equiprobable cross section surfaces for use in fast reactor simulations with temperature feedback

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