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Preliminary Generation of Windowed Multipole Covariance Data

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Abstract. A methodology for the generation of covariance data in the windowed multipole formalism for resolved resonance data was developed. Using this process, covariance matrices were created for oxygen-16, uranium-235, and uranium-238, such that sampled cross-sections would match a user-selected average standard deviation, set at 5% ± 0.5% for this work. Windowed multipole datasets were then sampled and used on a simple critical benchmark to demonstrate the use of WMP data in conjunction with the Total Monte Carlo method of uncertainty propagation.

1 Introduction

Nuclear data uncertainty quantification is an important tool in the reactor design process. Better understanding of the fundamental physics at work, and knowing the limits of that understanding, not only allow for the design of more efficient light-water reactors but for confident design and licensing of Generation IV reactor designs that do not have the same wealth of operating experience to look to [1].

Because evaluated nuclear data is calculated using experimental results fitted to theoretical models, the parameters presented in, for instance, the Evaluated Nuclear Data File (ENDF) to represent the cross-section of a nuclide in the resolved resonance range include covariance data generated during the process of fitting the experimental data [2]. The current most accurate method to propagate these experimental uncertainties further to parameters of interest for reactor design is total Monte Carlo (TMC). TMC consists of generating a large number of randomly sampled datasets and running a full Monte Carlo simulation using each, then using statistical methods to determine the uncertainty in quantities of interest as a result of this nuclear data uncertainty [1].

The main drawback of TMC is the computational load required. Not only does the time required to complete a calculation scale with the number of samples from the nuclear data used but all of these samples must be either pre-generated and stored, greatly increasing the memory requirement of a calculation, or generated as needed, at high computational cost. Though alternative schemes like Fast-TMC have been developed to address the first issue, the second remains [3].

The windowed multipole (WMP) formalism is a novel way of representing cross-section data in the resolved resonance region. Its primary benefit is that it allows Doppler broadening to account for the impact of temperature to be performed on-the-fly, rather than storing

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separate datasets at different temperatures and interpolating between them [4]. This makes the cross-sections calculated using WMP both more accurate and less memory-intensive than traditional representations (on the order of only 1% of the required memory). Unfortunately, windowed multipole covariance data does not exist, and converting it from existing data is quite complex [5].

In this paper, we will establish a methodology for generating covariances for windowed multipole data, demonstrate this using oxygen-16, uranium-235, and uranium-238, and use this data in a simple total Monte Carlo calculation.

2 Background

2.1 Multipole Formalism

In resonance interaction theory, the R-matrix formalism, which can be obtained by solving the Schrödinger equation, provides a full description of the possible interactions between a neutron and a nucleus, and their relative probabilities [6]. This is obviously a very powerful tool, but it is often impractical to use. As such, approximations such as the Single-Level Breit-Wigner (SLBW) and Reich-Moore formalisms have also been developed [2]. These reduce the computational complexity of computing resonance interactions, at the cost of being less physically accurate.

The multipole formalism, by contrast, is not in fact an approximation of R-matrix, but can be shown to be mathematically equivalent [7]. In this representation, cross-sections are a function of the poles and residues of a complex function. At $0K$:

$$\sigma(E) = \frac{1}{E} \sum_j \Re \left[\frac{-ir_j}{p_j - \sqrt{E}} \right] \tag{1}$$

where p_j and r_j are the complex pole and residue of resonance j, and the sum is over all of the resonances in the nuclide [8]. The real power of the multipole formalism, however, is that it makes it possible to Doppler broaden the cross-section on-the-fly [9].

2.2 Windowed Multipole

The pure mulipole formalism, however, still runs into performance issues [9]. Computing the contribution of every resonance to every point is very costly, especially for heavy nuclides with thousands of resonances. The windowed multipole (WMP) formalism solves this by recognizing that the cross-section at a given energy is only minimally impacted by resonances far away from that point. The energy range is therefore "windowed," and only the contributions of nearby resonances (those within the window) are calculated exactly. The rest are summed and approximated as a polynomial function of $\sqrt{E}$:

$$\sigma(E) = \frac{1}{E} \sum_{j \in \mathscr{W}(E)} \Re \left[\frac{-ir_j}{p_j - \sqrt{E}} \right] + \sum_{n=0}^{N-1} a_n \left(\sqrt{E} \right)^{n-2} \tag{2}$$

where $\mathscr{W}(E)$ is the set of poles in the same window as energy E and N is the number of polynomial curve-fit terms.

2.3 ENDF Resonance Data

For Evaluated Nuclear Data File (ENDF) nuclear data, resonance parameters are stored in the section of the evaluation known as File 2 [2]. A number of formalisms for representing this data, up to and including R-Matrix, are supported. The covariance for this data, when it is available, is stored in File 32. The data in both Files 2 and 32 is generated with a code like SAMMY, which uses a generalized least-squares method [10].

Also relevant are Files 3 and 33. File 3 provides continuous energy cross-sections, which must be added to the cross-section as calculated from File 2 where both are defined, and the covariance of this continuous-energy data is provided in File 33.

3 Methods

The goal of this covariance generation method will not be to convert directly from the resonance parameter covariances, but rather to match the resulting variance in the cross-section itself. The specific metric that will be prescribed is the root-mean-square (RMS) relative standard deviation in the cross-section at logarithmically spaced points across each window:

$$\varepsilon = \sqrt{\frac{1}{N}\sum_{n}\left[\frac{\mathrm{SD}[\sigma_n]}{\mathbb{E}[\sigma_n]}\right]^2} \tag{3}$$

where N is the number of points in the energy range, and $SD(\sigma_n)$ and $E(\sigma_n)$ are the standard deviation and mean the sampled cross-section at point n, respectively.

The fundamental assumption of the *windowed* multipole formalism, that the cross-section at a given energy will not be impacted by fluctuations in poles that it does not share a window with, can also be used to constrain the scope of covariance generation. It follows from this assertion that poles that do not share a window with each other should not be correlated, leading to a covariance matrix that will be blockwise along its diagonal. Nonetheless, there are still far more elements in the covariance matrix than there are window/channel combinations for which to evaluate the RMS deviation, meaning that the system is very underdetermined.

This metric means that any small perturbation of the position of the peak of a resonance (determined by the real part of the pole) will lead to a large RMS deviation. Analyzing the File 32 data for well determined nuclides like gadolinium-157, there is not actually much uncertainty at all in the peak energy, so the real part of the pole will not be varied, to prevent it from overcontributing to the RMS deviation.

3.1 Parameter sensitivities

In order to reduce the number of unknowns to the number of window/channel combinations, each element of the covariance matrix will be assigned to a single window/channel, and all the elements assigned to a window/channel will be scaled together. The question then becomes how to decide which window/channel a covariance parameter is assigned to, and what the ratios between parameters assigned to the same window/channel should be. Both of these will be determined by the sensitivity of each window/channel to each covariance parameter.

A small value will be assigned to each element of the covariance matrix individually, and the average RMS deviation in each window/channel will be recorded. The sensitivity of a window/channel to a covariance parameter will be defined as:

$$s = \frac{\varepsilon_0}{\sigma_0} \tag{4}$$

where s is the sensitivity, ε_0 is the RMS deviation, and σ_0 is the square-root of the perturbed covariance parameter (equal to the standard deviation for diagonal terms).

Each covariance parameter will be assigned to the window/channel that is most sensitive to it. All the covariance parameters assigned to a given window/channel will be proportional to the square of the sensitivity of that window/channel to the parameter, multiplied by a uniform scaling factor, k. The ratio between the standard deviations in parameters assigned to the same window/channel will therefore be fixed as the ratio between their sensitivities: a parameter that the cross-section is twice as sensitive to will vary twice as much.

In most windows, the deviation will be dominated by variance in the multipole parameters. In low energy windows, however, there may be windows without any poles. This is especially true for light nuclides. Some variance will therefore also be embedded in the constant term of the polynomial curve-fit for each window/channel. In windows with many poles, this will become negligible, and it will allow windows with few or no poles to still match the target variance. For simplicity, these fit parameters will be assumed to vary independently of each other.

3.1.1 Relative vs. Absolute Sensitivity

The idea that a parameter that is more sensitive to perturbation will vary more is an intuitively pleasing one, but there are in fact a number of ways this might reasonably be implemented, with non-trivially different results. An element of the final covariance matrix will take the general form:

$$\sigma_{ij}^2 = \left[k s_{ij} (\mu_i \mu_j)^n \right]^2 \tag{5}$$

where k is the scaling factor of the associated window and channel, and n is some arbitrary power.

If $n = 0$, the ratio between the *absolute* standard deviation in two parameters assigned to the same window will be set by the ratio of their sensitivities to an *absolute* perturbation:

$$\sigma_i = k s_{ii} = k \frac{\varepsilon_0}{\sigma_0} \tag{6}$$

If $n = 1$, the ratio between the *relative* standard deviation in two parameters assigned to the same window will be set by the ratio of their sensitivities to a *relative* perturbation:

$$\sigma_i = k s_{ii} \mu_i^2 \Rightarrow \sigma_i / \mu_i = k \frac{\varepsilon_0}{\sigma_0 / \mu_i} \tag{7}$$

Either of these choices is justifiable, but both turn out to have drawbacks: for $n = 0$, the covariances for heavy nuclides like uranium-235 and 238 fail to converge, and for $n = 1$, the datasets sampled have a large number of negative cross-sections, even in light nuclides like oxygen-16. By using an intermediate value of $n = 0.84$, both of these issues were (mostly) resolved. On its own, this led to negative cross-sections in windows with zero curve-fit, because for $n \neq 0$, there is also no variance in the curve-fit, and the multipole parameters were required to vary greatly to compensate. In these windows, the covariance was defined as:

$$\sigma_{ij}^2 = \left[k s_{ij} K \right] \tag{8}$$

where K is a uniformly applied scaling factor set at the lowest value that still prevents negative cross-sections. This was only necessary in uranium-238 and was set manually.

3.2 Window/Channel Scaling Factors

The only unknowns in the system are now the scaling factors that will be applied to each window and channel (and the associated covariance parameters). The initial guess for these values will be to find scaling factors that, in the absence of any of the parameters assigned to other windows or channels, will match the average RMS deviation of each window/channel to the target value. In reality, a window/channel will be impacted by both the parameters controlled by both adjacent windows and other channels in the same window, but this is a reasonably good starting point. An additional benefit of assigning each covariance parameter to the window and channel that is most sensitive to it is that the impact of the collective parameters assigned to a given window and channel on any other window/channel combination will necessarily be less than the impact on the controlling window/channel.

In order to find these "single-window factors," the scaling factor will be bounded and then converged using logarithmic bisection. First, an arbitrarily chosen starting factor will be tested. The RMS deviation will always be positively correlated with the scaling factor, so if the deviation for this test factor is too, high, it will be progressively decreased by factors of ten until both a value that yields too high of a deviation and one that yields too low of a deviation have been found. If the initial deviation is too low, the scaling factor will similarly be increased by factors of ten until the target deviation is bounded.

Once the target deviation has been bounded, the logarithmic midpoint of the bound will be tested. If the deviation is too low, this is set as the new lower bound, and if it is too high, it is set as the new upper bound. This process is repeated until a scaling factor is found for which the average RMS deviation is acceptably close to the target.

Once the single-window factors have been obtained for each window and channel, they are combined, and the actual deviation in each window/channel, accounting for the impact of the full covariance, is calculated. The factor for each window/channel is then multiplied by the ratio of the target deviation to the real deviation, e.g. the factor is decreased by 20% if the deviation is 20% too high. This process can be repeated iteratively to bring the results within a desired margin of the target deviation.

4 Results

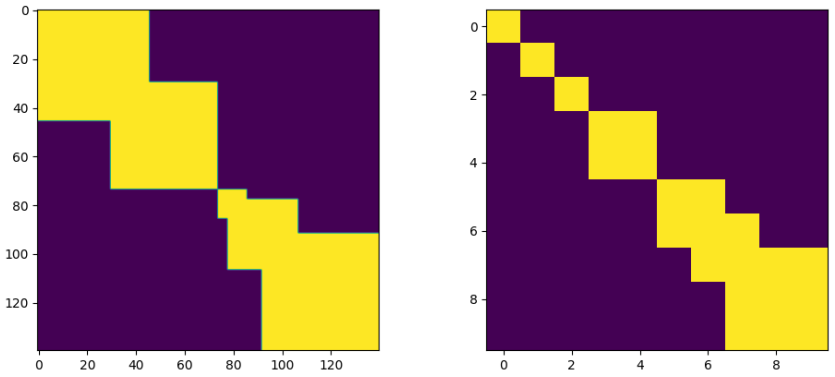
4.1 Covariance Generation and Sampling

As described above, poles that do not share a window will not be correlated. The structure of the densest possible covariance matrix will therefore mirror Figure 1(a), which shows the pole interactions in oxygen-16, or the equivalent for the nuclide in question.

The sparsest possible covariance would be entirely diagonal, and any number of configurations in between can be imagined, e.g. covariance only between real and imaginary parts of the same parameter, covariance between parameters within a pole but not between poles, etc. For this paper, diagonal covariance matrices were used.

Another simplification made for the purposes of this demonstration was the use of a uniform target deviation of 5%. In practice, this could be any value and need not even be the same across the energy range or between channels. The ultimate goal would be to match this to the deviation in cross-sections sampled from the existing File 32/33 data.

Using the methodology described in Section 3, covariance matrices were generated for oxygen-16, uranium-235, and uranium-238. For each, the average RMS deviation in the majority of windows and channels falls within 0.5% (absolute) of the target deviation of 5%. The windows/channels that fall outside this range are not consistent between samples, which would suggest a systemic issue, but are simply a result of the stochastic nature of the process. These results are shown in Figure 2.



(a) (b)

Figure 1: Oxygen-16: (a) Poles that share a window, (b) Windows that share poles

With these covariance matrices created, it is simple to sample windowed multipole datasets from them. Plots of the cross-sections, as sampled from these datasets, are shown in Figure 3, zoomed in to show detail.

4.2 Total Monte Carlo (TMC) with WMP

Total Monte Carlo, or TMC, is a method of Monte Carlo uncertainty propagation developed by A.J. Koning and D. Rochman [1]. The basic idea of TMC is to run a series of independent Monte Carlo simulations using different random samples of the nuclear data. The nuclear data variance is therefore:

$$\sigma^2_{ND} = \sigma^2_k - \bar{\sigma}^2_{stat} \tag{9}$$

where σ^2_k is the standard deviation in the values of k_{eff} returned by each of the simulations and $\bar{\sigma}^2_{stat}$ is the average of the statistical variance in k_{eff} for each simulation. For models that are already computationally intensive to run a single calculation, using TMC is infeasible, as the runtime scales with the number of samples, therefore a number of variations on the original TMC scheme have been developed to yield better performance [3].

To demonstrate the use of the covariance matrices generated with the procedure detailed above, TMC was implemented for the simple problem of a 20cm-radius bare sphere of 20% enriched UO_2. The calculations were performed in the open-source Monte Carlo transport code OpenMC, which supports WMP resonance data, and 500 data sets were sampled from the O-16, U-235, and U-238 covariance matrices. The impact of varying each nuclide individually, as well as all at the same time, was calculated. The results are tabulated in Table 1 and a histogram showing the distribution of k_{eff}, varying all cross-sections, is plotted in Figure 4.

5 Conclusions

Total Monte Carlo is a powerful tool for nuclear data uncertainty quantification, and the windowed multipole formalism allows for far better memory usage than traditional representations of resolved resonance data, through on-the-fly Doppler broadening. In this paper,

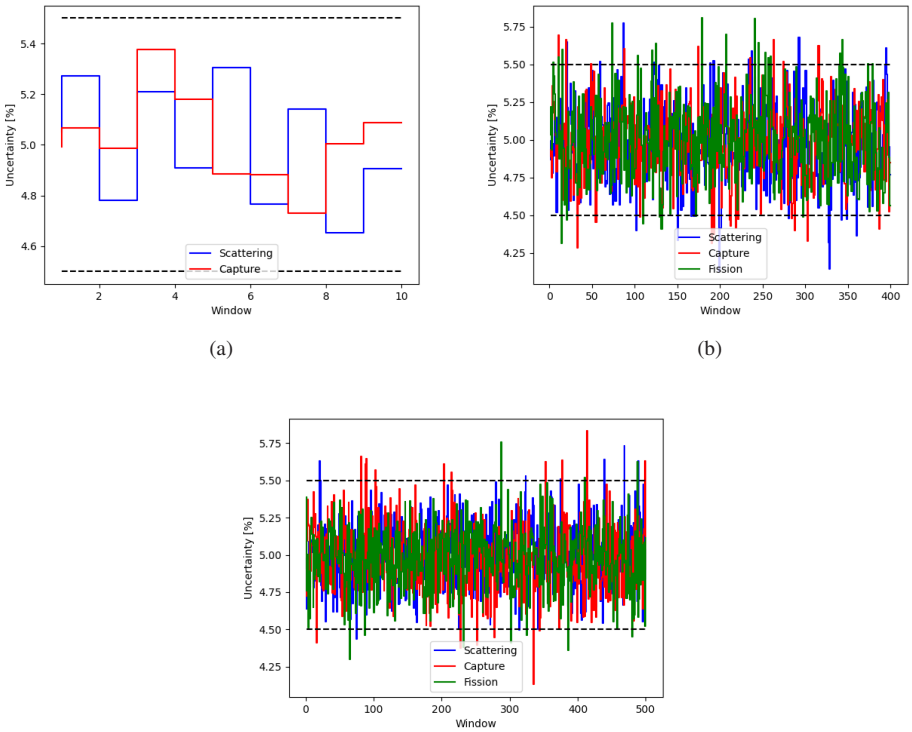


Figure 2: Average RMS deviation in (a) O-16 (b) U-235 (c) U-238

Table 1: Total Monte Carlo results for a 20cm-radius sphere of 20% enriched UO_2

Nuclides Varied	Uncertainty [pcm]	
	Nuclear Data	Statistical
O-16	253	59
U-235	37	59
U-238	29	59
U-235, U-238	36	59
O-16, U-235, U-238	251	59

a methodology to generate covariance matrices in the WMP formalism was developed and applied to oxygen-16, uranium-235, and uranium-238. The combination of these techniques (TMC and WMP) was then demonstrated on a simple problem.

Future work will involve eliminating the simplifications made in this paper, namely the inclusion of off-diagonal elements of the covariance matrix and matching the cross-section deviation to values representative of the actual ENDF covariance data, rather than an arbitrary uniform 5%, as well as comparing this approach with other methods. Even without these expansions, however, the potential of the windowed multipole formalism to improve the performance of Monte Carlo uncertainty quantification is clear.

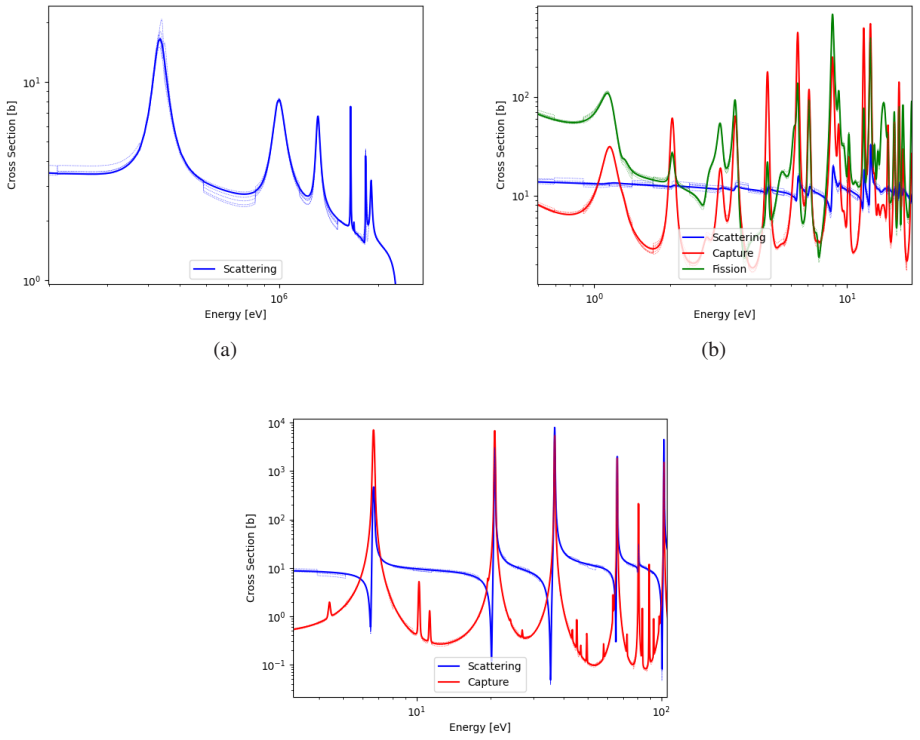


Figure 3: Cross-sections sampled from WMP covariances for (a) O-16 (b) U-235 (c) U-238, zoomed in to show detail

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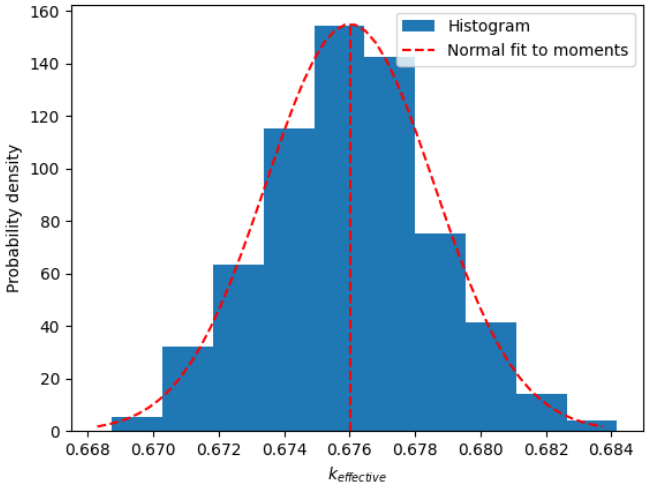

Figure 4: Histogram of k_{eff} for a 20cm-radius sphere of 20% enriched UO_2, varying the cross-sections of O-16, U-235, and U-238

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