Investigation of Uncertainty Propagation in the Resolved Resonance Range

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Abstract. This paper presents a comparative study using the first-order formula (also called "sandwich") and the multivariate sampling methodologies for propagating uncertainty in the resolved resonance region. A distinctive aspect of this work is the generation of random cross sections by sampling Resonance Parameters (RPs) taking in consideration their correlations provided in nuclear data libraries via the Resonance Parameter Covariance Matrix (RPCM). SCOOBY (**S**ampling **CO**variance **OB**servator**Y**), a newly developed sampling tool, is presented in this paper. This tool relies on the GAIA-2 nuclear data processing code to read and correct the RPCM and generate random cross sections.

The study compares the sandwich method that relies on sensitivity coefficients and covariance matrices, with the sampling method, which involves numerous Monte Carlo simulations with random cross sections. The comparison is tested on an ICSBEP benchmark, PU-MET-MIXED-002, chosen for its sensitivity to ^{239}Pu cross sections. The results indicate that both methods quantify similar uncertainties, confirming the reliability of both the SCOOBY module and the GAIA-2 code.

By using the PU-MET-MIXED-002 benchmark and sampling ^{239}Pu resonance parameters, this work demonstrates the effectiveness of these methodologies in estimating uncertainty in criticality safety calculations. The findings highlight the robustness of these approaches in uncertainty propagation, suggesting the need for further research on additional benchmarks and expanded uncertainty propagation studies.

1 Introduction

The generation of accurate nuclear Cross Sections (XSs) is fundamental to nuclear systems, significantly influencing reactor physics and criticality safety assessments. In the resolved resonance regions and for most nuclei, these XSs are reconstructed from the resonance parameters. This paper aims to assess the impact of uncertainties inherent in resonance parameters on nuclear systems using two methodologies for uncertainty quantification: the sandwich method and the multivariate sampling approach.

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Uncertainty propagation from input parameters in a system response can be done using the "sandwich rule." This rule assumes that parameter uncertainties are small, allowing for the use of a first-order Taylor expansion of the response around the mean values of these parameters. This approach establishes a mathematical relationship between the variance of the response, its sensitivity to the parameters, and the covariance matrix of these parameters.

The effective multiplication factor (k_{eff}) depends on numerous parameters, including cross sections reconstructed from resonance parameters by processing codes. A nuclear data evaluation in the resonance region for a given nucleus aims at estimating resonance parameters and their correlations, stored in the Resonance Parameter Covariance Matrix (RPCM). However, modern simulation tools only calculate sensitivities on multi-group cross sections, necessitating the use of the sandwich formula alongside a Cross Sections Covariance Matrix (CSCM). The conversion of RPCM to CSCM is performed by ERRORR (NJOY) [1] or PUFF-IV (AMPX) [2], which apply a first-order approximation, potentially neglecting non-linear effects.

Conversely, the multivariate sampling methodology employs RPCM to initially generate random RPs, which are subsequently reconstructed into random XSs. The sampling methodology enables bypassing both the sandwich rule, with its initial linear assumption, and the multigroup formalism, along with its assumption of weighting flux. This paper specifically concentrates on the generation of these random XSs.

This study also introduces the code SCOOBY (**S**ampling **CO**variance **OB**servator**Y**), a newly developed random sampling tool at IRSN. SCOOBY reads the RPCM and generates random cross sections by directly sampling resonance parameters based on their covariance data and uses GAIA-2 [3] to reconstruct XSs in the resolved resonance range. By comparing the sandwich method with the sampling method using SCOOBY, this research aims to evaluate the efficiency of these methodologies in propagating uncertainties within the resolved resonance region. The comparison is tested on an ICSBEP benchmark, specifically the PU-MET-MIXED-002, known for its sensitivity to ^{239}Pu cross sections. This benchmark provides a rigorous context to assess the implications of these methodologies on criticality safety evaluations, which is detailed in the following sections.

2 Methodology

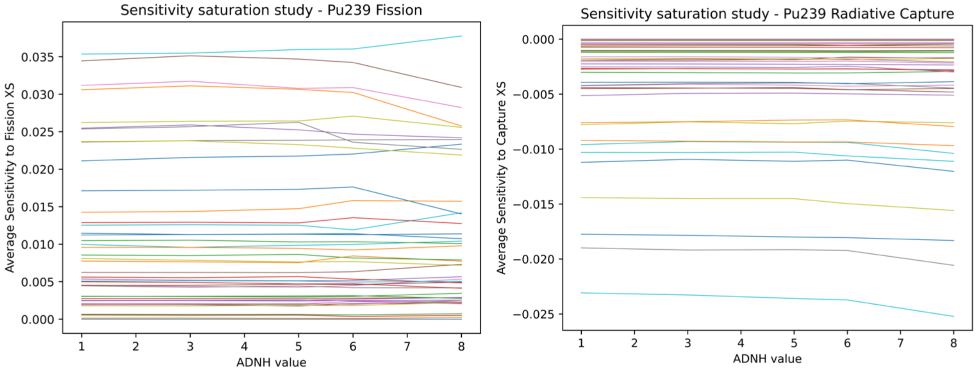
This study uses two methodologies for propagating uncertainty in the resolved resonance region: the sandwich method and the sampling approach. The following sections describe these methods in detail, including the tools and processes used.

2.1 Sandwich Method

The initial step in the sandwich method involved processing the covariance matrix for ^{239}Pu into a given energy mesh using the nuclear data processing code NJOY-2016.35. This procedure guarantees that sensitivity analysis performed using MORET-6 [4], the IRSN Monte Carlo code, produces sensitivity vectors consistent with the energy mesh of the covariance matrix produced by NJOY.

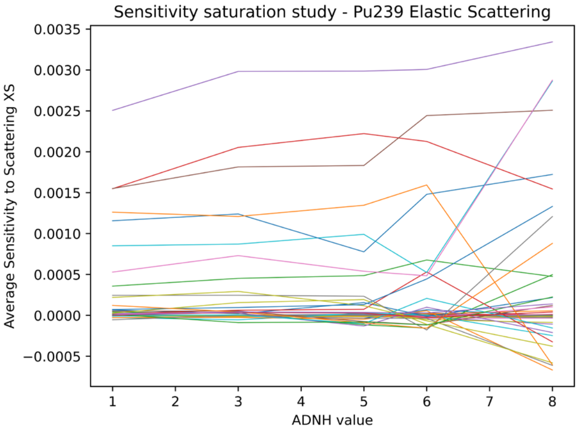
A preliminary study was conducted to guarantee the convergence of sensitivities, crucial for an accurate estimation of uncertainty using the sandwich methodology. The adjoint flux calculation relies on the number of "superhistories" generated in each cycle [5]. Each superhistory is the history of one neutron and all its progeny in a given number of generations per cycle which influences the neutron importance function [6]. The ADNH card in MORET-6 defines the number of superhistories initially requested and influences the convergence rate of the sensitivity coefficients sought. This convergence depends on the geometry of the system and must be studied for each benchmark.

Beginning with a 44-group structure, the study examined the convergence of the k_{eff} sensitivities to various cross sections within each energy bin by incrementally increasing the ADNH value from 1 to 8. This method entailed conducting 30 runs for each ADNH value while keeping a constant k_{eff} precision criterion of 20 pcm. Figure 1 illustrates the averaged sensitivity, with each colored line indicating the average sensitivity in one energy bin as a function of the ADNH. The study discussed, which is case 3 of the PMM-002 benchmark, indicates that the results may be relevant to the other four cases in the benchmark. Specifically, in this benchmark, Figures 1a and 1b show a convergence in sensitivity for the fission and capture cross-sections across all energy bins and ADNH values (with minimal influence from the lower ADNH values). The convergence of the elastic scattering response is more challenging to determine, but the sensitivity values are significantly lower, as depicted in Figure 2c.



(a) Average sensitivity of k_{eff} to fission XS.

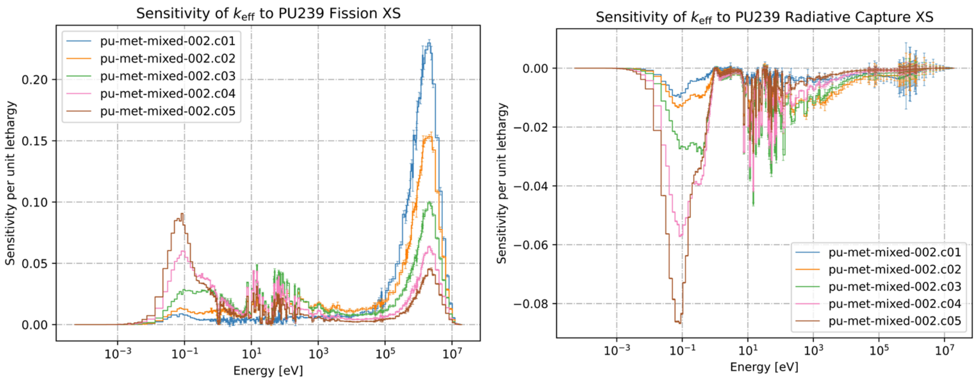
(b) Average sensitivity of k_{eff} to capture XS.



(c) Average sensitivity of k_{eff} to scattering XS

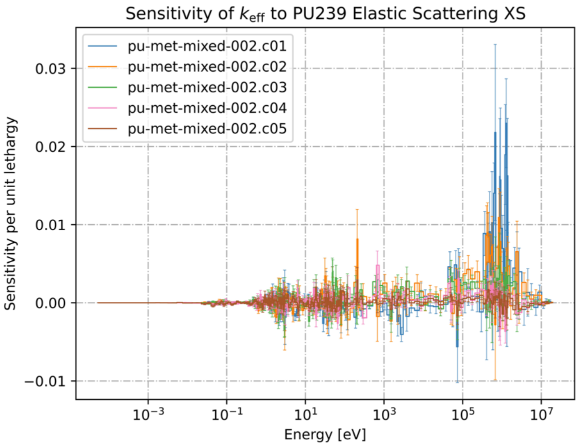
Figure 1: Sensitivity convergence study with varying adjoint flux parameters (ADNH card in MORET-6). Each line represents the average sensitivity in one energy bin.

A detailed sensitivity analysis has been carried out for the fission, capture, and elastic cross sections of ^{239}Pu across the studied cases, as shown in Figure 2. The sensitivity vectors have been calculated by MORET-6 using the 238 energy group structure of SCALE and ENDF/B-VIII.0 nuclear data library [7], with the ADNH parameter set to 4 in this study. It can be seen that out of the five studied cases, Case 3, Case 4, and Case 5 are quite sensitive to the XSs in the thermal and resolved resonance region, i.e., up to 2.5 keV. Therefore, these cases serve as classic examples of benchmarks that can provide reliable information on the impact of resonance parameter uncertainty.



(a) MT = 18; Fission.

(b) MT = 102; Radiative Capture.



(c) MT = 2; Elastic Scattering.

Figure 2: Group-wise Sensitivity plots of fission, capture, and elastic cross-sections of ^{239}Pu for the studied benchmark cases. These plots underscore the selection of these cases based on their sensitivity to ^{239}Pu cross-section variations.

Uncertainty quantification can then be performed via a first-order Taylor expansion of the variance on the multiplication factor, colloquially called the "sandwich formula" [8] :

$$\mathrm{Var}(k_{\mathrm{eff}}) = \mathrm{S} \cdot \mathrm{CSCM} \cdot \mathrm{S}^{\mathrm{T}} \tag{1}$$

Where Var(k_{eff}) is the variance of the computed k_{eff} introduced by the Pu-239 nuclear data, S is the sensitivity vector consisting of all reactions considered (MT = 2, 18, 102), S^T is the transpose of this vector, and CSCM is the cross-section covariance matrix consisting of variances and co-variances of all reactions considered.

The covariance matrices for ^{239}Pu, containing fission, capture, and elastic scattering cross sections were obtained by processing this nucleus from of ENDF/B-VIII.0 with NJOY using the same SCALE 238 energy mesh at 293.6 K.

The IRSN in-house tool CALINS (**CAL**culation and **I**nvestigation of **N**uclear data uncertainties and Sensitivities) has been used for uncertainty calculation using extracted sensitivity vectors and covariance matrices via the sandwich method, the results of which are presented in the next section.

2.2 Sampling Approach

The GAIA-2 nuclear data processing code includes a module that is designed to handle covariance matrices (COP). This module retrieves the covariance matrix from evaluations and applies mathematical adjustments to it. Subsequently, the SCOOBY code imports the corrected RPCM and generates sets of resonance parameters, maintaining the specified correlations among parameters. These random sets are then provided to the reconstruction module (DOP) of GAIA-2 which produces linearized cross sections. This direct use of the RPCM is used as our reference methodology for assessing the impact of resonance parameter uncertainties on XSs.

The sampling approach does not rely on the sandwich method. Instead, it involves running multiple Monte Carlo simulations with random cross sections [9]. Two sampling techniques have been implemented in SCOOBY, Simple Random Sampling (SRS) and Latin Hypercube Sampling (LHS). For this study, the LHS method has been used. LHS is a sampling method that ensures a more comprehensive exploration of the parameter space by dividing the cumulative distribution function of each parameter into equal intervals and sampling from each interval.

This study involved generating 300 sets of random parameters, each of which was then used to reconstruct cross sections, resulting in 300 evaluations. The convergence of the parameters sampled across numerous sets was verified to be consistent with their values in the original evaluation. The RPs sampled in each set comprised three types: energies, resonance widths, and scattering radii.

3 Results

3.1 Uncertainty due to varying cross section data library

In a supplementary study aimed solely at investigating the variation in simulation output due to changes in the nuclear data library, MORET-6 calculations were performed with a precision of 10 pcm for the five cases of the PMM-002 benchmark. This was done by exclusively changing the cross-section libraries to assess their impact on the calculated k_{eff}.

It is evident from Fig. 3 that the selection of cross-section libraries significantly impacts the calculated k_{eff}, which is compared to the experimental k_{eff}. The ENDF/B-VII.1 library provides the most accurate results. The discrepancies between the ENDF evaluations stem from the alterations to the ^{239}Pu cross-sections in ENDF/B-VIII.0 [10]. Although ENDF/B-VII.1 offers better outcomes, ENDF/B-VIII.0, being the more recent library, has been adopted as the foundational library for all subsequent calculations.

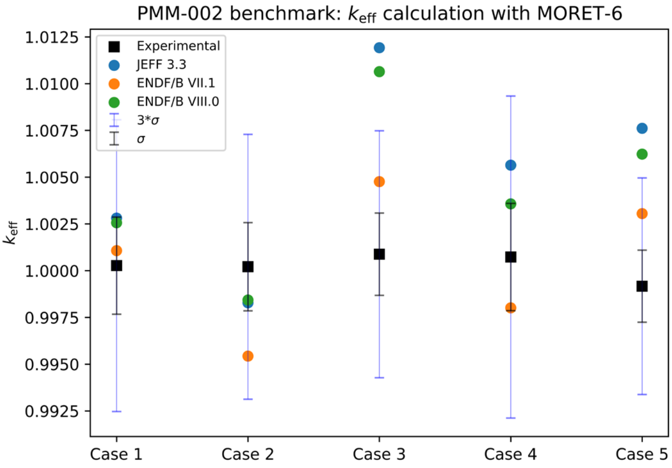


Figure 3: MORET-6 mean k_{eff} calculation for PMM-002 with different evaluations compared to the Experimental k_{eff}. The statistical uncertainty on the Monte Carlo simulation is 10 pcm.

3.2 Sandwich results

The initial step involved generating the covariance matrix for ^{239}Pu, set to 238 and 56 energy group structures of SCALE. For a fair comparison between the sandwich and sampling methods, only the resolved resonance region has been considered. In the sampling approach, only the cross sections in the resolved resonance region of ^{239}Pu, which spans up to 2.5 keV, were sampled. Consequently, the original group structures under study (238 groups and 56 groups) were truncated to energies only up to 2.5 keV, resulting in 175 groups and 39 groups, respectively. Covariance matrices were also processed for these truncated meshes with NJOY. This adjustment ensured that the remaining energies were removed from the group structure. Subsequently, the sensitivity coefficients obtained from MORET-6 simulations were used to carry out the sandwich.

The results for Cases 1-5 of the PMM-002 benchmark, which exhibit sensitivity to ^{239}Pu cross sections within the energy range pertinent to our study, are summarized in Tables 1 and 2. The k_{eff} values in Table 1 and 2 vary as different calculations were performed, and they are within the 20 pcm Monte Carlo uncertainty.

Table 1: Results of the Sandwich Method Applied to PU-MET-MIXED-002 Benchmark Cases 1-5 (238 groups and 56 groups). The statistical uncertainty on the Monte Carlo simulation is 20 pcm.

Studied Cases	k_{eff}	**Uncertainty [pcm]**	
		238 groups	**56 groups**
Case 1	1.00279	739	738
Case 2	0.99837	750	741
Case 3	1.01058	836	828
Case 4	1.00330	905	900
Case 5	1.00606	998	1000

Table 2: Results of the Sandwich Method Applied to PU-MET-MIXED-002 Benchmark Cases 1-5 (175 groups and 39 groups). The statistical uncertainty on the Monte Carlo simulation is 20 pcm.

Studied Cases	**Uncertainty [pcm]**	
	175 groups	**39 groups**
Case 1	194	195
Case 2	516	510
Case 3	759	758
Case 4	881	880
Case 5	998	986

It can be seen from Tables 1 and 2 that the different group structures of SCALE (238 and 56 groups) and the truncated group structures (175 and 39 groups) have minimal impact on the sandwich results, providing similar results. However, when the uncertainty is analyzed only for the 175 groups, cutting off at the resolved resonance region, the uncertainty obtained is lower, as expected, than the full spectrum of 238 groups, since the contribution of the remaining groups is removed. Given that sensitivity varies for the 175 groups considered for the five cases, the difference in uncertainty is also observed to differ. This 175-group uncertainty is compared with the sampling method results, which are also performed in the resolved resonance region.

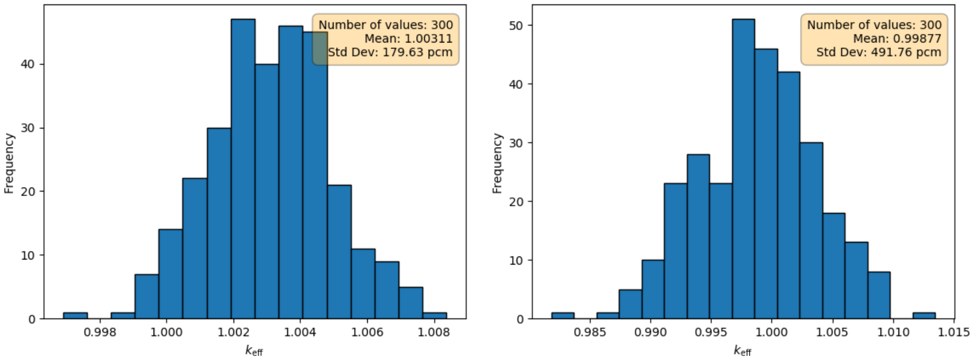
3.3 Sampling results

Following the presentation of the sandwich method outcomes, further analysis was conducted by examining the distributions of the results obtained through sampled cross sections. Histograms have been generated to visually represent the variations and trends within the data for each of the studied cases and are presented in Figure
4.

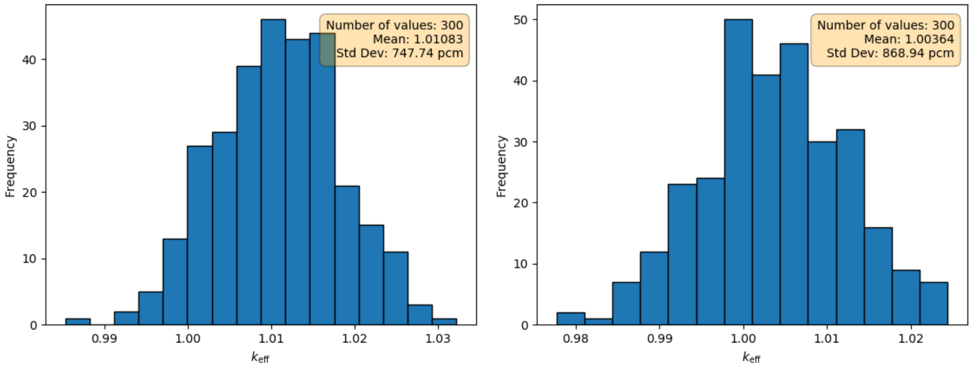
Figures 4a through 4e showcase the distribution of results for Cases 1-5 of the PMM-002 benchmark respectively, illustrating the variability in k_{eff} induced by sampling the RPs of the Pu-239 evaluation, further highlighting the importance of carefully considering these uncertainties in criticality calculations. It is important to note that the spread in the distribution encompasses both the Monte Carlo simulation uncertainty, fixed at 20 pcm, and the nuclear data uncertainty. Despite this compounded uncertainty, the observed variance in the sampling case offers valuable insights into the potential magnitude of uncertainty one might anticipate when employing the uncertainties present in the RPCM.

3.4 Comparison of Sandwich and Sampling Methods

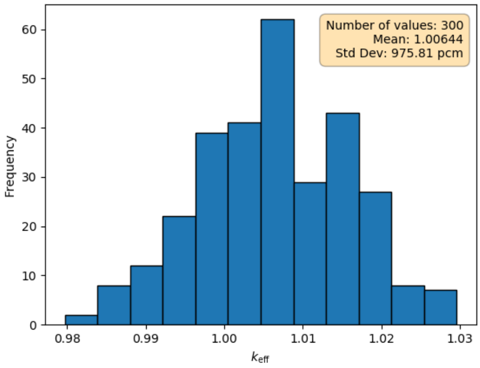
The comparison of the uncertainty results from the sandwich method and SCOOBY sampling for the PU-MET-MIXED-002 benchmark cases 1-5 is summarized in Table 3. As the case number increases, the benchmarks show greater sensitivity to the neutron energy spectrum below 2.5 keV, leading to increasing uncertainties due to the Pu-239 resolved resonance region. The results indicate that both the sampling and sandwich methods provide similar uncertainty estimates, with differences generally within the range of 10-30 pcm. This demonstrates the consistency of both methodologies in propagating uncertainties in the resolved resonance region. To further validate these methodologies, it is recommended to test them on a broader



(a) Case 1 (b) Case 2



(c) Case 3 (d) Case 4



(e) Case 5

Figure 4: Distributions of k_{eff} values when sampling resonance parameters for the studied cases of the PU-MET-MIXED-002 benchmark. The statistical uncertainty on Monte Carlo simulations are 20 pcm.

series of ICSBEP benchmarks and other nuclides. Furthermore, exploring more RPCMs will enhance the robustness of nuclear data processing methods and contribute to the advancement of criticality safety standards. These efforts will ensure a more comprehensive understanding of uncertainty propagation, ultimately improving the reliability and safety of nuclear systems.

Table 3: Comparison of Uncertainty Results from Sampling Methodology and Sandwich Method for PU-MET-MIXED 002 Benchmark Cases 1-5

Studied Cases	**SCOOBY Sampling [pcm]**	**Sandwich Method**		**Difference**	
		175 groups [pcm]	**39 groups [pcm]**	**Sampling - 175 groups [pcm]**	**Sampling - 39 groups [pcm]**
Case 1	180	194	195	14	15
Case 2	492	516	510	24	18
Case 3	748	759	758	11	10
Case 4	869	881	880	12	11
Case 5	976	998	986	22	10

4 Conclusion

The study emphasizes the dynamics and consequences of using both the sandwich method and the sampling approach to propagate uncertainties in the resolved resonance region. Both methods produce comparable outcomes for the PU-MET-MIXED-002 benchmark across its five cases. This offers a detailed insight into the possible variations in criticality safety assessments when including uncertainties originating from the initial nuclear data evaluation, specifically those arising from the Resonance Parameter Covariance Matrix (RPCM). The consistent outcomes of these methods highlight their reliability and efficacy in assessing the influence of resonance parameter uncertainties on cross-section computations.

Furthermore, this study confirms the efficacy of the GAIA-2 processing capabilities and demonstrates the robustness of the SCOOBY tool in implementing the sampling approach using Latin Hypercube Sampling (LHS). Both methods have been shown to be effective in propagating uncertainties, highlighting their robustness and utility in nuclear data analysis.

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