Continuous Energy Cross Section Adjustment: a New Method to Generalize Nuclear Data Assimilation for a Wider Range of Applications

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Abstract -
This work presents a new method to perform continuous-energy cross section adjustment. The proposed method is based on recently developed Monte Carlo perturbation capabilities with continuous-energy sensitivity functions implemented in an extended Serpent version. The generation of continuous energy basis functions as eigendecomposition of the covariance matrices and the Generalized Least Squares method applied to these functions are described. The new approach is verified against standard, multi-group adjustment methodologies in a case study involving four different response functions in Jezebel. The results obtained by the two approaches for the selected case study are presented and compared in term of adjusted cross sections, adjusted covariance matrices, and uncertainty reduction.

I. INTRODUCTION

In the past years, research efforts were devoted to the development of methods and tools for the consistent use of integral experiments and nuclear data covariances for data assimilation purposes [1] [2] [3]. Usually, these methods involve the calculation of multi-group sensitivities to generalized response functions by means of deterministic neutron transport codes, and the use of discretized covariance matrices. These approaches proved useful for experiment representativity analysis, for uncertainty studies via the generation of adjusted covariance matrices, and, more in general, for the purposes of providing precious information to nuclear data evaluators. Nonetheless, adjusted multi-group cross sections and covariance matrices depend on the choice of the energy dependent weighting function, and are of little help in producing adjusted continuous-energy cross sections, e.g., to be adopted in Monte Carlo neutron transport codes. An attempt has also been made to use the integral experiments to adjust nuclear parameters in order to provide fundamental information on the evaluated nuclear data files [4, 5]. However, that approach is rather complex and a more practical method has been investigated.

In fact, recently, continuous energy Monte Carlo codes have been extended to allow the calculation of multi-group sensitivities for generalized response functions (e.g., see [6, 7, 8]). While this improves the accuracy of the produced results, it does not overcome the limitations related to the adoption of discretized sensitivity profiles and covariance matrices. Moreover, the statistical error of Monte Carlo sensitivity estimates rapidly increases when adopting finer energy grids.

For these reasons, an innovative and powerful method for data assimilation based on continuous energy cross section adjustment is under development and is presented here. The proposed method makes use of continuous energy sensitivity functions, instead of group-averaged cross sections sensitivities, as the bases of the data adjustment process.

The proposed approach is preliminary demonstrated for the purpose of this summary adopting the criticality benchmark Jezebel-^{239}Pu as case study, and ENDF/B-VII covariances.[1] Four different response functions are considered in the present work: the effective multiplication factor and 3 spectral indeces measure in the center of the assembly: F28/F25, F37/F25, and F49/F25.

Results of the nuclear data uncertainty estimate and the adjustment process are compared to deterministic results.

II. PROJECTING NUCLEAR DATA COVARIANCES AND GENERALIZED SENSITIVITY PROFILES ONTO CONTINUOUS ENERGY FUNCTIONS

The first step for the proposed method consists in the projection of the cross section uncertainties (i.e., nuclear data covariance matrices) and the generalized sensitivity profiles onto a set of continuous-energy basis functions.

This step represents the "discretization-free" counterpart of the cross section and covariances "collapsing" into few groups, adopted in deterministic tools. The new approach was made possible by new capabilities implemented in an extended version [9] of the Serpent Monte Carlo code [10], which allows calculating the sensitivities of generalized responses to arbitrary, double differential continuous functions.

In particular, the present work investigates the adoption of basis functions obtained from the eigendecomposition of continuous energy covariance matrices.

Considering a single cross section $\Sigma(E)$, for simplicity, the continuous-energy first-order uncertainty propagation formula is:

$$Var\left[R\right] = \int_{E_{min}}^{E_{max}} \int_{E_{min}}^{E_{max}} S_{\Sigma}^{R}(E) \cdot COV\left[\Sigma(E), \Sigma(E')\right] \cdot S_{\Sigma}^{R}(E') \, dE \, dE'$$

(1)

$COV\left[\Sigma(E), \Sigma(E')\right]$ represents the continuous-energy relative covariance matrix for the considered reaction cross section Σ.

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[1] ENDF/B-VII uncertainties are not provided as continuous energy covariance data. For this reason the result of the adjustment, adopting the continuous-energy methodology proposed, suffers from the fine-grid discretization present in the input data.

$S_\Sigma^R(E)$ is the energy-dependent sensitivity density function for the generic response R. In the present work, response functions in the form of k_{eff} and reaction rate ratios are considered.

After eigendecomposition of the relative covariance matrix:

$$COV\left[\Sigma(E), \Sigma(E')\right] = \sum_{j=1}^{\infty} U_j(E) \cdot V_j \cdot U_j(E') \qquad (2)$$

the first-order uncertainty propagation formula becomes:

$$Var[R] = \sum_{j=1}^{\infty} V_j \cdot \left(\int_{E_{min}}^{E_{max}} U_j(E) \cdot S_\Sigma^R(E) \, dE\right)^2 \qquad (3)$$

where V_j are the eigenvalues of the continuous energy covariance matrix corresponding to the eigenfunctions $U_j(E)$.

The next step of the continuous-energy adjustment method consists in the calculation of the integrals $\int U_j(E) S_\Sigma^R(E) \, dE$ via Monte Carlo Perturbation Theory. These integral sensitivities $\left(S_{U_j}^R\right)$ are obtained via the eXtended Generalized Perturbation Theory (XGPT) approach [9], which allows estimating the sensitivities of generalized responses to continuous-energy functions, within a single Monte Carlo run, via the collision-history approach.

Adopting these eigenfunctions sensitivities, the uncertainty from nuclear data in the response function R can be obtained, without any multi-group energy discretization:

$$Var[R] = \sum_{j=1}^{\infty} V_j \cdot \left(S_{U_j}^R\right)^2 \simeq \sum_{j=1}^{n} V_j \cdot \left(S_{U_j}^R\right)^2 \qquad (4)$$

The choice of the number n of eigenfunctions adopted for the uncertainty propagation process determines the accuracy of the variance estimation and, thus, the adjustment process.

The truncation error introduced by the adoption of a finite number n of basis functions might seem similar to the discretization error introduced by the choice of the energy discretization for the calculation of the sensitivity coefficients in the standard, multi-group approaches. On this point, it should be noted that it is common to experience exponential convergence toward the exact value for the variance estimates, when increasing the number of eigenfunctions adopted. As an example, Fig. 1 shows the contribution to the total variance in Jezebel for each basis functions obtained from the eigenvalue decomposition of ENDF/B-VII ^{239}Pu covariance matrices, considering different response functions. It can be appreciated that there is a reduction of several orders of magnitude of the "importance" of the basis functions within the first 50. For comparison, increasing the number of energy groups for the sensitivities calculations lead to a much slower convergence.

Moreover the higher efficiency of the new approach lies in the fact that the statistical precision of the Monte Carlo estimates for the sensitivities does not depend on the number of eigenfunction considered, whereas the increase in the number of energy bins in the standard approach leads to higher statistical errors in the multi-group sensitivities.
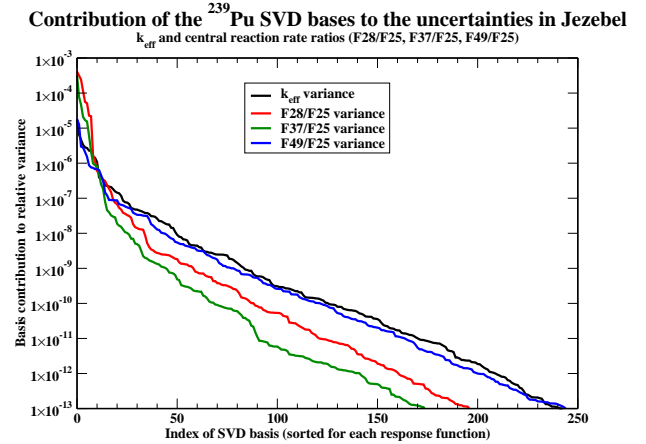

Fig. 1. Eigenfunctions contribution to the total variances in Jezebel. Response functions: k_{eff}, F28/F25, F37/F25, F49/F25. (^{239}Pu ENDF/B-VII covariances).

The major contributors to the uncertainty in Jezebel for k_{eff} and F28/F25 among the eigenfunctions of the covariance matrices, for the considered case study, are presented in Fig. 2. It is worth noting a few important feature of these basis function. The strong anti-correlation between ^{239}Pu elastic and inelastic scattering uncertainties in the ENDF/B-VII covariance data is clearly reflected in the most important functions of the eigendecomposition. At high energies (i.e., above 2-3 MeV), the eigenfunctions appear smooth and "continuous" in energy. At lower energies, the basis functions present stair-like trends. Unfortunately, this is not related to the method proposed, but to the discretization in the input ENDF/B-VII covariances, that are not provided in a fine enough structure. This "multi-group" aspect of the eigenfunctions in certain energy regions propagates to whole adjustment process. In a previous work [9], it has been shown that the adoption of fully continuous energy covariance matrices (e.g., derived from random nuclear data evaluations) is able to produce continuous basis functions for the uncertainty quantification and nuclear data adjustment processes.

Another limitation related to the adoption of ENDF/B-VII covariance data relates to the fact that the available ^{239}Pu matrices present negative eigenvalues. Correlation matrices need to be positive semi-definite and negative eigenvalues represent unphysical correlations. In order to proceed in the continuous energy adjustment approach, the ENDF/B-VII covariances where fixed finding the nearest symmetric positive semidefinite matrices in the Frobenius norm to the original ones [11].
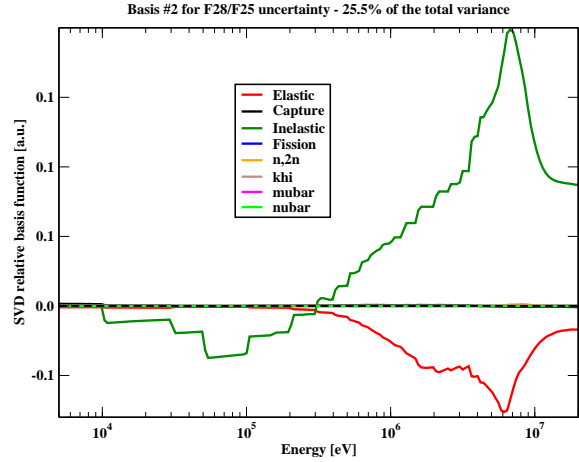
III. CONTINUOUS-ENERGY CROSS SECTION ADJUSTMENT

The previous step of the proposed method provides all the elements required to proceed with the adjustment process. The C/E for the considered response functions R and the experimental uncertainties and correlations are equivalent to
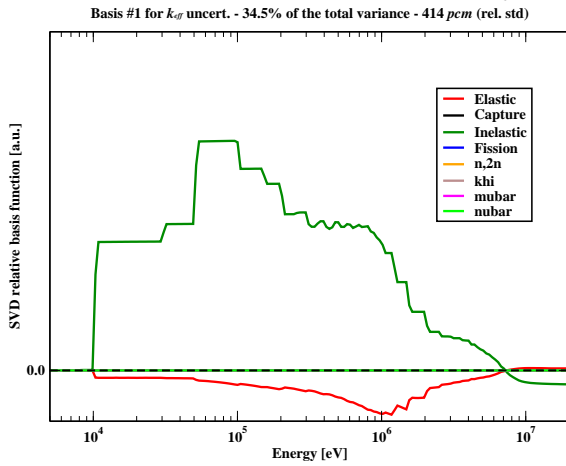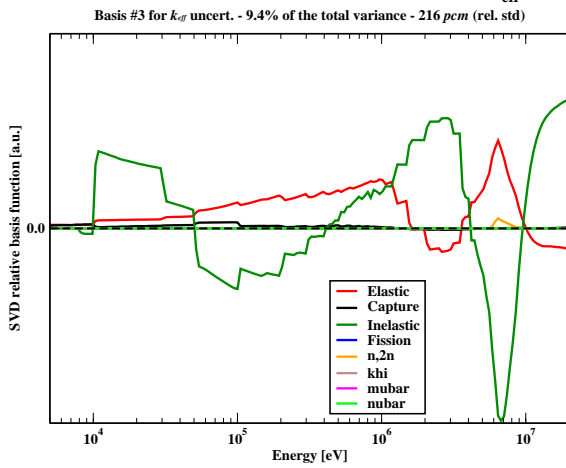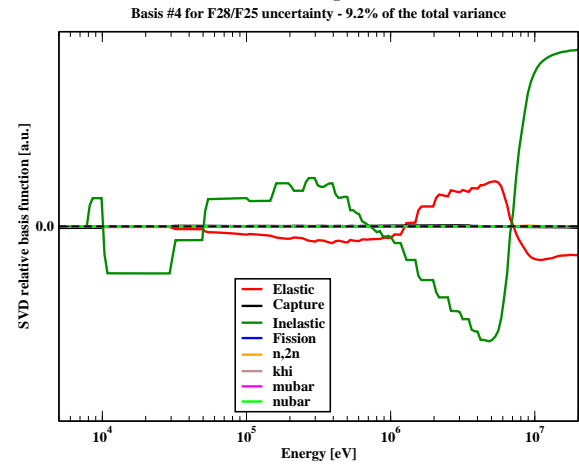
Fig. 2. Four functions from the eigendecomposition of the ^{239}Pu ENDF/B-VII covariances.

their counterparts in the standard, multi-group approach. The other elements required for the adjustment are the coefficients for the projection of the covariance matrices and the sensitivity profiles onto the continuous energy basis functions.

In the standard approach, the main inputs for the adjustment process are the multi-group sensitivity coefficients:

$$\mathbf{S_\Sigma^R} = \left(S_{\Sigma_1}^R, S_{\Sigma_2}^R \cdots S_{\Sigma_N}^R \right) \qquad (5)$$

and the (prior) multi-group covariance matrices for the considered cross sections:

$$\mathbf{COV}[\Sigma,\Sigma] = \begin{bmatrix} Var(\Sigma_1) & COV[\Sigma_1,\Sigma_2] & \cdots & COV[\Sigma_1,\Sigma_N] \\ COV[\Sigma_2,\Sigma_1] & Var(\Sigma_2) & \cdots & COV[\Sigma_2,\Sigma_N] \\ \vdots & \vdots & \ddots & \vdots \\ COV[\Sigma_N1,\Sigma_1] & COV[\Sigma_N,\Sigma_1] & \cdots & Var(\Sigma_N) \end{bmatrix} \qquad (6)$$

where $\Sigma_1, \Sigma_2 \dots \Sigma_N$ are the multi-group cross sections and nuclear data.

In the continuous-energy approach, $\mathbf{S_\Sigma^R}$ and $\mathbf{COV}[\Sigma,\Sigma]$ are replaced by the vector of eigenfunctions sensitivities:

$$\mathbf{S_U^R} = \left(S_{U_1}^R, S_{U_2}^R \cdots S_{U_n}^R \right) \qquad (7)$$

and the projection of the (prior) covariance matrices:

$$\mathbf{COV}[U,U] = \begin{bmatrix} V_1 & 0 & \cdots & 0 \\ 0 & V_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & V_n \end{bmatrix} \qquad (8)$$

It should be noted that because the eigenfunctions $U_1, U_2 \dots U_n$ are produced via eigendecomposition of the covariance matrices, $\mathbf{COV}[U,U]$ is a diagonal matrix composed by the eigenvalues $V_1, V_2 \dots V_n$. In case the continuous-energy functions are not produced as eigenvectors of $COV[\Sigma(E),\Sigma(E')]$ (e.g., obtained from a previous analysis), $\mathbf{COV}[U,U]$ would be a full $n \times n$ matrix, as in the multi-group case. The scaling of the continuous functions is arbitrary, as long as there

is consistency between each U_j and V_j (i.e., Eq. (2)). The continuous-energy adjustment methodology proceeds with the standard solution of the Generalized Least Squares Method, as done for the multigroup cross section case [3] to find the adjustment parameters $\mathbf{\Delta_U} = [\Delta_{U_1}, \Delta_{U_2} \cdots \Delta_{U_n}]^T$:

$$\mathbf{\Delta_U} = \mathbf{M} \, \mathbf{G}^T \left[\mathbf{G} \, \mathbf{M} \, \mathbf{G}^T + \mathbf{V_e} + \mathbf{V_m} \right]^{-1} \mathbf{D_R} \quad (9)$$

where $\mathbf{M}$ is the prior covariance of the continuous functions $^{prior}\mathbf{COV}\,[\mathbf{U}\,,\mathbf{U}]$. $\mathbf{V_e}$ and $\mathbf{V_m}$ represent the matrices of the experimental and modeling errors for the considered response functions. $\mathbf{D_R}$ is the vector containing the relative differences between the calculated and measure experiments.

$\mathbf{G}$ is the matrix of the sensitivities, containing the sensitivity of each response to each continuous functions:

$$\mathbf{G} = \begin{bmatrix} \mathbf{S_U^{R_1}} \\ \mathbf{S_U^{R_2}} \\ \vdots \\ \vdots \\ \mathbf{S_U^{R_N}} \end{bmatrix} \quad (10)$$

It is worth mentioning that the sensitivities for all the basis and responses R can be obtained in a single Monte Carlo criticality calculation per each experiment. Also, the possibility of calculating continuous energy sensitivities to all the possible response functions (k_{eff}, reaction rate ratios, and bi-linear ratios), thanks to the XGPT implementation, is thought of great importance for the flexibility of this approach.

Δ_{U_j} represents the projection of the change in the continuous-energy cross sections, along the direction of the eigenfunction U_j. This way, the adjusted nuclear data can be reconstructed as:

$$^{adjusted}\Sigma(E) \simeq {}^{prior}\Sigma(E) \cdot \left(1 + \sum_{j=1}^{n} \Delta_{U_j} \cdot U_j(E) \right) \quad (11)$$

Recalling that the prior covariance matrix was decomposed as:

$$^{prior}COV\,[\Sigma(E)\,,\Sigma(E')] \simeq \sum_{j=1}^{n} U_j(E) \cdot V_j \cdot U_j(E') =$$

$$= \begin{bmatrix} U_1(E) & \dots & U_n(E) \end{bmatrix} \begin{bmatrix} V_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & V_n \end{bmatrix} \begin{bmatrix} U_1(E') \\ \vdots \\ U_n(E') \end{bmatrix} \quad (12)$$

In a similar way, the adjusted covariance of the continuous functions $^{adjusted}\mathbf{COV}\,[\mathbf{U}\,,\mathbf{U}]$ via the Generalized Least Squares Method is obtained as:

$$^{adjusted}\mathbf{COV}\,[\mathbf{U}\,,\mathbf{U}] \; - \; {}^{prior}\mathbf{COV}\,[\mathbf{U}\,,\mathbf{U}] =$$

$$= \mathbf{M} \, \mathbf{G}^T \left[\mathbf{G} \, \mathbf{M} \, \mathbf{G}^T + \mathbf{V_e} + \mathbf{V_m} \right]^{-1} \mathbf{G} \, \mathbf{M} \quad (13)$$

$^{adjusted}\mathbf{COV}\,[\mathbf{U}\,,\mathbf{U}]$ contains the correlations among the basis functions introduced by the experiments.

Finally, the adjusted cross-section covariance matrix is obtained from the adjusted covariance of the eigenfunctions:

$$^{adjusted}COV\,[\Sigma(E)\,,\Sigma(E')] \simeq$$

$$\simeq \begin{bmatrix} U_1(E) & \dots & U_n(E) \end{bmatrix} {}^{adjusted}\mathbf{COV}\,[\mathbf{U}\,,\mathbf{U}] \begin{bmatrix} U_1(E') \\ \vdots \\ U_n(E') \end{bmatrix} \quad (14)$$

IV. RESULTS: A CROSS-SECTION ADJUSTMENT CASE STUDY

The case study presented in this work involves four different response functions in Jezebel: k_{eff} and three spectral indeces measured in the center of the assembly (F28/F25, F37/F25, and F49/F25). ^{239}Pu is the main isotope involved in the adjustment process, and eight different nuclear data were considered for this isotope: elastic scattering, inelastic scattering, fission, capture, (n,2n), fission spectrum (chi), first Legendre moment of the elastic scattering angular distribution, average number of neutrons emitted per fission (nubar). Also, the fission cross sections for the following isotopes were included in the adjustment process: ^{235}U, ^{238}U, and ^{237}Np. The results obtained with the proposed continuous energy approach are compared to multi-group results obtained with ERANOS and the standard adjustment methodology, adopting a 33 energy group structure.

To provide a demonstrative comparison of the input uncertainties and covariance matrices adopted by the two approaches, Fig. 3 and Fig. 4 show the ^{239}Pu capture cross uncertainties and correlation matrices adopted by the continuous and multi-group adjustment processes. While the differences between the two input uncertainties is remarkable, it should be noted that in some energy regions, the ENDB/B-VII data present a multi-group like aspect that prevents reaching fully "continuous" adjustment capabilities.
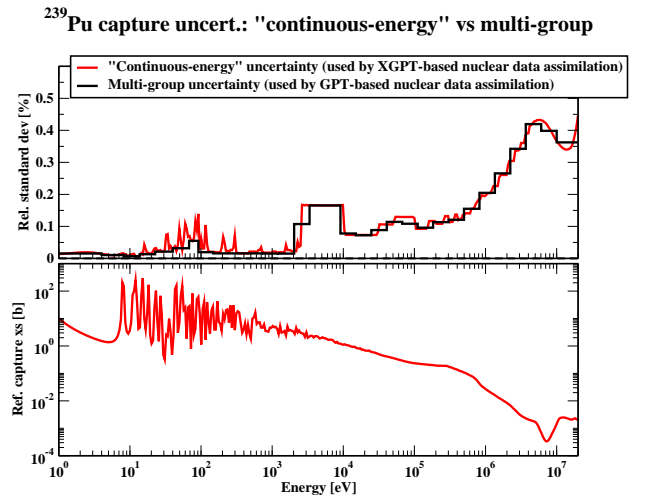

Fig. 3. Comparison between ^{239}Pu capture cross section relative uncertainty adopted as input by the "continuous" and multi-group approaches. For better clarity, the ^{239}Pu capture cross section is plotted below the uncertainties.
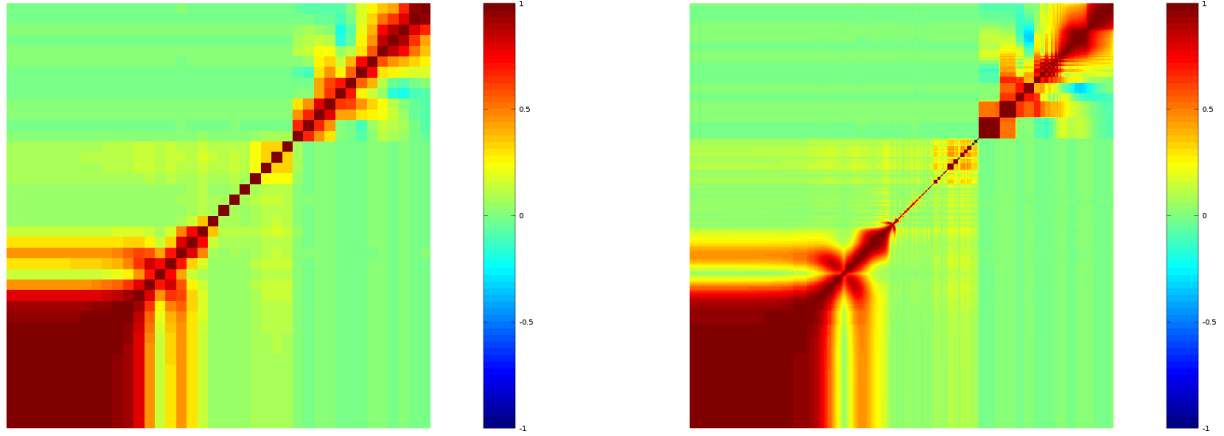
Fig. 4. Comparison between the multi-group (left) and continuous (right) ^{239}Pu capture cross correlation matrices adopted in the adjustment process.

In Table I and Table II, the adopted experimental and modeling uncertainties and correlation matrices are reported. They represent the $\mathbf{V_e}$ and $\mathbf{V_m}$ matrices that enter in the adjustment process in Eq. (9) and Eq. (13).

Relative experimental uncertainties

k_{eff}	F28/F25	F37/F25	F49/F25
0.002	0.011	0.014	0.009

Experimental correlation matrix

	k_{eff}	F28/F25	F37/F25	F49/F25
k_{eff}	1.00	0.00	0.00	0.00
F28/F25	0.00	1.00	0.32	0.23
F37/F25	0.00	0.32	1.00	0.23
F49/F25	0.00	0.23	0.23	1.00

TABLE I. Experimental uncertainties and correlation matrix for the four considered response functions (from [3]).

Table III show the calculated and experimental values for k_{eff} and the three considered central reaction rate ratios. These values, along with the continuous functions sensitivities calculated via XGPT adopting the extended Serpent version constitute the necessary elements for the adjustment process. In a similar way, the standard multi-group adjustment process was carried out adopting the Generalized Perturbation Theory capabilities available in ERANOS to calculate sensitivities coefficients for multi-group nuclear data. The results of the two processes are presented in the following.

In Table IV , the estimated nuclear data uncertainties for the considered response functions, before and after the adjustment process, are presented for the two methods. Continuous energy adjusted results are in very good agreement with deterministic estimates. In both cases, the final uncertainties are close to the input experimental and modeling uncertainties. The prior uncertainties for the different response functions are affected by the specific treatment of the input ENDF/B-VII

Relative modeling uncertainties

k_{eff}	F28/F25	F37/F25	F49/F25
0.0018	0.0090	0.0030	0.0030

Modeling correlation matrix

	k_{eff}	F28/F25	F37/F25	F49/F25
k_{eff}	1.00	0.00	0.00	0.00
F28/F25	0.00	1.00	0.50	0.50
F37/F25	0.00	0.50	1.00	0.50
F49/F25	0.00	0.50	0.50	1.00

TABLE II. Modeling uncertainties and correlation matrix for the four considered response functions (from [3]).

	Exp.	Calc. (this work)	Calc. (from [3])
k_{eff}	1.0000	0.99976	0.99986
F28/F25	0.2133	0.20871	0.20839
F37/F25	0.9835	0.97155	0.97071
F49/F25	1.4609	1.42435	1.42482

TABLE III. Experimental and calculated values.

covariances, from which where removed negative eigenvalues. While nuclear data covariances require to be symmetric positive semidefinite matrices, unphysical negative eigenvalues are sometime present in the available data. Their removal introduce differences in the prior uncertainties for some response function. For example, the Jezebel k_{eff} uncertainty obtained with the standard firs order uncertainty propagation formula, without covariance matrices correction is about 646 pcm, that is approximately 10% lower than the estimate from corrected matrices.

The reduction of the estimated uncertainties after the adjustment process in the considered case study derives mainly from reduction of the ^{239}Pu inelastic and elastic scattering un-
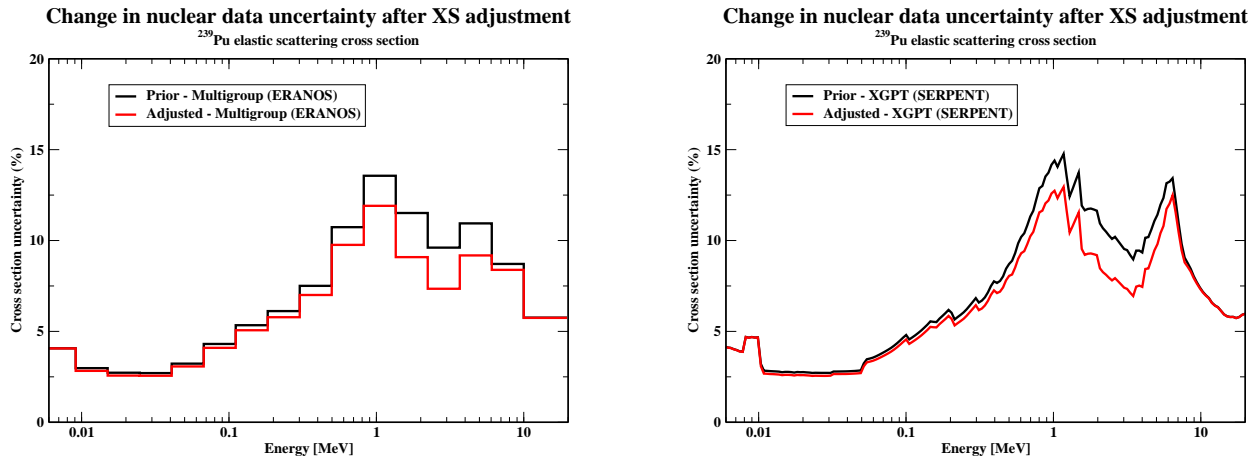
Fig. 5. ^{239}Pu elastic scattering uncertainty before and after the adjustment process. Multi-group (left) and continuous energy (right) results.
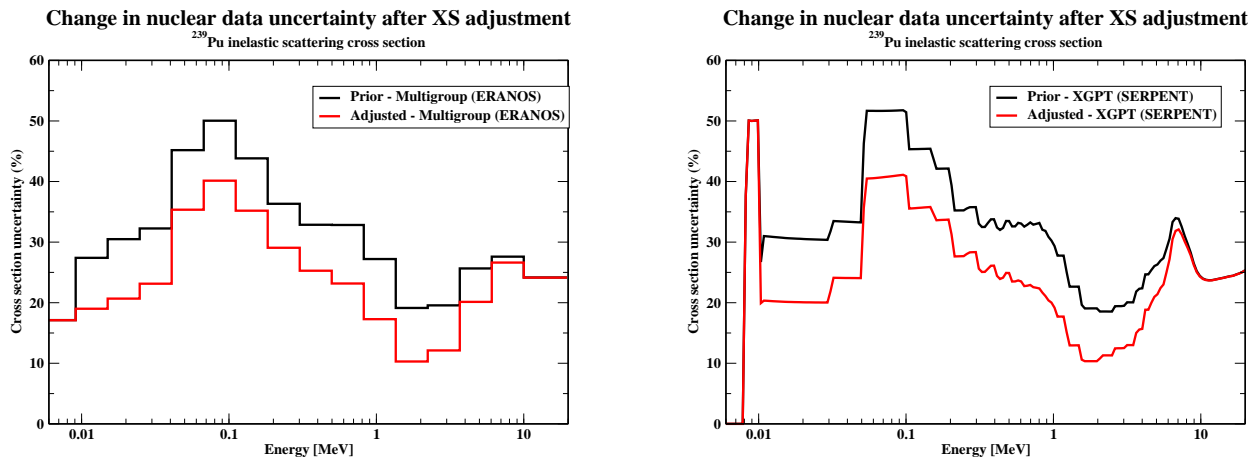

Fig. 6. ^{239}Pu inelastic scattering uncertainty before and after the adjustment process. Multi-group (left) and continuous energy (right) results.

certainties, and from the introduction of negative correlations.

In 5 and Fig. 6, the effect of the adjustment process on cross section uncertainties is presented. For both reactions, continuous energy results (right) closely follow the general trend of multi-group data (left), showing a good agreement between the two approaches. Moreover, at high energies, where the ENDF/B-VII ^{239}Pu covariances present a fine discretion, also the adjusted uncertainties preserve a smooth profile.

The negative correlations introduced by the adjustment process can be appreciated in Fig. 7 for the ^{239}Pu inelastic scattering. A large part of the reduction in the final uncertainties for some of the response functions comes from the new, post-adjustment (negative) correlations, rather than from the reduction in uncertainties alone.

The comparison for the adjusted C/E, as obtained after the Generalized Least Squares minimization, is presented in Table V. The two methods lead to very similar post C/E, despite slightly difference in the input C/E. The most important part of the adjustment of the nuclear data involves elastic and inelastic scattering on ^{239}Pu. Comparisons of relative cross sections adjustments predicted by the two approaches for these two reactions are shown in 8 and 9. Multi-group adjustment results obtained with ERANOS and continuous energy estimates from the XGPT extended Serpent version

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[2]The multi-group adjustment process is based on deterministic ERANOS S_N sensitivity calculations. Nonetheless, the C/E factors adopted in the Generalized Least Square adjustment are obtained from continuous-energy Monte Carlo correction factors from [3].
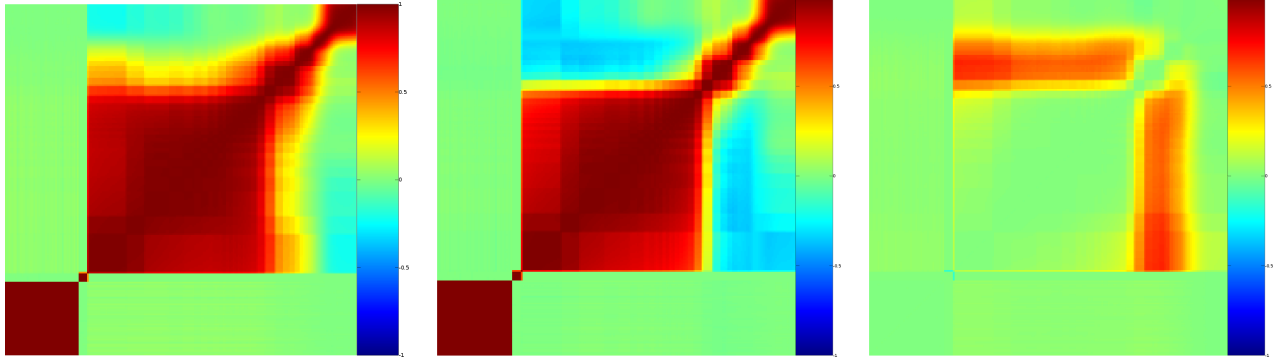
Fig. 7. ^{239}Pu inelastic scattering correlation matrix in the 1 keV – 20 MeV energy region. Before (left) and after (center) the continuous energy adjustment process, and Prior – Post difference is shown on the right.

	Prior rel. uncert. (%)		Post rel. uncert. (%)	
	multi-group	XGPT	multi-group	XGPT
k_{eff}	0.733	0.704	0.191	0.190
F28/F25	3.731	3.581	1.298	1.291
F37/F25	3.631	3.573	1.307	1.306
F49/F25	0.825	0.797	0.558	0.547

TABLE IV. Comparison of prior (input) and post (adjusted) nuclear data uncertainties estimated by the multi-group and continuous approaches for the four response functions.

	Prior C/E		Post C/E	
	multi-group [2]	XGPT	multi-group	XGPT
k_{eff}	0.99986	0.99976	1.00001	1.00000
F28/F25	0.977	0.979	0.995	0.995
F37/F25	0.987	0.988	0.996	0.996
F49/F25	0.975	0.975	0.985	0.984

TABLE V. Comparison of prior and post C/E estimated by the multi-group and continuous approaches for the four response functions.

are in good agreement. At high energy, the relative change introduced by the process follows a smooth "continous energy" profile. In the energy regions where the original ENDF/B-VII data presented coarse, multi-group-like input covariances, the adjustment can't produce continuous results.

V. DISCUSSION AND CONCLUSIONS

This work presents a new approach to perform continuous-energy cross section adjustment. The proposed method is based on recently developed Monte Carlo perturbation capabilities with continuous-energy sensitivity functions implemented in an extended Serpent version.

The new approach, that offers the possibility to produce continuous adjusted cross sections, has been compared against standard, multi-group-based results obtained via ERANOS deterministic calculations.
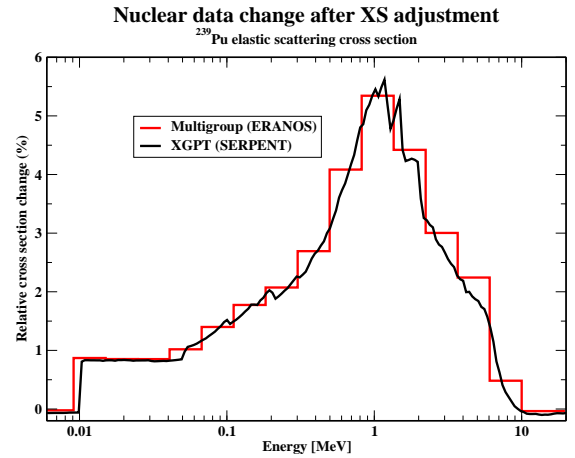

Fig. 8. ^{239}Pu elastic scattering cross section before and after the adjustment process. Multi-group (red) and continuous energy (black) results.

The considered case study involved four different response functions in the Jezebel critical assembly. A very good agreement between the proposed approach and the standard adjustment methodology is shown for what concerns adjusted covariances, adjusted cross sections, and uncertainty reduction.

The method requires to perform the eigendecomposition of input covariance matrices. For this reason, unphysical negative eigenvalues in the ^{239}Pu ENDF/B-VII correlation matrices had to be removed before the adjustment. Moreover, the adopted input data presented a fine discretization or "continuous"-like covariances only in certain energy regions. When the input data show multi-group-like uncertainties, this discretization is propagated through the steps of the adjustment process. In a previous work ([9]), fully continuous sensitivity functions were adopted, obtained from random nuclear data evaluations.

The adjusted data in Fig. 8 and Fig. 9 are given as examples of the results that can be expected using the proposed
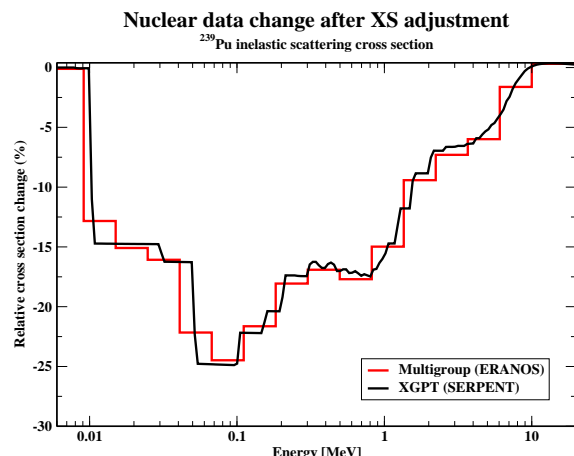
Fig. 9. ^{239}Pu inelastic scattering cross section before and after the adjustment process. Multi-group (red) and continuous energy (black) results.

method. An adjustment with a larger integral database would be needed to infer realistic data modifications. Thanks to the promising results obtained in the present work, further tests of this approach with a broader range of integral experiments and wider sets of applications are foreseen in the near future.

Moreover, a parallel research activity made available the capability to calculate sensitivities of generalized response functions to resonance parameters in a Serpent Monte Carlo implementation [12]. Future activities will consider the possibility to include directly these parameters in the adjustment process.

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