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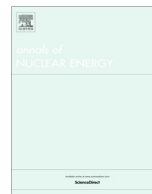
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XGPT: Extending Monte Carlo Generalized Perturbation Theory capabilities to continuous-energy sensitivity functions



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ABSTRACT

The XGPT method extends the Generalized Perturbation Theory capabilities of Monte Carlo codes to continuous-energy sensitivity functions. In this work, this method is proposed as a new approach to nuclear data uncertainty propagation. XGPT overcomes some of the limitations of legacy perturbation-based approaches. In particular, it allows the nuclear data uncertainty propagation to be performed adopting continuous energy covariance matrices, instead of discretized (multi-group) data. The XGPT capabilities are demonstrated in three simple fast criticality benchmarks for ^{239}Pu and ^{208}Pb cross section uncertainties. The new method is also applied in selected cases to estimate higher moments of the k_{eff} distribution, starting from *TENDL* random evaluations. The XGPT estimates, when compared against reference Total Monte Carlo (TMC) results, show a good agreement and a significant reduction in computational requirements with respect to the TMC approach. Finally, the capabilities for uncertainty propagation involving adjoint-weighted response functions are demonstrated.

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1. Introduction

Interest in sensitivity and uncertainty analysis within the nuclear community is continuously increasing, and recently there has been a wide spread effort to develop and consolidate tools and methods for uncertainty propagation (e.g., see [Cacuci, 2005](#); [Aliberti et al., 2006](#); [Rochman et al., 2011](#)).

Nuclear data uncertainty propagation for reactor response functions is typically performed using the Generalized Perturbation Theory (GPT) inside deterministic codes. GPT allows calculating the effect of several perturbations on reactor parameters in a single step instead of separate direct perturbation calculations. Legacy deterministic approaches adopt discretized nuclear data for both the neutron transport solution (i.e., multi-group cross sections) and the uncertainty propagation process (i.e., multi-group covariance matrices). These approaches were extensively adopted for data assimilation and cross section adjustment studies (e.g., [Palmiotti et al., 2009](#)¹), also benefiting from the fact that cross sections and covariances are adopted in a consistent multi-group form. Recently, interest in perturbation calculations in Monte Carlo has risen, and several codes have gained the capability to calculate

multi-group sensitivities, adopting continuous energy cross sections for the solution of the neutron transport problem (e.g., [Perfetti, 2012](#); [Kiedrowski and Brown, 2013](#); [Truchet et al., 2013](#); [Perfetti and Rearden, 2014](#); [Aufiero et al., 2015](#)). Nevertheless, using these codes for uncertainty propagation purposes still requires discretized, multi-group covariance matrices, and the applications of these techniques for data adjustment studies is complicated by the inconsistency between the continuous energy cross sections adopted as input, and the multi-group sensitivities obtained as output from the sensitivity calculations.

The purpose of this work is to present a new perturbation-based approach to nuclear data uncertainty propagation in Monte Carlo codes, which overcomes some of the limitations of available methods. A collision-history based method was recently implemented in Serpent ([Aufiero et al., 2015](#)) for sensitivity/perturbation calculations. Differently from other approaches, this method allows for the calculation of effects of perturbations of nuclear data on generalized response functions as k_{eff} , reaction rate ratios and bi-linear ratios (e.g., adjoint-weighted kinetics parameters and reactivity worth). Moreover, the method provides fully continuous (in energy and angle) estimators for sensitivity calculations involving Legendre moments of scattering distributions, with no requirement for angular discretization. This is obtained via weighting the scattering events in particle histories with continuous functions of the scattering cosine (i.e., the Legendre polynomials, see [Aufiero et al., 2015](#)).

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¹ For more recent information on data assimilation and cross-section adjustment methodology the reader is referred to the WPEC/SG-39 website, <https://www.oecd-nea.org/science/wpec/sg39/>.

The present work presents a generalization of such approach and a new method is proposed to perform sensitivity/perturbation calculations with no requirement for multi-group discretization of the energy-dependent sensitivity profiles or the covariance matrices. This new method is named XGPT as it extends Monte Carlo Generalized Perturbation Theory capabilities to continuous-energy sensitivity functions. The proposed method is demonstrated performing nuclear data uncertainty propagation studies in fast criticality benchmarks. The case studies involve cross section uncertainties in ^{208}Pb and ^{239}Pu . The application of the method to estimate higher moments of the response distributions is also presented. All results were obtained through a purpose-made extension of the code Serpent version 2.1.24 (SERPENT, 2011), and show a drastic reduction in computational requirements, compared to modern approaches based on the Total Monte Carlo method.

2. Standard methods for nuclear data uncertainty propagation: covariance- and TMC-based approaches

A common way to propagate nuclear data uncertainties is to use the so-called first-order uncertainty propagation formula (or *sandwich rule*, Cacuci, 2005):

$$\text{Var}[R] = \underline{S}_x^R \text{Cov}[\underline{x}] \left(\underline{S}_x^R\right)^T \quad (1)$$

where $\text{Var}[R]$ is the variance of the generic response function R and \underline{x} ; $\text{Cov}[\underline{x}]$ is the covariance matrix of the vector \underline{x} of considered nuclear data parameters (e.g., multi-group cross sections); \underline{S}_x^R is the vector of sensitivity coefficients describing the effect of perturbations on x on the response R , and defined as follow (Williams, 1986):

$$\underline{S}_x^R \equiv \frac{dR/R}{dx/x} \quad (2)$$

Methods for calculating continuous-energy accurate estimates of k_{eff} (and sometime other response functions) sensitivity coefficients are available in multiple Monte Carlo codes (e.g., Perfetti, 2012; Kiedrowski and Brown, 2013; Truchet et al., 2013; Perfetti and Rearden, 2014; Aufiero et al., 2015). These codes make use of continuous-energy cross sections data for neutron transport, overcoming some of the limitations related to the use of multi-group data in deterministic codes. Nevertheless, the propagation of nuclear data uncertainty requires introducing a discretization and score group-wise integrals of \underline{S}_x^R on a given energy grid. Increasing the accuracy of the energy discretization requires calculating a higher number of energy-integrated sensitivity coefficients. Moreover, the statistical error of Monte Carlo estimates rapidly increases when \underline{S}_x^R are scored on a finer energy grid. For these and other reasons, beyond few hundreds groups it is impractical to calculate discretized sensitivity profiles using Monte Carlo, and most often no more than few tens of groups are used.

The Total Monte Carlo method (TMC, Koning and Rochman, 2008; Rochman et al., 2011) is a different approach to nuclear data uncertainty propagation. In TMC, a large number of independent ENDF files are randomly generated starting from resonances and nuclear models parameters and their uncertainties (e.g., with TALYS, Koning et al., 2007). These files are then processed with NJOY to produce a set of formatted continuous-energy cross sections (i.e., ACE files), and independent Monte Carlo neutron transport simulations are run with these different ACE files as input. Finally, the distributions of the response functions of interest are obtained directly from the results of the Monte Carlo runs.

Despite several improvements to the TMC method (Zwermann et al., 2012; Rochman et al., 2014), this approach is often considered an inefficient way of propagating nuclear data uncertainties, when adopted in combination with Monte Carlo neutron transport

codes. Covariance-based method presents important advantages for several applications, especially when different sources of uncertainties are to be investigated separately. On the other hand, clear advantages of the TMC method over classical approaches are that (1) no artificial multi-group covariance matrices are required, and (2) higher moments of the response distributions can be easily obtained. This method also allows to easily take into account source of uncertainties that are often neglected (e.g., secondary angular distributions) and to propagate uncertainties to virtually any response function.

3. The XGPT method for nuclear data uncertainty propagation

In this work, the XGPT method is proposed to extend Monte Carlo Generalized Perturbation Theory capabilities to continuous-energy sensitivity functions. The new method allows for nuclear data uncertainty quantification with no requirements for energy discretization. It enables efficient estimation of higher moments of the probability distributions of the considered response functions, if adopted in combination with TMC-like random evaluation files. The XGPT method is based on the projection of both the nuclear data uncertainties and the perturbation/sensitivity calculations on a set of continuous-energy basis functions.

The practice of adopting a reduced subspace is common in uncertainty propagation (e.g., see Abdel-Khalik et al., 2008; Chen et al., 2015). Nonetheless, previously available methods in Monte Carlo neutron transport codes are not able to provide unbiased sensitivity estimators for the continuous-energy bases forming the uncertainty projection subspace. Thus, legacy approaches require either the multi-group discretization of the nuclear data uncertainties (i.e., covariance matrices) or the adoption of computationally expensive direct perturbation techniques.

The key point of the new approach is the possibility to score the continuous Monte Carlo sensitivity estimates on an arbitrary defined set of bases. This approach has been previously implemented and tested in Serpent for sensitivity to scattering angular distributions, the continuous basis functions being related to the Legendre Polynomials of the scattering cosine (Aufiero et al., 2015; Aufiero and Fratoni, 2016).

In the following sections, the XGPT method and the adopted Monte Carlo estimators are briefly presented. Different case studies are used to test the XGPT results for cross sections uncertainties propagation against reference TMC results. XGPT capabilities were implemented in a purpose-made extension of the Serpent Monte Carlo code, version 2.1.24.

3.1. Cross section uncertainties in the form of random nuclear data files

The TMC approach makes use of random nuclear data evaluations as the input of the independent Monte Carlo runs for the uncertainty propagation process. As example, in Fig. 1, fifty TENDL-2013 random evaluations for the ^{208}Pb elastic scattering cross section are shown. The independent TENDL evaluations were randomly generated by varying nuclear data parameters (e.g., resonances parameters, optical model parameters, etc.) according to their estimated expected values and uncertainties. The description of the processes adopted for the generation of the random evaluations is beyond the scope of this work. A detailed description of the TMC approach can be found in (Koning and Rochman, 2012). It is worth noting that although the quality of the uncertainty propagation always depends on the assumptions employed for the generation of the input uncertainties, the XGPT method is meant to be adopted independently from the specific approach used to produce the random evaluations or the continuous energy covariance matrices.

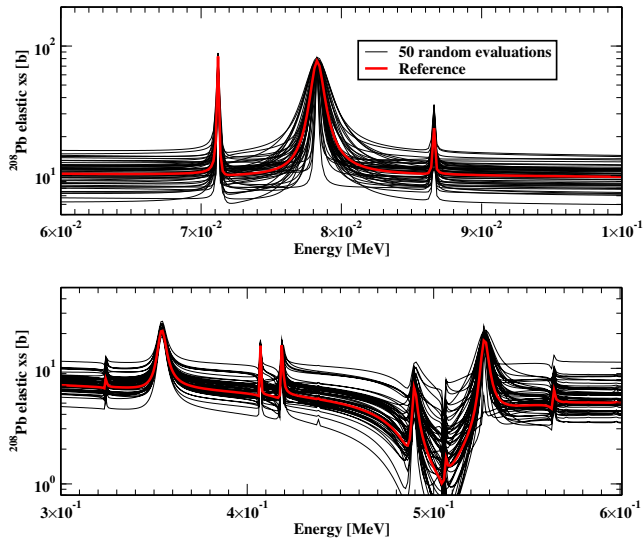


Fig. 1. TENDL-2013 ^{208}Pb random scattering cross section. Top: 60–100 keV interval. Bottom: 300–600 keV interval. Red curve represents the reference TENDL-2013 value. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this article.)

In order to present the XGPT approach, approximately 3000 independent ^{208}Pb ACE files were produced with *NJOY* adopting the reference TENDL-2013 evaluation along with the *MF2-MT151* and *MF3-MT1,2,16,51–57,102* sections of random ENDF files. This way, 3000 continuous energy ^{208}Pb nuclear data sets were produced with random elastic scattering, ($n, 2n$), inelastic scattering, and capture cross sections.

Cross sections standard deviation and correlation matrices were obtained as continuous function of the incident neutron energy, directly from the random TENDL-2013 evaluations by processing the independent ACE files. Fig. 2 shows elastic scattering relative standard deviation as obtained for ^{208}Pb . Details of the energy range between 65 and 90 keV are presented in Fig. 3. The sharp increase in the cross section relative standard deviation in the region of the tails of the 78.25 keV resonance and the decrease close to the resonance peak are clearly visible. Calculating average effective values of group-wise cross section uncertainties and sensitivities in resonances regions is a sensitive task and one of the most challenging steps for the classical approach to nuclear data uncertainty propagation, based on multi-group energy discretization. Both the TMC approach and the proposed XGPT method do not require this error-prone step.

The continuous-energy *MT2/MT2* correlation matrix obtained from the 3000 random evaluations is presented in Fig. 4. For comparison, the multi-group correlation matrix is presented in Fig. 5, adopting approximately 100 energy groups (retrieved from the OECD/NEA software JANIS-4.0). As expected, the two correlation matrices show very similar values. Nonetheless, the artificial structures introduced by the multi-group discretization are clearly visible in Fig. 5.

3.2. Projecting the cross section covariances onto a set of continuous basis functions

The first step for the discretization-free XGPT method for nuclear data uncertainty propagation consists in the projection of the cross section uncertainties onto a set of continuous-energy basis functions.

Considering for sake of simplicity only the elastic scattering reaction channel, the set of random-generated cross sections

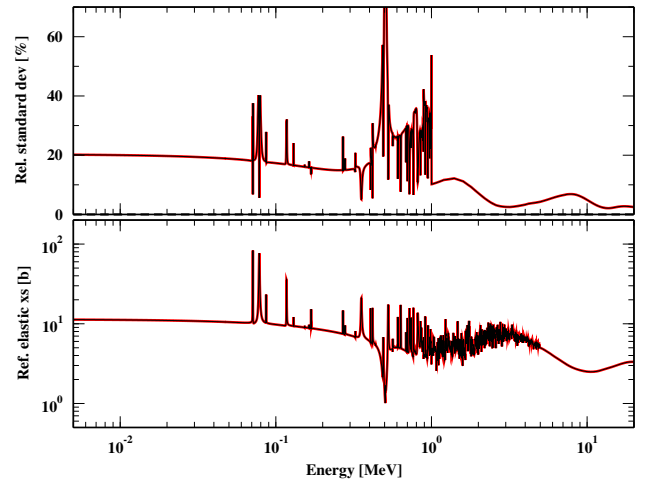


Fig. 2. ^{208}Pb elastic scattering relative standard deviation (top). ^{208}Pb TENDL-2013 reference elastic scattering cross section (bottom).

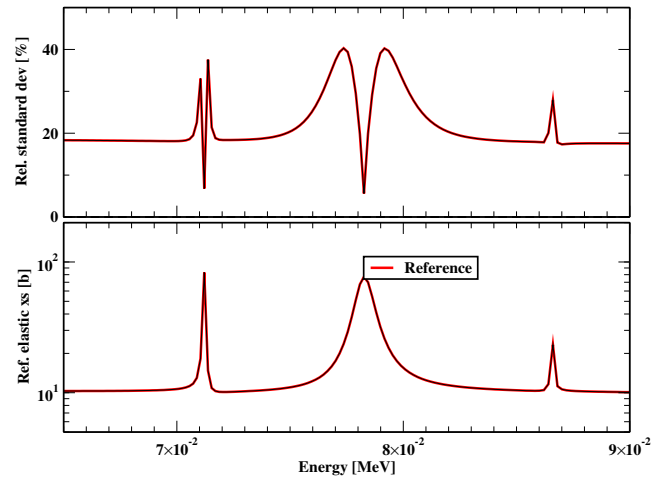


Fig. 3. ^{208}Pb elastic scattering relative standard deviation, details of the 65–90 keV energy region.

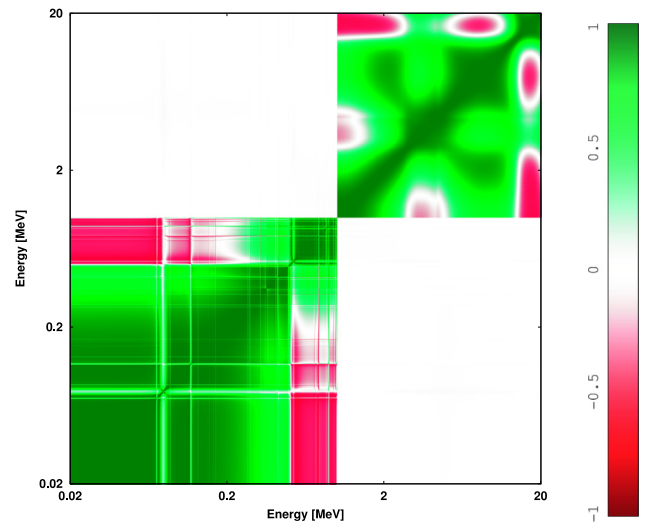


Fig. 4. ^{208}Pb *MT2/MT2* continuous energy correlation matrix.

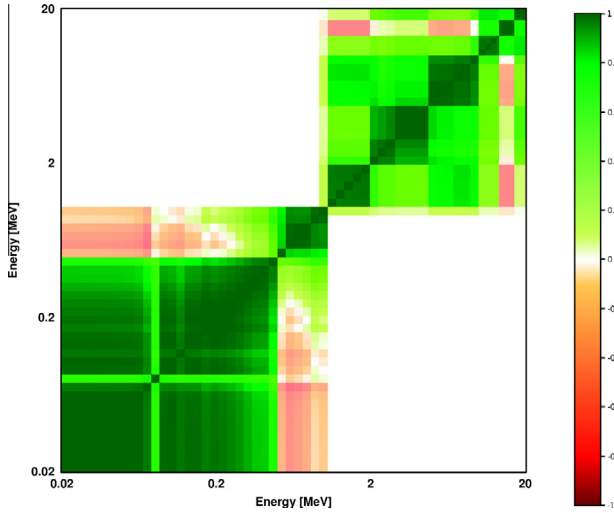


Fig. 5. ^{208}Pb MT2/MT2 multi-group correlation matrix (retrieved from OECD/NEA software JANIS-4.0).

$\{\Sigma_1, \Sigma_2, \Sigma_3 \dots \Sigma_N\}$ can be rewritten in the form of relative cross section differences:

$$\underline{A}_N = \{d_{\Sigma,1}(E), d_{\Sigma,2}(E), d_{\Sigma,3}(E) \dots d_{\Sigma,N}(E)\} \quad (3)$$

where:

$$d_{\Sigma,i}(E) = \frac{\Sigma_i(E) - \Sigma_0(E)}{\Sigma_0(E)} \quad (4)$$

with $\Sigma_0(E)$ being the reference cross section. In the present case study, N is equal to 3000 and $\Sigma_0(E)$ is the reference TENDL-2013 elastic scattering cross section for ^{208}Pb .

Using the *method of snapshots* (Volkwein, 2011) for the Proper Orthogonal Decomposition (POD) of \underline{A}_N , an optimal set of orthogonal basis functions for the projection of the cross section variability is produced. This method only requires that an inner product for the relative cross section difference function can be defined, so that the elements k_{ij} of the snapshot correlation matrix $\underline{\mathbf{K}} \in \mathbb{R}^{N \times N}$ can be calculated as $k_{ij} = \langle d_{\Sigma,i}, d_{\Sigma,j} \rangle$. Several definitions for the inner product $\langle d_{\Sigma,i}, d_{\Sigma,j} \rangle$ could be adopted in the form:

$$\langle d_{\Sigma,i}, d_{\Sigma,j} \rangle \equiv \int_{E_{\min}}^{E_{\max}} \omega(E) \cdot d_{\Sigma,i}(E) \cdot d_{\Sigma,j}(E) dE \quad (5)$$

by choosing an optimal weighting function $\omega(E)$. The present work assumes a simple weighting function uniform in lethargy over the whole energy domain.

By computing a truncated eigen-decomposition of the snapshots correlation matrix $\underline{\mathbf{K}}$, a set \underline{B}_n of n relative basis functions for the cross section Σ can be reconstructed²:

$$\underline{B}_n = \{b_{\Sigma,1}(E), b_{\Sigma,2}(E), b_{\Sigma,3}(E) \dots b_{\Sigma,n}(E)\} \quad (6)$$

This way, each random continuous-energy cross section can be approximated as a linear combination of the basis functions:

$$d_{\Sigma,i}(E) \simeq \widetilde{d}_{\Sigma,i}(E) = \sum_{j=1}^n \alpha_i^j \cdot b_{\Sigma,j}(E) \quad (7)$$

where α_i^j is the linear combination coefficient obtained by projecting $d_{\Sigma,i}(E)$ onto the basis function $b_{\Sigma,j}(E)$.

Fig. 6 shows three basis functions obtained from the POD of the 3000 random ^{208}Pb cross sections data. Joint basis functions were

² Volkwein (2011) provides a clear description of the snapshot method with weighted inner products, along with the simple steps required to perform the Proper Orthogonal Decomposition.

produced for all the reactions considered in the present uncertainty propagation study, meaning that each basis contains information on all the perturbed cross sections, fully accounting for the cross terms in the nuclear data correlations. For sake of simplicity, only elastic scattering values are presented.

Those bases represent the continuous-energy functions on which the uncertainties are projected. The three bases of Fig. 6 were selected for illustrative purposes: the basis functions are not constructed directly from the uncertainties in nuclear data parameters, but from the derived uncertainties in the continuous energy cross sections, minimizing the average squared projection errors of the random evaluations. Nevertheless, the basis functions carry physical information from the underlying process adopted to create the random cross sections. For example, it might be guessed that the basis function # 3 in Fig. 6a is representative of uncertainties in the optical model parameters, whereas basis functions 4 and 5 (Fig. 6b and c) appear to relate to uncertainties in resonance parameters.

The ^{208}Pb MT2/MT2 continuous energy correlation matrices obtained from the random cross sections reconstructed via Eq. (7) (i.e., after the orthogonal decomposition of the nuclear data uncertainties) are presented in Fig. 7. Plots are included for different number n of orthogonal basis functions $b_{\Sigma,j}$. A simple comparison of Fig. 7d and Fig. 4 suggests that 20 basis functions are able to fully represent the ^{208}Pb elastic scattering covariance matrix. For a more rigorous analysis, the eigenvalues obtained from the Proper Orthogonal Decomposition are presented in Fig. 8. These eigenvalues are often considered proportional to the relative covariance information carried by each POD basis. The usual trend with exponential decrease of the relative information is noticeable.

In the present approach, the Proper Orthogonal Decomposition (POD) of the random cross sections could be replaced directly with the eigenvalue decomposition of the continuous energy covariance matrix, with no need for generation of random evaluations. Moreover, the adoption of XGPT in combination with available fine multi-group covariance matrices is preliminary tested, as well, and shows promising efficiency.

The next step of the XGPT method for nuclear data uncertainty propagation involves scoring Monte Carlo sensitivities estimates on the same basis functions generated via the POD or eigendecomposition of cross section uncertainties. The adopted MC estimators are presented in the following Section.

3.3. Collision history-based generalized sensitivity estimators

We will consider a generic response function R defined as the ratio of two arbitrary Monte Carlo estimates:

$$R = \frac{E[e_1]}{E[e_2]} \quad (8)$$

As an example, e_1 and e_2 can be two Monte Carlo reaction rate detectors, if the response function R is a reaction rate ratio:

$$R = \frac{\langle \Sigma_1, \phi \rangle}{\langle \Sigma_2, \phi \rangle} \quad (9)$$

In the collisions rejection and particle weight perturbation framework presented in Aufiero et al. (2015), the sensitivity of R to the cross section Σ can be estimated as:

$$S_{\Sigma}^R(E) = \frac{\text{COV} \left[e_1, \sum^{\text{history}} (ACC_{\Sigma,E} - REJ_{\Sigma,E}) \right]}{E[e_1]} - \frac{\text{COV} \left[e_2, \sum^{\text{history}} (ACC_{\Sigma,E} - REJ_{\Sigma,E}) \right]}{E[e_2]} \quad (10)$$

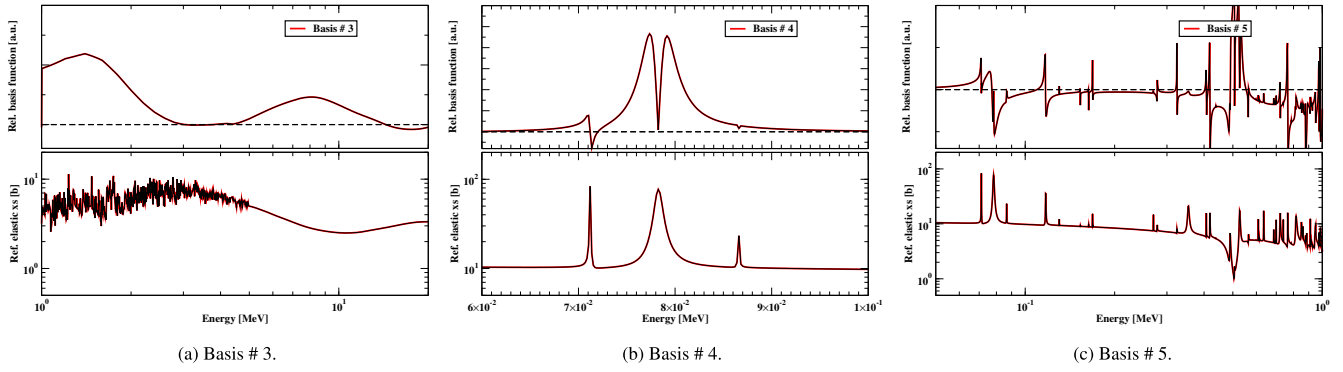


Fig. 6. Basis functions number 3, 4, and 5 from the POD decomposition of the ^{208}Pb elastic scattering uncertainty (top plots). Reference TENDL-2013 cross section (bottom plots).

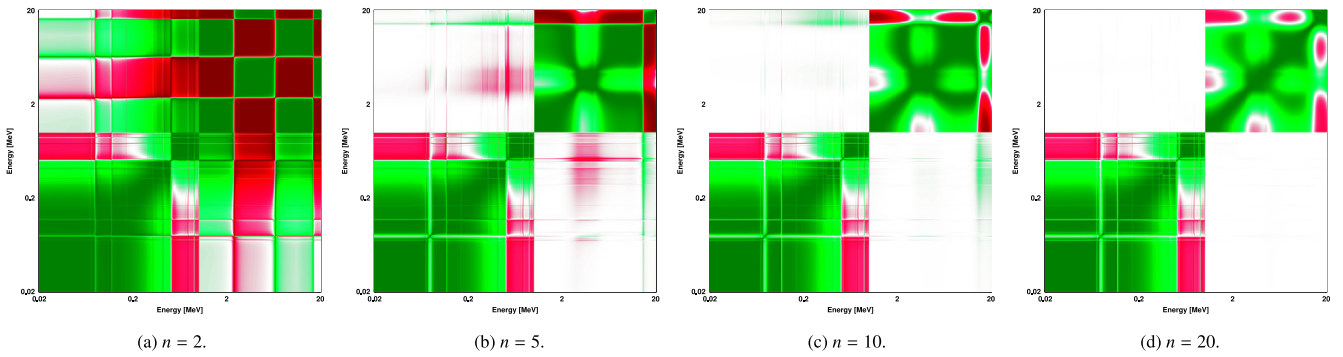


Fig. 7. ^{208}Pb MT2/MT2 continuous energy correlation matrix reconstructed after POD decomposition of the random elastic scattering cross sections, for different number n of orthogonal basis functions $b_{\Sigma,j}$.

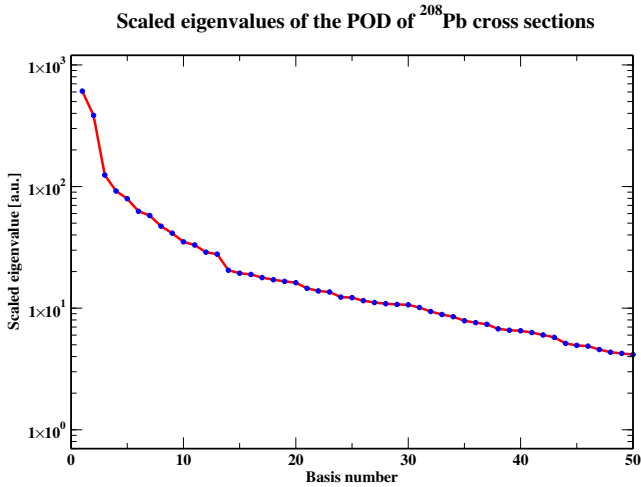


Fig. 8. Eigenvalues of the Proper Orthogonal Decomposition of the ^{208}Pb cross section uncertainties.

where $\text{COV}[X, Y] \equiv E[X \cdot Y] - E[X] \cdot E[Y]$ represents the covariance between the quantities X and Y associated to each particle, estimated over the whole neutron population. $S_{\Sigma}^R(E)$ is the sensitivity density function, $\text{ACC}_{\Sigma,E}$ and $\text{REJ}_{\Sigma,E}$ represent the accepted and rejected events with an incident neutron energy E , and is related to the cross section Σ in the history of each particle. In continuous energy Monte Carlo transport, the probability of occurrence of a collision at the exact energy E is zero. For this reason, energy-resolved sensitivity profiles are obtained by calculating group-wise integrals of $S_{\Sigma}^R(E)$:

$$S_{\Sigma,g}^R = \int_{E_g}^{E_{g+1}} S_{\Sigma}^R(E) dE \quad (11)$$

The sensitivity coefficient $S_{\Sigma,g}^R$ of the response R to the cross section Σ in the energy group g can be estimated from the accepted and rejected events in the collision histories of the neutron population, occurred within the energy boundaries E_g and E_{g+1} . In most cases (e.g., for scattering cross sections), the efficiency of the analog Monte Carlo sensitivity estimators is directly related to the number of collisions that occur within the boundaries of the considered energy group, per number of source particle. For this reason, the statistical error of Monte Carlo estimates rapidly increases when S_x^R are scored on a finer energy grid.

3.4. Basis functions sensitivities

The XGPT approach to nuclear data uncertainty propagation involves the Monte Carlo estimation of basis functions sensitivities $S_{b_{\Sigma,j}}^R$ where $S_{b_{\Sigma,j}}^R$ represents the relative change in the response function R due to a perturbation of the cross section $\Sigma(E)$ equal to the relative basis function $b_{\Sigma,j}(E)$, and can be expressed as:

$$S_{b_{\Sigma,j}}^R = \int_{E_{\min}}^{E_{\max}} b_{\Sigma,j}(E) \cdot S_{\Sigma}^R(E) dE \quad (12)$$

Extending the collision history-based approach presented in (Aufiero et al., 2015) and recalled in the previous section, $S_{b_{\Sigma,j}}^R$ can be estimated from the covariance between the terms of the response function R and the collisions related to the cross section Σ , weighted by $b_{\Sigma,j}(E)$:

$$S_{b_{\Sigma,j}}^R = \frac{\text{COV} \left[e_1, \sum^{history} G_{b_{\Sigma,j}} \right]}{E[e_1]} - \frac{\text{COV} \left[e_2, \sum^{history} G_{b_{\Sigma,j}} \right]}{E[e_2]} \quad (13)$$

where $G_{b_{\Sigma,j}}$ represents a score equal to $b_{\Sigma,j}(E)$, evaluated at the collision energy E , which is added to the particle history buffer in case of accepted collisions, and subtracted in case of rejected collisions.

The effective multiplication factor k_{eff} and the effective prompt lifetime ℓ_{eff} are the two responses considered in the present study. In case of k_{eff} being the response function, adopting the Iterated Fission Probability (IFP, Nauchi and Kameyama, 2010) adjoint estimators, Eq. (13) can be simplified to:

$$S_{b_{\Sigma,j}}^{k_{\text{eff}}} = E \left[\sum \left((-\gamma) G_{b_{\Sigma,j}} \right) \right] \quad (14)$$

where $\sum \left((-\gamma) G_{b_{\Sigma,j}} \right)$ is the sum of the weighted $G_{b_{\Sigma,j}}$ scores, collected during the γ^{th} previous neutron generation, and γ represents the number of latent generations adopted for the convergence of the adjoint estimators (Kiedrowski et al., 2011).

Adopting the IFP for the effective prompt lifetime described in (Leppänen et al., 2014), Eq. (13) is reduced to:

$$S_{b_{\Sigma,j}}^{\ell_{\text{eff}}} = \frac{\text{COV} \left[(-\gamma) l, \sum^{history} G_{b_{\Sigma,j}} \right]}{E[(-\gamma) l]} \quad (15)$$

$(-\gamma) l$ is the lifetime of the γ^{th} neutron ancestor of the present population.

3.5. First order uncertainty propagation with XGPT

The simplest way to perform continuous-energy uncertainty propagation with the proposed XGPT method involves the adoption of the first-order uncertainty propagation formula or *sandwich rule*:

$$\text{Var}[R] = \underline{S}_{b_{\Sigma}}^R \text{Cov}[\underline{\alpha}] \left(\underline{S}_{b_{\Sigma}}^R \right)^T \quad (16)$$

where $\underline{S}_{b_{\Sigma}}^R$ is the vector of the sensitivities of R to the set \underline{b}_n of the first n basis functions $b_{\Sigma,j}(E)$, obtained adopting the Monte Carlo estimators presented in Eq. (13); $\underline{\alpha}$ is the vector of linear combination coefficients α^j for the projection of the Σ cross section uncertainties onto the set \underline{b}_n . $\text{Cov}[\underline{\alpha}]$ can be calculated directly from the projections of the N $d_{\Sigma,i}(E)$, obtained from the random cross sections Σ_i . In case POD is adopted to produce the set of basis functions \underline{b}_n , the matrix $\underline{\alpha} \in \mathbb{R}^{N \times n}$, whose elements α_i^j are the linear combination coefficients for the relative cross section difference $d_{\Sigma,i}(E)$ and the basis function $b_{\Sigma,j}(E)$, is easily obtained after the eigendecomposition of \underline{K} . Moreover, thanks to the Proper Orthogonal Decomposition, the linear combination coefficients α^j are linearly uncorrelated, and Eq. (16) simplifies to:

$$\text{Var}[R] = \sum_{j=1}^n \text{Var}[\alpha^j] \cdot \left(S_{b_{\Sigma,j}}^R \right)^2 \quad (17)$$

In a similar way, the continuous energy basis functions can be obtained from the eigenvalue decomposition of relative covariance matrices. Eq. 1 can be rewritten in continuous form, considering a single cross section $\Sigma(E)$, for simplicity:

$$\text{Var}[R] = \int_{E_{\text{min}}}^{E_{\text{max}}} \int_{E_{\text{min}}}^{E_{\text{max}}} S_{\Sigma}^R(E) \cdot \text{COV}[\Sigma(E), \Sigma(E')] \cdot S_{\Sigma}^R(E') dE dE' \quad (18)$$

After eigendecomposition of the relative covariance matrix:

$$\text{COV}[\Sigma(E), \Sigma(E')] = \sum_{j=1}^n U_j(E) \cdot V^j \cdot U_j(E') \quad (19)$$

Eq. (18) becomes:

$$\text{Var}[R] = \sum_{j=1}^n V^j \cdot \left(\int_{E_{\text{min}}}^{E_{\text{max}}} U_j(E) \cdot S_{\Sigma}^R(E) dE \right)^2 \quad (20)$$

where V^j are the eigenvalues of the continuous energy covariance matrix corresponding to the eigenfunctions $U_j(E)$. Adopting the basis function sensitivity defined in the previous section, the uncertainty from nuclear data in the response function R can be obtained as:

$$\text{Var}[R] = \sum_{j=1}^n V^j \cdot \left(S_{U_j}^R \right)^2 \quad (21)$$

which is equivalent to Eq. (16). If the continuous energy covariance matrices were produced numerically from a set of random evaluations, the Proper Orthogonal Decomposition of the random nuclear data and the eigenvalue decomposition of the covariance matrix produce the same set of orthogonal functions.

Apart from changing the set of parameters from the multi-group cross sections to the continuous energy basis functions, the XGPT approach can be adopted in combination with the solid methods developed from classical linear perturbation theory (e.g., see Salvatores et al., 2013). This could disclose the possibility to perform experiment data assimilation and cross sections adjustment studies with continuous-energy cross sections, adopting legacy Generalized Linear Least Squares (GLLS) approaches.

As pointed out in the previous Sections, one of the advantages of the TMC approach is the possibility to easily obtain higher moments of the response function distributions due to nuclear data uncertainties. For example, the adoption of the ^{208}Pb uncertainties from TENDL-2013 random evaluations lead to highly skewed k_{eff} distributions, in the case studies presented in the following sections. These distributions are not well represented by the standard deviation alone. For this reason, the XGPT method was adopted to obtain higher moments of the response function distributions.

3.6. XGPT and POD as a reduced order model for TMC

The nuclear data Proper Orthogonal Decomposition allows to approximate every random cross section $\Sigma_i(E)$ as a function of the reference cross section $\Sigma_0(E)$ and a linear combination of the orthogonal basis functions $b_{\Sigma,j}(E)$:

$$\Sigma_i(E) \simeq \widetilde{\Sigma}_i(E) = \Sigma_0(E) \cdot \left(1 + \sum_{j=1}^n \alpha_i^j \cdot b_{\Sigma,j}(E) \right) \quad (22)$$

adopting the XGPT method, the value for the response function R obtained adopting a random cross section Σ_i as input can be approximated as follows:

$$R_{\Sigma_i} \simeq \widetilde{R}_{\Sigma_i} = R_{\Sigma_0} \cdot \left(1 + \sum_{j=1}^n \alpha_i^j \cdot S_{b_{\Sigma,j}}^R \right) \quad (23)$$

where R_{Σ_i} is the value for the response calculated for the random cross section $\Sigma_i(E)$, R_{Σ_0} is the value of R for the reference cross section $\Sigma_0(E)$ and $S_{b_{\Sigma,j}}^R$ are the R sensitivities to the basis functions $b_{\Sigma,j}(E)$ calculated via the Monte Carlo estimators presented in the previous sections.

The XGPT method allows estimating values of any response function R for each of the N considered random cross sections set, within a single criticality source Monte Carlo run. The present implementation of the XGPT approach involves the calculations of only the first-order sensitivity coefficients, as common in nuclear

data uncertainty propagation. The impact of this approximation is discussed in the following Section.

4. Verification of the XGPT results against TMC estimates

In this Section, nuclear data uncertainty propagation results obtained using the XGPT approach are compared to TMC results for several criticality benchmarks.

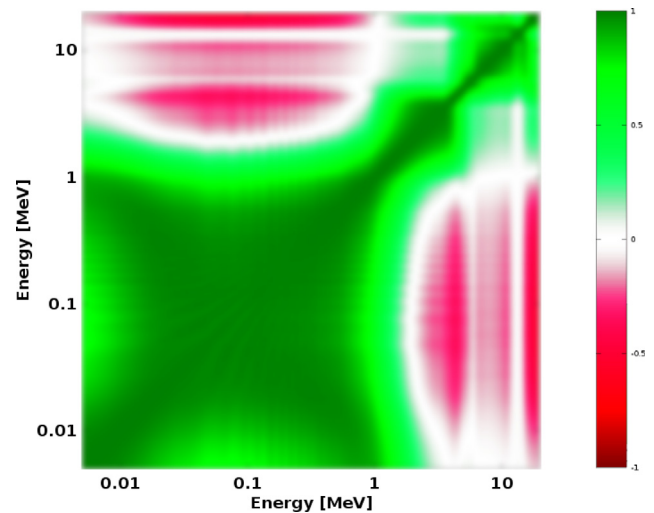
4.1. k_{eff} uncertainty from continuous energy covariance matrix in Jezebel

The first verification case study involves the propagation of ^{239}Pu fission cross section uncertainties in a bare metallic plutonium sphere (Jezebel, PU-MET-FAST-001 from NEA Nuclear Science Committee, 2011), using continuous energy *MT18/MT18* covariance matrix. For this purpose, approximately 650 TENDL-2013 (Koning and Rochman, 2012a) evaluations were processed with NJOY, adopting random *MF3-MT18* sections in the *ENDF* files. For consistency, the ^{239}Pu random *ACE* files were read with Serpent and all the fission cross sections from the independent evaluations were scored on the same energy grid (5000 uniform lethargy bins between 2.5 keV and 20 MeV). The ^{239}Pu *MT18/MT18* relative covariance matrix was produced directly from the 650 cross sections set. The obtained continuous energy correlation matrix is presented in Fig. 9, and compared to the multigroup values from TENDL-2013 *MF33* file.

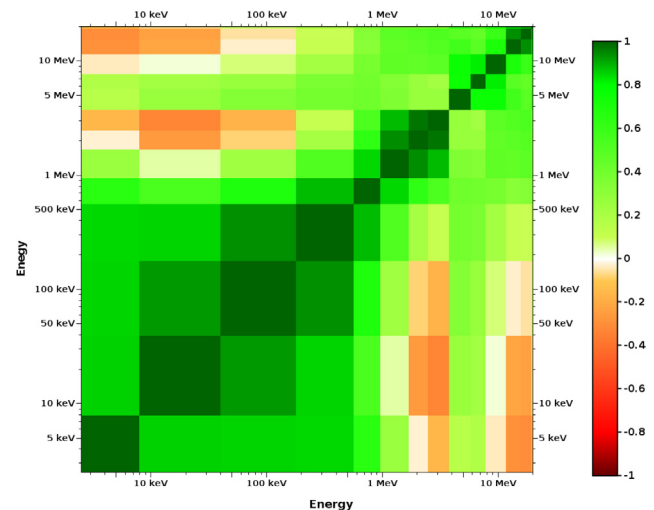
The eigenvalue decomposition of the continuous energy covariance matrix was performed adopting the first 150 eigenpairs, to allow the XGPT estimate of the ^{239}Pu fission cross section contribution to the k_{eff} uncertainty in Jezebel via Eq. (21). XGPT estimates were obtained adopting five latent generations for the convergence of the adjoint estimators and are compared to TMC reference results in Table 1. The Total Monte Carlo simulations were run on a 20 cores machine equipped with two Intel(R) Xeon(R) CPU E5-2670 v2 processors @ 2.50 GHz, using 4×10^8 active particles per run, for a total of approximately 130 h wall-clock time (650 runs). The statistical uncertainty on the Monte Carlo k_{eff} estimates in each simulation was around 5 pcm, which resulted to be negligible compared to the k_{eff} uncertainty derived from the fission cross section TENDL-2013 data. The relative statistical error in the TMC uncertainty estimate was calculated as $\simeq \sqrt{1/2(n-1)}$, where $n = 650$ represents the number of samples (Ahn and Fessler, 2003). The XGPT results were obtained with a single extended Serpent run on a laptop machine with Intel(R) Core (TM) i7-5500U CPU (two cores), adopting 4×10^7 active particles (approx. 6 min wall-clock time). This resulted in statistical error for the k_{eff} uncertainty similar to the TMC result (± 1 pcm).

This simple uncertainty propagation case study shows a very good agreement between XGPT and reference TMC results. Nonetheless, it should be noted that this test is only meant to be considered as verification case, and similar studies performed adopting other covariance data (e.g., from *ENDF/B-VII.1*) showed a smaller contribution of ^{239}Pu fission to k_{eff} uncertainty in Jezebel (e.g., see Zhu et al., 2015). For a better understanding of the presented results, Fig. 10 shows the TMC k_{eff} distribution from random ^{239}Pu *MF3/MT18* uncertainties. The continuous line shows a normal distribution having the standard deviation obtained from the XGPT results.

The effect of the eigenvalue expansion truncation on the accuracy of the XGPT uncertainty estimate for the considered case study is presented in Fig. 11. Few basis functions are required to reduce the truncation error to a low level and below statistical uncertainties (i.e., around 1 pcm). Despite the fact that more complex cases are expected to require more functions to reach the required accuracy, the good converging properties of this approach



(a) Continuous energy correlation matrix obtained numerically from the random TENDL-2013 fission cross sections.



(b) TENDL-2013 multigroup correlation matrix (*MF33* file). Retrieved from OECD/NEA-JANIS-4.0.

Fig. 9. Continuous energy and multigroup ^{239}Pu *MT18/MT18* TENDL-2013 correlation matrix.

Table 1

^{239}Pu fission cross section contribution to the k_{eff} uncertainty (standard deviation) in Jezebel. XGPT and eigendecomposition of the continuous covariance matrix vs. TMC.

Method	Uncertainty (<i>MT18</i>)	Uncert. stat. err.
TMC	828 pcm	± 1 pcm
XGPT + eig.	827 pcm	± 1 pcm

is intrinsically related to the usual behavior of rapidly decreasing eigenvalues in eigendecomposition of covariance matrices. It is worth noting that the number of orthogonal functions required (i.e., the number of sensitivity coefficients to be calculated with Monte Carlo) should be compared to the standard practice for GPT-based uncertainty propagation, which adopts a much larger number of multi-group sensitivity coefficients.

4.2. Higher moments of responses distributions adopting XGPT and POD

In this Section, the capabilities of the XGPT method to estimate higher moments of the uncertain response function distributions

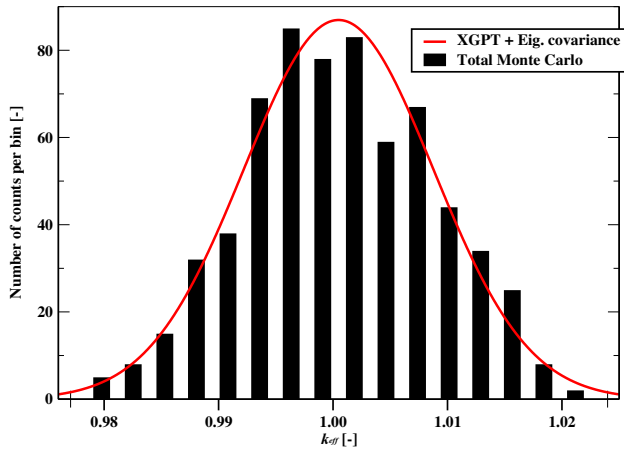


Fig. 10. k_{eff} distribution from ^{239}Pu MF3/MT18 uncertainties (TENDL-2013). XGPT and eigendecomposition of the continuous covariance matrix vs. Total Monte Carlo.

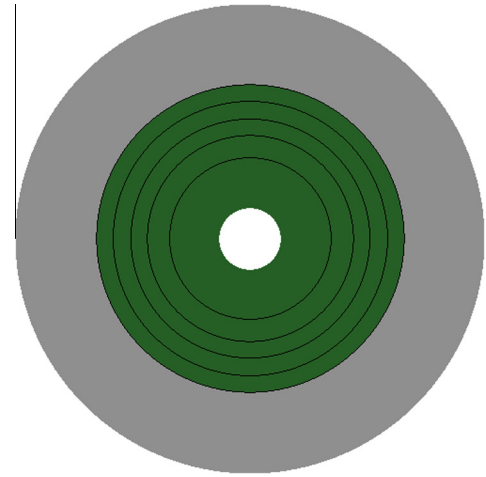


Fig. 12. Simplified geometrical description of the PMF-35 criticality safety benchmark from (NEA Nuclear Science Committee, 2011). The central plutonium core is depicted in green. The lead reflector is shown in gray color. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this article.)

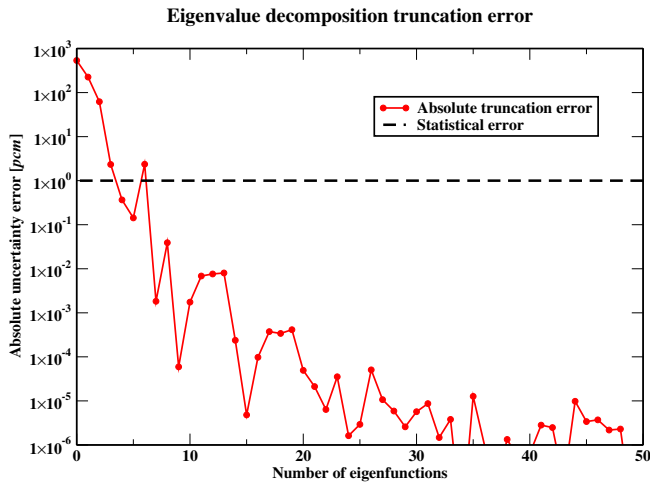


Fig. 11. Truncation error in the XGPT uncertainty estimate due to the adoption of a finite number of eigenfunctions. k_{eff} uncertainty in Jezebel due to ^{239}Pu fission cross section (TENDL-2013).

are presented. For this purpose, the ^{208}Pb nuclear data were considered. Previously published TMC results showed highly skewed k_{eff} distribution for cases involving this nuclide (e.g., see Alhassan et al., 2015).

The case studies considered in this Section are two lead-reflected criticality benchmarks: PU-MET-FAST-035 and HEU-MET-FAST-064 from (NEA Nuclear Science Committee, 2011). The PMF-35 is a critical assembly consisting of a concentric shells of metallic ^{239}Pu (δ , 98%) of 6 cm radius, reflected by 3.15 cm of lead (see Fig. 12). The HMF-64 is a critical assembly consisting of a cylinder of alternating layers of highly enriched uranium (96 at. %) and lead with a lead reflector (see Fig. 13).

Reference k_{eff} distributions were obtained with the standard TMC approach: 3000 independent ^{208}Pb ACE files were produced with NJOY adopting the TENDL-2013 evaluation (Koning and Rochman, 2012a) along with the MF2-MT151 (resonance parameters) and MF3-MT1,2,16,51,52,53,54,55,57,102 sections of random ENDF files. This way, 3000 continuous energy ^{208}Pb nuclear data sets were produced with random elastic scattering, inelastic scattering, ($n, 2n$) and capture cross sections.

The random ACE files were also adopted to numerically derive the joint probability distributions of the ^{208}Pb continuous energy cross sections for the considered reactions, scored on a 5000 uni-

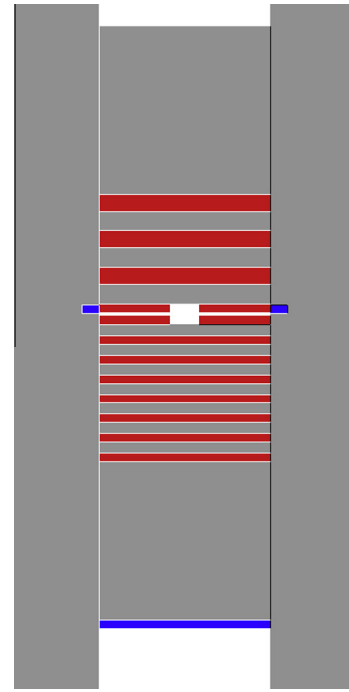


Fig. 13. Simplified geometrical description of the HMF-64 criticality safety benchmark from (NEA Nuclear Science Committee, 2011). The highly enriched uranium disks are presented in red. Lead is shown in gray. Other materials in blue. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this article.)

form lethargy bins grid. The Proper Orthogonal Decomposition was adopted to produce basis functions for the XGPT uncertainty propagation process. In the presented case studies, a single set of orthogonal functions was produced. Thus, the information on the cross terms covariances (e.g., representing the correlation between elastic scattering and capture) is implicitly embedded in the linearly uncorrelated multi-reaction bases.

XGPT estimates for the k_{eff} distributions were obtained in both cases with a single criticality source calculation by the modified Serpent version. This extended version includes the capability to calculate orthogonal basis sensitivities to reconstruct a reduced

order model approximation of response function distributions, as presented in the previous Section.

Using Eq. (23), the k_{eff} values for the 3000 random evaluations were estimated via XGPT from the basis functions sensitivities and the coefficients of the POD decomposition. Fig. 14 shows the XGPT results in the PMF-35 case study versus reference values obtained with independent Monte Carlo runs. Results are expressed as differences from the average k_{eff} over 3000 random samples. The XGPT run adopted 8 latent generations for the convergence of the IFP adjoint estimators and 150 POD bases. Fig. 15 shows the errors in the XGPT estimates ($k_{\text{eff}}^{\text{XGPT}} - k_{\text{eff}}^{\text{TMC}}$). The error bars represent $\pm 1\sigma$ statistical uncertainty, accounting for both the k_{eff} error in each independent TMC simulation and the statistical uncertainty in the continuous functions k_{eff} sensitivity coefficients in XGPT. For the few extreme cases of random cross sections sets leading to a system reactivity excess beyond 1500 pcm from the average value, a slight underestimation of the XGPT results can be noticed. These differences are likely related to non-linear perturbation effects that are not taken into account in the present implementation. Nonetheless, most of the 3000 estimates obtained via XGPT lie within ± 20 pcm from the reference TMC results.

The PMF-35 k_{eff} distribution derived from TENDL-2013 uncertainties for the main reaction cross sections in ^{208}Pb is presented in Fig. 16. The histogram plot compares XGPT and TMC results, showing a good agreement between perturbation-based and reference results.

As reported in previous works related to the TENDL-based TMC analysis of lead isotopes (e.g., see Alhassan et al., 2015), the k_{eff} distribution appears to be highly skewed. The sample standard deviation and higher moments of the distribution are presented in Table 2. Estimating higher moments of the uncertain k_{eff} distributions represents one of the most interesting advantage of the Total Monte Carlo method, compared to legacy multi-group perturbation-based approaches.

The simple case studies considered in the present work show that the XGPT method can reproduce the TMC distributions with fairly good accuracy, in a more computationally efficient way. Fig. 17 presents the statistical convergences of the XGPT and TMC estimators for the standard deviation, the skewness and the kurtosis of the considered PMF-35 case, as function of the total number of active particles. The Monte Carlo sampling-based TMC approach shows slow convergence compared to perturbation-

PMF-35 - k_{eff} estimates - XGPT errors

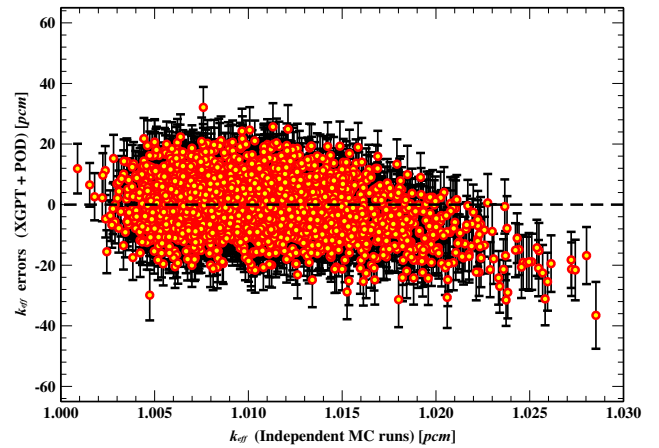


Fig. 15. Errors in the 3000 k_{eff} XGPT estimates. PMF-35 case study.

PMF-35 - k_{eff} uncertainty - XGPT + POD vs. TMC

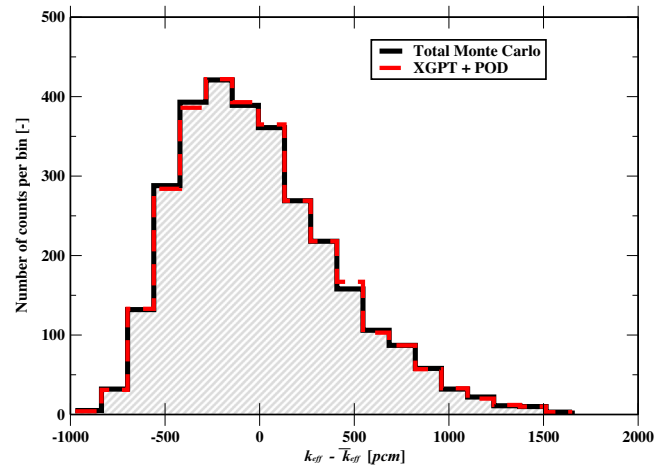


Fig. 16. PMF-35 k_{eff} distribution from TENDL-2013 ^{208}Pb cross section data. Histogram bins size is approximately 150 pcm.

PMF-35 - k_{eff} estimates - XGPT + POD vs. TMC

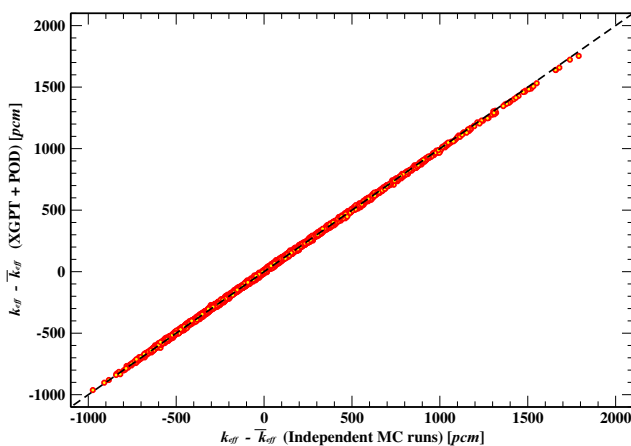


Fig. 14. Comparison between XGPT estimates for the k_{eff} for each random ^{208}Pb cross section and reference results from independent Monte Carlo runs. PMF-35 case study. Results expressed as differences from the average k_{eff} over 3000 samples.

Table 2

Standard deviation, skewness and kurtosis of the PMF-35 k_{eff} distribution from TENDL-2013 ^{208}Pb cross section data.

Methods	Standard deviation	Skewness	Kurtosis
TMC	426 pcm	0.81	3.62
XGPT	423 pcm	0.80	3.58

based results, especially for higher moments of the distributions. The difference is mainly related to the fact that the TMC method requires a large number of independent Monte Carlo transport simulations to reach satisfactory convergence. It should be noted that a relatively high number of active particles (2×10^8) was adopted in the TMC runs, to reach few pcm statistical uncertainty in the k_{eff} estimates, for better comparison with the XGPT results. For the simple purpose of estimating the moments of k_{eff} distribution, the number of active particle in the TMC runs could be reduced.

As a further demonstration of the capabilities of the XGPT approach, the HMF-64 k_{eff} distribution from TENDL ^{208}Pb cross section uncertainties and its first four moments are presented in Fig. 18 and Table 3, respectively. Compared to the previous case

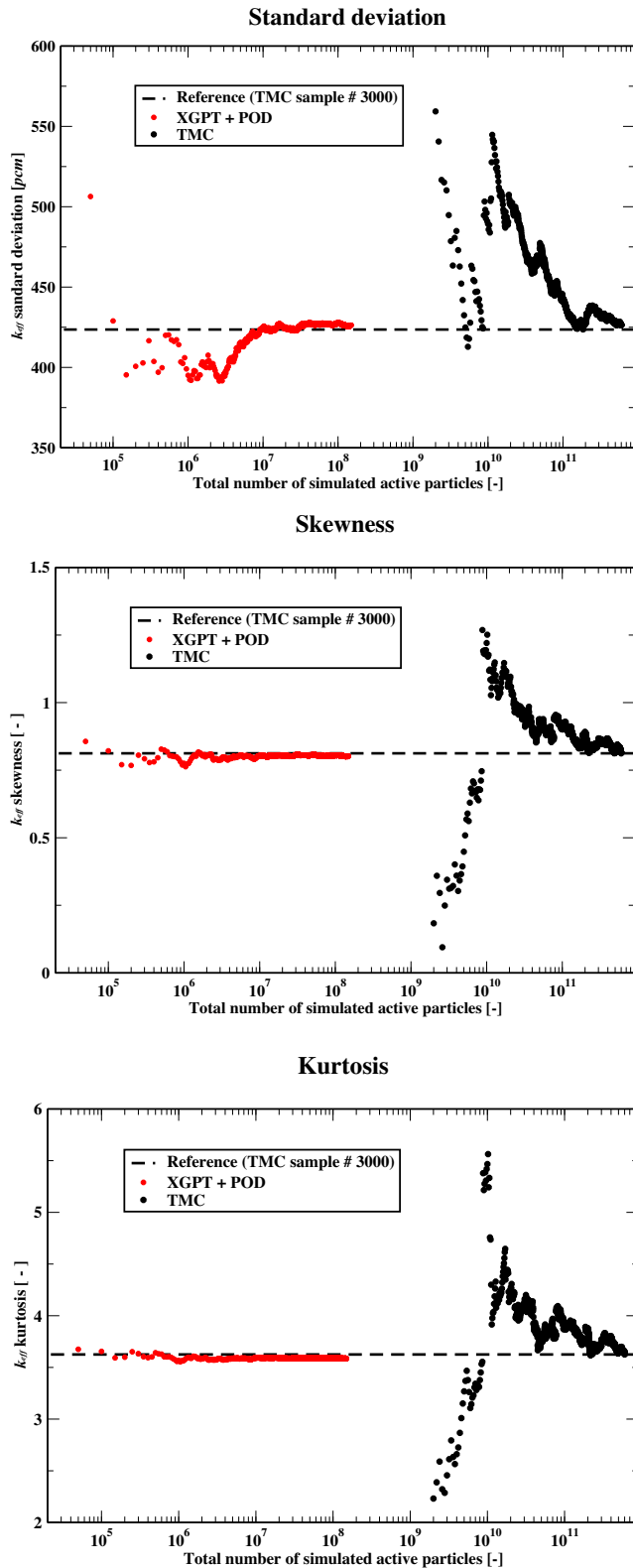


Fig. 17. Convergence of sample estimators for the standard deviation, skewness and kurtosis of the PMF-35 k_{eff} distribution versus the total number of simulated active particles.

study, in this criticality safety benchmark, the content of lead is greatly increased, and it is present not only as reflector, but also between the highly enriched metallic uranium disks (see Fig. 13).

The XGPT run was performed adopting the same orthogonal basis functions produced for the previous cases, along with 10

HMF-64 - k_{eff} uncertainty - XGPT + POD vs. TMC

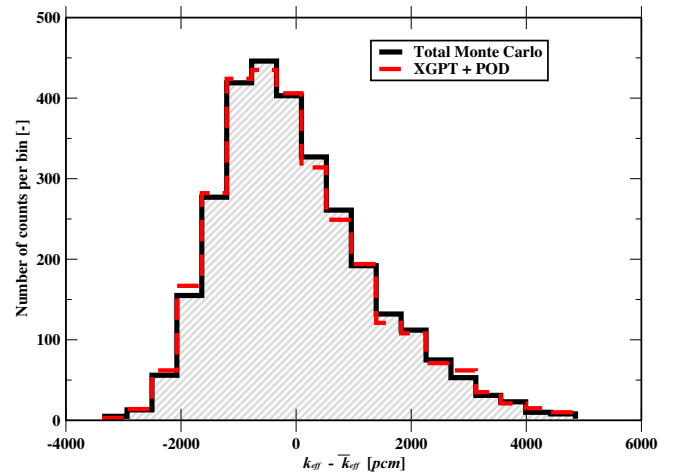


Fig. 18. HMF-64 k_{eff} distribution from TENDL-2013 ^{208}Pb cross section data. Histogram bins size is approximately 450 pcm.

Table 3

Standard deviation, skewness and kurtosis of the HMF-64 k_{eff} distribution from TENDL-2013 ^{208}Pb cross section data.

	Standard deviation	Skewness	Kurtosis
TMC	1326 pcm	0.74	3.49
XGPT	1371 pcm	0.81	3.65

latent generations for the convergence of the adjoint IFP estimators. This case study shows a very large impact of ^{208}Pb nuclear data uncertainties on k_{eff} , leading to an uncertainty in the order of 1300 pcm. This result is rather unexpected to the authors, taking into account that a single, non-fissile isotope was considered in the uncertainty propagation study. Nonetheless the result is consistent with uncertainty quantification studies that used similar TMC input uncertainties for lead (Alhassan et al., 2015). Despite larger differences between XGPT and reference results compared to the PMF-35 benchmark, also this case study confirms a good agreement between the proposed perturbation-based approach and the TMC method, especially considering the large reduction in computational time requirements.

One of the foreseen application of the XGPT approach involves assimilation, data adjustment and representativity studies. Recently, Rochman et al. (2015) and Alhassan et al. (2016) proposed a new approach to incorporate integral experiment information in the TMC methodology. This TMC-based approach requires a separate Monte Carlo run per each integral experiment, per each random nuclear data evaluation. Thus, the adoption of the proposed perturbation-based method is expected to lead to a great reduction in CPU time, while still relying on the same random evaluations adopted in the TMC approach, without the assumptions and approximations related to the generation of multi-group covariance matrices and the use of the first order propagation formula. As a simple example, Fig. 19 shows the k_{eff} correlation between HEU-MET-FAST-064 and PU-MET-FAST-035, considering ^{208}Pb cross section uncertainties.

The collision history-based approach to Generalized Perturbation Theory calculations proposed in (Aufiero et al., 2015) allows to estimate the effect of nuclear data perturbation on virtually any quantity from the output of standard Monte Carlo runs, included adjoint-weighted response functions. These capabilities, not available in other continuous energy Monte Carlo codes, are

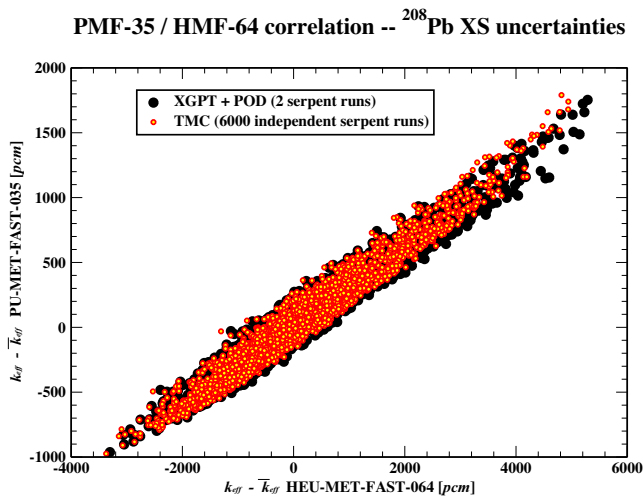


Fig. 19. Correlation between HMF-64 and PMF-35 k_{eff} estimates, considering TENDL-2013 ^{208}Pb cross section uncertainties.

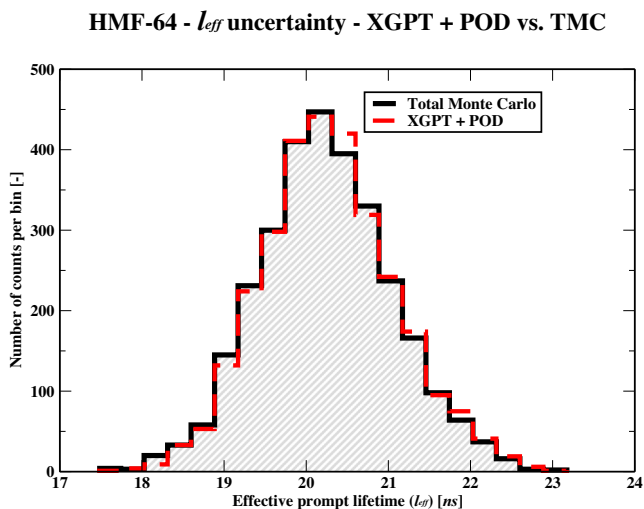


Fig. 20. HMF-64 l_{eff} distribution from TENDL-2013 ^{208}Pb cross section data. Histogram bins size is approximately 0.3 ns.

adopted in the present work to estimate the HMF-64 effective prompt lifetime uncertainty due to ^{208}Pb cross sections.

The l_{eff} sensitivity coefficients to the continuous energy orthogonal functions were calculated via Eq. (15). The distribution of the effective prompt lifetime reconstructed via XGPT is presented for the 3000 random cross sections sets in Fig. 20, and compared to reference TMC results. The relative l_{eff} uncertainty (1σ) predicted by the two methods, from the same random TENDL data is 4.01% and 3.99%, respectively. This simple test case confirms that the XGPT approach could be extended beyond k_{eff} uncertainty quantification.

5. Conclusions and ongoing development

In this work, we presented the Monte Carlo eXtended Generalized Perturbation Theory (XGPT) approach to nuclear data uncertainty propagation. This new method was implemented into a modified version of the Serpent code. It extends the previously implemented generalized perturbation capabilities to continuous basis functions sensitivity calculations.

The new capabilities allow the uncertainty propagation process to be performed with continuous-energy covariance matrices. This

possibility was demonstrated adopting a well known criticality safety benchmark (Jezebel, PU-MET-FAST-001) and ^{239}Pu MF3-MT18 (fissions cross section) uncertainties, as case study. The continuous energy covariance matrix was produced numerically, processing random TENDL-2013 evaluations via NJOY. The random ACE files were also adopted, along with the Total Monte Carlo (TMC) method, to produce reference uncertainty estimates for the considered case study. The XGPT k_{eff} uncertainty for this simple case was found to be in good agreement with reference TMC results, showing that XGPT can be effectively used for discretization-free uncertainty propagation studies, with no requirement for multi-group discretization of the covariance matrices. Moreover, whereas the TMC method requires a few hundreds independent Monte Carlo criticality source simulations, the XGPT approach adopts a single Serpent run, ensuring a significant reduction in computational requirements.

The continuous energy basis functions for the Jezebel case study were produced via truncated eigenvalue decomposition of the cross section relative covariance matrix. Other options are available for the selection of the bases for the sensitivity calculations. As a further investigation of the XGPT capabilities, the new method was adopted along with the Proper Orthogonal Decomposition (POD) of random TENDL ^{208}Pb evaluations, to reproduce higher moments of uncertain response functions probability distributions in two lead-reflected fast systems (PU-MET-FAST-035 and HEU-MET-FAST-064). Previous TMC-based studies highlighted that Pb nuclear data uncertainties lead to highly skewed k_{eff} distributions in lead-reflected fast systems. The case studies presented in this work show that XGPT can accurately reproduce these skewed probability distributions, with a good agreement between TMC and XGPT estimate of higher moments.

In conclusion, the new Monte Carlo XGPT method offers the possibility to overcome some of the limitations of legacy perturbation-based approaches to nuclear data uncertainty quantification, which require the discretization of uncertainties into multi-group covariance matrices and are unable to estimate higher moments of the response distributions. At the same time, when compared to the TMC approach, which does not suffer from major approximations, the new XGPT method showed to be significantly more efficient from the point of view of computational requirements. In this sense, XGPT provides a reduced order model approximation that can be employed as fast-running TMC surrogate or as a preliminary analysis tool, prior to a full TMC study. It is worth noting that the description of continuous-energy covariance matrices is not available in the legacy ENDF format. This is likely due to the fact that existing codes do not make use of continuous-energy covariance matrices. A wide adoption of the XGPT method will require the generation of such data.

The authors are currently involved in several research activities related to the adoption of XGPT for nuclear data assimilation and uncertainty studies. The direct calculation of resonance parameters sensitivities was successfully tested in simple 2D PWR pin-cell case studies (Aufiero et al., 2016). In this case, the continuous basis functions for the perturbation calculations are the cross sections sensitivities to the resonance parameters (e.g., total resonance width and partial resonance widths). Adopting this new approach, uncertainty propagation in the resolved resonance region can be performed directly through MF32-MT151 files (covariance information for resonance parameters). The same method is being tested for the quantification of uncertainties related to the thermal scattering parameters for $S(\alpha, \beta)$ tables.

The XGPT method is also being used for research activities related to cross section adjustment and nuclear data assimilation. This approach involves the adoption of basis functions from the eigendecomposition of covariance matrices and the related

sensitivities within the Generalized Linear Least Square (GLLS) adjustment methodology, replacing the legacy multi-group approach.

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