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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.

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/.

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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):

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

where $Var[R]$ is the variance of the generic response function R and $\underline{x}$; $Cov[\underline{x}]$ 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):

$$S_x^R \equiv \frac{dR/R}{dx/x} \tag{2}$$

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 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 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.

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