Sensitivity and Uncertainty Analysis of Nuclear Data Based on Sampling Methods

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Abstract

Nuclear data constitutes the primary source of uncertainty in nuclear reactor physics calculation results. Investigating the impact of nuclear data uncertainty on results can improve the accuracy of nuclear reactor physics calculations, thereby ensuring the economic efficiency and safety of nuclear reactor systems. This study utilizes the nuclear data sampling tool SANDY to perform multiple sampling perturbations on nuclide cross sections within the limits permitted by covariance, and based on the BEAVRS commercial pressurized water reactor benchmark hot zero-power core physics model, combined with the Monte Carlo transport calculation code OpenMC, calculates the perturbed effective multiplication factor (keff). By fitting the keff distribution curve, the impact of nuclide cross-section uncertainty in the nuclear data library on keff is quantitatively analyzed and evaluated. The results indicate that under BEAVRS benchmark hot zero-power conditions, the fission cross section of 235U is the most sensitive, with a sensitivity coefficient of 0.45; the uncertainty of the inelastic scattering cross section of 238U has the most significant impact on keff, with the standard deviation of keff reaching 91*10-5. Through comparison of the calculation results, the feasibility and applicability of the SANDY-based statistical sampling method for uncertainty analysis of nuclear data cross sections are demonstrated.

Full Text

Preamble

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Sensitivity and Uncertainty Analysis of Nuclear Data Based on Sampling Method

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Abstract

[**Background**] The input parameters for nuclear reactor physics calculations primarily include nuclear data, geometric dimensions, and fuel enrichment, among others. Among these, nuclear data is widely recognized as one of the most significant sources of uncertainty impacting the accuracy of reactor analysis. Consequently, quantitative research on the propagation of nuclear data uncertainty enhances the precision of nuclear reactor physics calculations, thereby ensuring the safety of nuclear reactor systems and improving their economic efficiency. [**Purpose**] This study aims to introduce a highly adaptable method for analyzing nuclear data uncertainty. This method enables the perturbation of nuclear databases and generates perturbation files with broad applicability, which can be utilized to conduct uncertainty analysis across various computational tools and models. [**Methods**] This study first employed the direct numerical perturbation method to conduct a sensitivity analysis on typical nuclide cross-sections, thereby validating the feasibility of the nuclear data sampling tool SANDY for perturbing nuclide cross-sections. Subsequently, within the range permitted by covariance, SANDY was utilized to perform multiple sampling perturbations on nuclide cross-sections, constructing multiple sets of perturbed nuclear databases for uncertainty analysis. To validate the effectiveness of the method, the study selected the BEAVRS benchmark, a commercial pressurized water reactor with complex geometric features, and calculated the effective multiplication factor (keff) for each perturbed database based on its hot zero-power core physics model using the Monte Carlo transport code OpenMC. To enhance computational efficiency, the sampling process was optimized: the parallelizable application perturbation module in SANDY was isolated and ProcessPoolExecutor was used to accelerate the generation of perturbation files; simultaneously, the OpenMC calculation process was parallelized using MPI technology on a supercomputing cloud platform. Finally, by fitting the distribution curve of keff, the impact of nuclide cross-section uncertainties in the nuclear database on keff was quantified. [**Results**] Under the hot zero-power condition of the BEAVRS benchmark, the sensitivity coefficients, ranked from highest to lowest, are as follows: ^{235}U fission cross-section, ^{238}U capture cross-section, ^{1}H elastic scattering cross-section, ^{235}U capture cross-section, and ^{238}U fission cross-section. Among these, the ^{235}U fission cross-section exhibits the highest sensitivity, with a sensitivity coefficient of 0.45. The uncertainties, ranked from largest to smallest, are as follows: ^{235}U fission cross-section, ^{238}U capture cross-section, ^{235}U capture cross-section, and ^{238}U inelastic scattering cross-section. Notably, the uncertainty of the ^{238}U inelastic scattering cross-section has the most significant impact on keff, with a standard deviation of up to 91$×10^{-5}$. [**Conclusions**] This study proposes a nuclear data cross-section uncertainty analysis method based on SANDY. Through validation with the BEAVRS benchmark, the feasibility of this method

under complex geometric conditions has been demonstrated. Furthermore, the perturbation files generated by SANDY support both ACE and HDF5 formats, rendering them compatible with various Monte Carlo programs such as OpenMC and MCNP. This underscores the method' s robust cross-tool and multi-model application capabilities, highlighting its strong adaptability. The research indicates that the sampling method based on SANDY not only effectively perturbs nuclear databases but is also compatible with multiple Monte Carlo computational tools, rendering it suitable for uncertainty analysis across models and under various operational conditions.

Keywords: Nuclear data; BEAVRS benchmark; Effective multiplication factor; Uncertainty analysis; Sampling method

1. Introduction

In recent years, modern numerical computing technology has advanced rapidly, coupled with the widespread application of high-performance computing platforms, enabling the construction of increasingly accurate and efficient mathematical-physical models for complex physical processes within nuclear reactor systems. This technological progress has not only enhanced simulation precision but also significantly reduced computational time, thereby delivering substantial advantages for commercial nuclear reactor systems in critical areas such as safety and economics. Simultaneously, the improvement in simulation accuracy has imposed more stringent requirements on numerical uncertainty quantification. Among various uncertainty sources, nuclear data is widely recognized as a primary contributor to uncertainty in reactor analysis. Therefore, quantitative investigation of nuclear data uncertainty propagation not only improves the accuracy of nuclear reactor physics calculations but also plays a vital role in ensuring system safety and enhancing economic performance.

1.1 Research Background

Currently, the methods widely used internationally for uncertainty quantification and propagation can be broadly categorized into two classes, as illustrated in [Figure 1: see original paper]. The first class comprises deterministic methods based on relative sensitivity coefficients. The fundamental principle involves calculating the relative covariance matrix of responses using the "Sandwich Rule" approach, which combines the relative sensitivity coefficient vector of the response with respect to input parameters and the relative covariance matrix of the input parameters. The critical component of deterministic methods is sensitivity analysis, with widely adopted techniques including perturbation theory methods and direct numerical perturbation methods.

Depending on the analysis object, perturbation theory methods can be further divided into Classical Perturbation Theory (CPT) and Generalized Perturbation Theory (GPT). CPT is exclusively applicable to eigenvalue sensitivity analysis, whereas GPT is required for other responses such as few-group homogenized parameters and power distributions. The primary advantage of perturbation theory lies in its high efficiency when the number of responses in the simulation system is significantly smaller than the number of input parameters. However, for different nuclear reactor physics codes and response types, perturbation theory necessitates the development of corresponding perturbation equations and modifications to the source code to incorporate the required computational functionalities. Consequently, this approach exhibits strong dependence on and requires substantial alterations to the source program, resulting in limited applicability.

The Direct Numerical Perturbation Method (DNPM) employs difference quotients to approximate partial derivatives for calculating relative sensitivity coefficients. This method requires artificially applying specific perturbations to the input parameters of the simulation system and recording the perturbed responses to determine the relative sensitivity coefficients. For different response types, DNPM requires no additional processing steps, offering strong applicability, and has consistently served as a benchmark method for validating the accuracy of perturbation theory-based sensitivity analysis results.

The second class encompasses Statistical Sampling Methods (SSM), which can be further subdivided based on the uncertainty propagation pathway into input parameter uncertainty propagation methods and output parameter uncertainty extrapolation methods. The currently predominant approach is the input parameter uncertainty propagation method, whose core concept involves selecting a certain number of sample points within the distribution range of input parameters as inputs to the simulation system, executing calculations to obtain corresponding response values, and subsequently performing statistical analysis on all response samples to acquire response uncertainty and related information, thereby achieving uncertainty quantification. Statistical sampling methods treat the simulation system as a "black box" without requiring source code modifications, thus demonstrating strong applicability. However, this method demands large sample sizes, making the uncertainty quantification process relatively time-consuming.

A comparative analysis of these two common uncertainty analysis methods reveals that deterministic methods, despite their higher computational efficiency in specific scenarios, fundamentally rely on first-order linear approximations, exhibiting significant limitations when handling large perturbations and nonlinear problems. Moreover, they require additional modeling for different responses, making it difficult to meet cross-model adaptation requirements. In contrast, statistical sampling methods do not depend on low-order approximations and can more accurately capture system response characteristics under nonlinear conditions and large perturbations. Although this method requires substantial sample sizes resulting in longer computational times, the individual computational tasks are completely independent, a limitation that can be effectively mitigated through parallel computing or cloud computing technologies. Therefore, this study will employ statistical sampling methods for relevant research.

1.2 Research Status

Currently, uncertainty analysis programs developed based on statistical sampling methods have achieved certain progress, such as the SAMPLER program from Oak Ridge National Laboratory and the UNICORN program from Xi' an Jiaotong University. Wan Chenghui et al. implemented a "two-step" uncertainty propagation study based on the UNICORN program, which essentially adopted statistical sampling methods and avoided statistical errors through two-stage sampling. However, resampling remains necessary when changing computational models, indicating that its applicability requires further improvement. Sun Jingyu et al. employed SANDY with statistical sampling methods to investigate the impact of nuclear data uncertainty on the effective multiplication factor calculation for the Japan Research Reactor No.3 Modified (JRR-3M). Nevertheless, research reactors feature relatively simple geometric designs and low power levels, with analysis processes that differ from commercial reactors, such as computational optimization approaches.

Based on the above analysis, it is evident that few studies have applied sampling methods to analyze cross-section uncertainty for nuclear data in commercial reactors with complex geometric structures. Additionally, in nuclear database cross-section uncertainty analysis, avoiding separate modeling for each application scenario and achieving unified code analysis for different reactor systems can reduce workload and error accumulation caused by repeated model generation. Furthermore, supporting the use of multiple computational tools (such as OpenMC, MCNP, etc.) enables comparison of results across different tools, thereby providing more reliable theoretical foundations for nuclear database cross-section impact analysis. In response to these research gaps and requirements, developing a highly adaptable process holds practical significance and necessitates relevant research.

This study first employs the direct numerical perturbation method to conduct sensitivity analysis on selected key nuclides to validate SANDY' s feasibility. Subsequently, based on the commercial pressurized water reactor benchmark Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS), the nuclear data sampling tool SANDY is utilized to perturb nuclide cross-sections within the limits permitted by covariance, combined with OpenMC to calculate the perturbed keff. Python scripts are developed to quantify and display the fitted keff distribution. To address the low computational efficiency for large sample sizes, this study accelerates OpenMC calculations through supercomputing servers and develops Python scripts to overcome SANDY's limitation of being unable to generate multiple sampling samples simultaneously, thereby significantly improving computational efficiency.

2. Theoretical Model

SANDY is a Python package for reading and writing ENDF-6 format nuclear data files, producing a set of perturbed ENDF-6 format files as output. This uncertainty propagation approach can be used for brute-force uncertainty propagation and is applicable to any model, response, or computer code compatible with ENDF-6 format files. Moreover, perturbed files are not constrained by any implicit effects arising from processing, such as multi-group approximations, resonance self-shielding, or temperature effects. This section first identifies nuclides of interest through sensitivity analysis, then employs statistical sampling methods using SANDY and OpenMC to complete sampling and calculations, and finally utilizes Python scripts to implement curve fitting for uncertainty analysis.

2.1 Sensitivity Analysis

To validate the feasibility of SANDY for nuclear data cross-section perturbation, this study screened several typical nuclide cross-sections as research objects through literature review and theoretical analysis. Direct numerical perturbation method was employed for sensitivity analysis of key nuclides, and the feasibility was verified by comparing analysis results. The direct numerical perturbation method uses the difference quotient shown in Equation 1 to approximate the differential and obtain the sensitivity coefficient of output parameters.

$$\frac{dR/R}{d\sigma/\sigma}$$

where R represents the model output, such as keff, and σ represents the microscopic cross-section of the nuclide.

2.2 Sampling Principle

SANDY extracts random nuclear data samples based on the cross-section covariance matrix (MF=33) from ENDF-6 format files. However, the ENDF-102 manual does not explicitly specify the distribution function type for nuclear reaction cross-sections, though the mathematical form of the covariance matrix is highly compatible with the statistical characteristics of normal distributions. Therefore, to simplify statistical processing and quantify nuclear data uncertainty, nuclear reaction cross-sections are typically assumed to follow a normal or approximately normal distribution. This assumption is widely applied in Monte Carlo sampling and other nuclear data processing tools.

This study further assumes that nuclide cross-sections follow a multivariate normal distribution, with correlations defined by the covariance matrix provided in ENDF-6 files. First, SANDY extracts the covariance matrix Σ from ENDF-6 format files and constructs a multivariate normal distribution $N(0, \Sigma)$. To sample from this multivariate normal distribution, an $m \times n$ matrix X must first be generated:

$$X = \begin{pmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{m1} & \cdots & x_{mn} \end{pmatrix}$$

where each column consists of independent random variables following the standard normal distribution $N(0,1)$, n is the sample size, and x_{ij} represents sample values.

To transform X into samples K that follow the target distribution $N(0,\Sigma)$, a linear operator L is defined such that $K = LX$. The linear operator L has two key properties: (1) The linearity of L ensures the distribution shape remains unchanged and does not alter the distribution mean; (2) Through linear algebra derivation, we obtain $KK^T = LXX^TL^T = LL^T = \Sigma$.

Since XX^T is an identity matrix, $E(LX(LX)^T) = LE(XX^T)L^T = LL^T = \Sigma$. To find a linear operator L satisfying this equation, SANDY employs eigenvalue decomposition: $\Sigma = S\Lambda S^T$, where $L = S\Lambda^{1/2}$.

After obtaining sample K, SANDY shifts the distribution mean to the unit vector to obtain the final sample matrix $P = K + 1$. Therefore, P is an $m \times n$ matrix following the $N(1,\Sigma)$ distribution. Taking column j as an example, each column element represents one sample, with a total of n samples, and each sample consists of perturbation values corresponding to m energy points:

$$P_j = \begin{pmatrix} p_{1j} \\ \vdots \\ p_{mj} \end{pmatrix}$$

2.3 Sampling Times

The key to statistical sampling methods is effective coverage of the sample space. Wilks' formula can determine the required minimum sample size based on specified confidence and probability levels, as shown in the following equation:

$$1 - \alpha^N \geq \beta$$

where α, β, and N represent the confidence level, probability level, and minimum required sampling times, respectively. Calculations show that with both confidence and probability levels at 99%, the minimum required sampling times is 663. To achieve higher computational accuracy, this study selects 1000 sampling times.

2.4 Calculation Process

Considering the enormous computational load of 1000 samplings and SANDY' s lack of support for Message Passing Interface (MPI) parallelization, the parallelizable application perturbation module in the program was isolated and ProcessPoolExecutor was employed to simultaneously generate 64 sets of ACE files at different temperature points on a supercomputing server, which were then converted to HDF5 files. Experimental results demonstrate that with 64 node cores, each set of 1000 samplings requires approximately 160 CPU core-hours, with an actual time of about 2.5 hours, significantly reducing computational time. The overall calculation flow is illustrated in [Figure 2: see original paper], which can be divided into three steps: (1) **Sampling Stage**: SANDY downloads ENDF-6 format files as input and calls Python APIs to perform data processing including cross-section reconstruction, matrix reading, sampling execution, and perturbation application. Finally, SANDY generates ACE files at various temperature points through the `get_{ace}` function. (2) **Calculation Stage**: OpenMC' s `ace-to-hdf5` script converts each set of ACE files into corresponding HDF5 files, which replace the original unperturbed files in the database. OpenMC then calculates and generates statepoint files for the replaced nuclear database. (3) **Statistical Stage**: Python scripts batch-read the statepoint files, fit the keff distribution curve, and perform uncertainty quantification analysis through mean and variance calculations.

3. Results and Discussion

3.1 BEAVRS Benchmark

The BEAVRS benchmark is a commercial pressurized water reactor core neutronics calculation model constructed based on actual nuclear power plants and holds significant importance in the validation of reactor analysis tools. The core consists of 193 17$\times$17 fuel assemblies, comprising 264 fuel rod lattice cells categorized into three enrichment levels of ^{235}U: 3.1%, 2.4%, and 1.6%. The remaining 25 lattice cells outside fuel cells include instrumentation tubes, burnable poison rods, and control rods. Instrumentation tubes are dispersedly arranged in assemblies at different positions, while the number and arrangement of burnable poison rods are related to assembly location. Control rods can be divided into power regulation rods (types A, B, C, D) and shutdown rods (types SA, SB, SC, SD, SE).

The core exhibits quarter-rotational symmetry overall, with high-enrichment fuel assemblies surrounding the periphery and medium- to low-enrichment fuel assemblies arranged alternately in the interior. The radial and axial geometric structures of the BEAVRS model plotted using OpenMC are shown in Figure 3: see original paper and (b). This study selected the condition with control rod D fully inserted and set the boron concentration to 902 ppm (parts per million) to calculate keff under Hot Zero Power (HZP) conditions. The cross-section database used was ENDF/B-VII.1, with 1 million neutrons per generation, 500 total generations, and the first 100 generations skipped to exclude initial inactive generation effects. The calculated reference keff value is 1.00173 $\pm$ 0.00003. In comparison, Tang Xiao et al. calculated keff as 1.00080 $\pm$ 0.00004 using OpenMC under identical conditions. Considering differences in database versions and BEAVRS model versions, the discrepancy of 93$×10^{-5}$ remains within acceptable limits.

3.2 Sensitivity Analysis

Since the direct numerical perturbation method has certain limitations on perturbation magnitude, this study used SANDY to extract the standard deviation σ of each nuclide cross-section and set the perturbation value to 1% based on the 3σ rule of normal distribution to ensure perturbation rationality. Considering numerical error cancellation issues, OpenMC calculations were configured with 1 million neutrons per generation and 500 total generations to achieve higher precision results.

Hassan et al. investigated keff sensitivity to nuclide cross-sections for the BEAVRS benchmark under all-rods-out conditions using perturbation theory, demonstrating that the ^{235}U fission cross-section is the most sensitive with a sensitivity coefficient of 0.437, indicating that keff increases most dramatically with increasing fission cross-section. The ^{238}U capture cross-section also shows relatively high sensitivity but with a negative coefficient, indicating that keff decreases with increasing capture cross-section. Based on these findings and considering the nuclear fuel composition characteristics of BEAVRS, this study selected several key nuclide cross-sections for validation research as listed in . The sensitivity coefficients calculated using Equation 1 are compared in [Figure 4: see original paper].

records the specific keff values and sensitivity coefficients after perturbing each cross-section. Comparison with Hassan' s sensitivity coefficients reveals consistent trends in magnitude, though numerical values differ slightly due to minor condition variations, which remains within reasonable bounds. Consequently, the feasibility of SANDY for cross-section perturbation has been validated.

3.3 Uncertainty Analysis

Given the substantial computational requirements for 1000 OpenMC runs, the number of neutrons per generation, total neutron generations, and inactive generations were adjusted to 200,000, 100, and 20, respectively, while maintaining unchanged control rod insertion and boron concentration. The reference keff under these settings became 1.00129 ± 0.00023.

Experiments showed that each set of 1000 sampling calculations requires approximately 4000 CPU core-hours. To reduce actual computational time, MPI parallel technology supported by OpenMC was employed on a supercomputing server to complete the calculations. The uncertainty distributions for the four selected nuclide cross-sections are shown in [Figure 5: see original paper]. records the mean and standard deviation of the uncertainty distributions for the four cross-sections after sampling calculations.

The results indicate that although the sensitivity coefficients of ^{235}U fission and

^{238}U capture cross-sections are significantly higher, their uncertainties differ little from that of the ^{235}U capture cross-section, consistent with Hassan et al.' s findings. Notably, the ^{238}U inelastic scattering cross-section exhibits an extremely small sensitivity coefficient (<0.01), yet its uncertainty distribution shows a relatively large standard deviation of approximately 100$×10^{-5}$. This occurs because high nuclide sensitivity does not necessarily imply high cross-section standard deviation. Taking ^{235}U fission and ^{238}U inelastic scattering cross-sections as examples, the standard deviation distributions shown in [Figure 6: see original paper] reveal that the ^{238}U inelastic scattering cross-section standard deviation is indeed significantly larger than that of ^{235}U fission cross-section across most energy ranges, leading to scenarios of high sensitivity but low uncertainty. Therefore, the SANDY-based sampling method demonstrates feasibility for investigating the impact of nuclear data uncertainty on commercial reactors.

3.4 Applicability Analysis

Through SANDY' s `get_{ace}` function, perturbed ACE files at different temperature points can be generated. By setting the required temperature points, a set of perturbed ACE files for the same nuclide cross-section can be produced. These perturbed files are then converted to HDF5 format (.h5 files) using the `openmc-ace-to-hdf5` command, which can directly replace the unperturbed files in the original database to create a single-perturbation database. To study uncertainty distributions under simultaneous perturbations of multiple nuclear data, no additional work is required—simply replacing the original unperturbed files with these perturbed files suffices. Since the perturbed files are in HDF5 format supported by OpenMC, these perturbed databases can be directly applied when using OpenMC for any benchmark calculation.

For other computational tools, only format conversion from ACE to the supported file format is needed. Therefore, whether using OpenMC or other Monte Carlo simulation software, the perturbed data generated through this method is universal and applicable to other computational tools and models.

This paper presents a nuclear data cross-section uncertainty analysis workflow based on SANDY and validates its feasibility under complex geometries using the commercial pressurized water reactor benchmark BEAVRS. The research process comprises three stages: First, direct numerical perturbation method was employed for sensitivity analysis of selected key nuclides. Results show that under BEAVRS hot zero-power conditions, the ^{235}U fission cross-section is the most sensitive with a coefficient of 0.45, consistent with actual conditions and other studies, validating SANDY' s effectiveness in generating nuclide cross-section perturbations. Second, within the covariance limits of nuclide cross-sections, ProcessPoolExecutor was used to accelerate SANDY sampling and perturbation file generation, with supercomputing servers and parallel technology accelerating OpenMC calculations. Results demonstrate that ^{238}U inelastic scattering cross-section uncertainty most significantly impacts keff with a standard deviation of 91×10^{-5}, aligning with actual conditions and confirming the feasibility of SANDY-based sampling methods for commercial reactor nuclear data cross-section uncertainty analysis. Additionally, by plotting standard deviation comparison charts for ^{235}U fission and ^{238}U inelastic scattering cross-sections, the conclusion that high nuclide sensitivity does not necessarily imply high uncertainty was derived. Finally, the perturbed ACE files generated by SANDY can be converted to HDF5 or other formats, making them compatible with various Monte Carlo programs including OpenMC and MCNP, and supporting cross-model and multi-condition analyses, demonstrating strong applicability.

In summary, this study proposes a SANDY-based nuclear data cross-section uncertainty analysis workflow and validates its feasibility for quantifying nuclear data cross-section uncertainty under complex geometries through sensitivity and uncertainty analysis. The research demonstrates that this method can effectively perturb nuclear databases and generates highly applicable perturbed files suitable for uncertainty analysis across different computational tools and models.

Author Contribution Statement

Cai Zhoutong: Drafted the manuscript; performed modeling and validation; analyzed and interpreted data. Liu Xiaojing: Developed research concepts; critically reviewed intellectual content. Zhang Tengfei: Provided theoretical guidance; supervised writing and review; acquired research funding.

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Note: Figure translations are in progress. See original paper for figures.