A new efficient sampling method for quantifying and propagating nuclear data uncertainty in CUSA

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Abstract: Uncertainty inevitably exists in nuclear data and correlation exists between different nuclear reactions, which are always represented by the relative covariance matrix. For the statistical sampling method, the major technical challenge is to generate a desirable input sample space by using an efficient sampling method based on the relative covariance matrix. In this paper, an efficient sampling method of Latin Hypercube Sampling combined with Singular Value Decomposition Conversion (LHS-SVDC) is proposed based on rigorous mathematical derivation and especially the correlation information between different cross sections is represented precisely. TMI-1 pin-cell case of OECD UAM benchmark was employed to verify this new method with respected to the reference solution generated by TSUNAMI-1D module. The numerical results indicate that the new LHS-SVDC method can generate a desirable sample space of multi-group cross sections quickly and effectively, which can further propagate the uncertainty in multi-group cross sections to the target parameters more accurately.

Keywords: nuclear data; uncertainty; correlation; efficient sampling method; SVD

1 Introduction

There has been an increasing demand for the uncertainty and sensitivity analysis for the numerical results from complicated nuclear reactor system, because the uncertainty inevitably exists in input parameters and computing models [1]. For nuclear reactor physical calculation, the uncertainty in nuclear data becomes the major uncertainty source and needs to be quantified by applying sensitivity and uncertainty analysis method. At present, two primary kinds of methods are widely used, *e.g.*, the perturbation method and statistical sampling method, to propagate and quantify uncertainty in nuclear data. Although, the perturbation theory establishes a good mathematical equation between the multi-group cross sections and output parameters, such as eigenvalue. But it is a first order approximation method and the adjoint equation must exists and easy to be solved. So for quantifying uncertainty of control rod worth and power distribution propagated from nuclear data, the perturbation method will fail because of inexistence of the solution of the adjoint equation or the difficulty in obtaining it. An alternative method is the statistical sampling method, which provides less approximation and has no limit to the system responses.

For the statistical sampling method, the major technical challenge is to generate a desirable input sample space by using an efficient sampling method. Several sampling methods have been developed over the years for conducting uncertainty analysis of nuclear data and these methods, such as Latin Hypercube Sampling (LHS) and Simple Random Sampling (SRS), have been implemented in some famous codes, such as SAMPLER [2], UNICORN [3], VSOP-UQ [4], CUSA [5]. The CUSA is a self-developed code system, in which LHS, SRS, Latin Hypercube Sampling combined with Cholesky Decomposition Conversion (LHS-CDC) has been successfully imple- mented to generate a reasonable sample space. And it can be coupled with other nuclear reactor physics calculation code for uncertainty analysis. Although, these three methods can be used to generate a reasonable sample space based on relative multi-group cross-section covariance matrix, the correlation infor- mation between different cross sections is not fully taken into account.

In this paper, an efficient sampling method of Latin

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Hypercube Sampling combined with Singular Value Decomposition Conversion (LHS-SVDC) is proposed based on rigorous mathematical derivation and especially the correlation information between different cross sections is represented precisely. By using this method, the sample space can represent the uncertainty information of nuclear data more accurately. At the same time, the uncertainty data generation module 'Guide' in CUSA has been updated based on the work presented in this paper.

2 Research ideas

The mathematic model for nuclear reactor physics calculation can be briefly written as:

$$R = f(\mathrm{X}) \tag{1}$$

where f is the response function; R indicates responses, such as k_{eff}; X indicates inputs. In this work, the inputs are multi-group cross sections, which obeys the multivariate normal distribution $X \sim N_{nX}(\mu,\Sigma)$, where μ is the mean value of cross sections. Σ is multi-group nuclear cross-section covariance matrix. The SRS or LHS methods can be used to generate a random sample space with a certain dimension, which are input parameters for nuclear reactor physics calculation. Actually, it is quite difficult and complicated to generate the samples satisfactory to the original matrix by directly using the covariance matrix Σ, because different cross sections are dependent and coordinated variation of samples for different parameters should be considered. An alternative approach is to generate an independent sample space from multivariate standard normal distribution $Z \sim N_{nX}(0,\mathrm{I})$, that will produce a population of vectors when multiplied by the original input vector. Its mean is equal to the reference and its elements have dependencies as given by the covariance matrix, as shown in Eq. (2).

$$X = AZ + \mu \tag{2}$$

The matrix A can be numerically solved by Cholesky factorization for symmetric positive-definite matrix or by singular value decomposition. In this way, the success of this method should meet the following two conditions: 1) the correlation matrix associated with Z is very close to the $nX \times nX$ identity matrix; 2) the mean vector is a zero vector.

A normally-distributed random sample space Z can be generated from multivariate standard normal distribution $N_{nX}(0,\mathrm{I})$ by applying LHS method. The correlation coefficient matrix C of sample space can be obtained by statistical analysis. The form of C is shown as follows:

$$C = \begin{bmatrix} c_{1,1} & c_{1,2} & \cdots & c_{1,\mathrm{nX}} \\ c_{2,1} & c_{2,2} & \cdots & c_{2,\mathrm{nX}} \\ \vdots & \vdots & \ddots & \vdots \\ c_{\mathrm{nX},1} & c_{\mathrm{nX},2} & \cdots & c_{\mathrm{nX},\mathrm{nX}} \end{bmatrix} \tag{3}$$

where $c_{i,j}$ is the correlation coefficient between parameters, $c_{i,j} = c_{j,i}$ and $c_{i,i} = 1$. Taking multi-group nuclear cross-section covariance matrix of $^{238}U(\mathrm{n},\gamma)$ [6] for example, the matrix C is shown in Fig. 1:

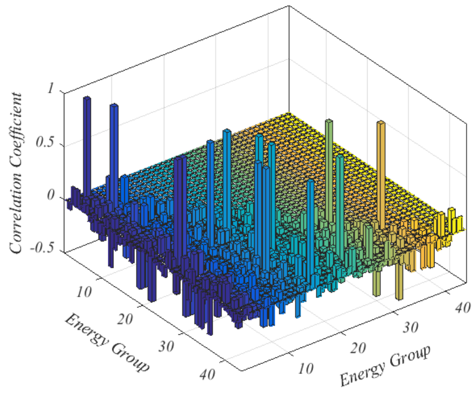

Fig.1 The correlation information between the parameters in the sample space Z obtained by LHS.

The diagonal elements are set to 0 manually, only the upper triangular part or the lower triangular part of correlation coefficient matrix is given.

The correlation coefficient matrix will not always be the identity matrix due to the correlation constraint is not considered in this process. In order to reduce the correlation between parameters of sample space, the LHS-CDC method [5] was proposed in the previous study. The specific implementation is shown as following:

$$C = QQ^T \tag{4}$$

where C is a symmetric positive-definite matrix, the upper triangular matrix Q can be obtained by Cholesky factorization for C, then the random sample space Z is transformed one by one, as shown in Eq. (5):

$$Z^* = Q^{-1}Z \tag{5}$$

The correlation coefficient matrix C^* of sample space Z^* is closer to the unit matrix compared with C, which indicates that parameters of sample space Z^* are much closer to independence. So in this way, the statistical correlation between different parameters is effectively reduced by the Cholesky decomposition transformation, as shown in Fig. 2:

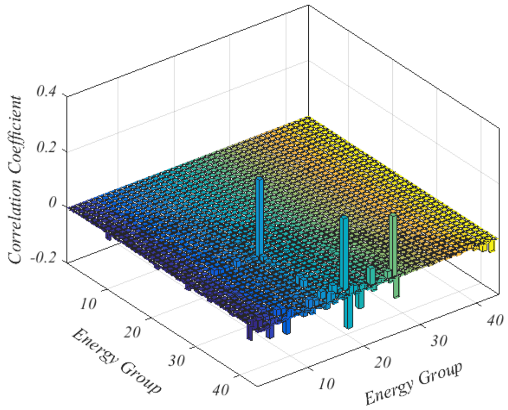

Fig. 2 The correlation information between the parameters in the sample space Z^* obtained by LHS-CDC.

Although the LHS-CDC method is a good method to generate a reasonable sample space, it is still an approximate method and there is some significant correlation between some parameters. In order to optimize this method, an efficient sampling method based on rigorous mathematical theory is proposed in this paper. The details of this new method is described as following:

A sample space Z_s can be generated by using the LHS method, and the covariance matrix Σ_s of the sample space is given as:

$$\Sigma_s = \frac{1}{n} Z_s^T Z_s - \frac{1}{n^2} Z_s^T H Z_s \tag{6}$$

where n is the number of sample space. H is a $n \times n$ full matrix with all elements are 1. Then the covariance matrix Σ_s can be decomposed by using the singular value decomposition as:

$$\Sigma_s = USV^T \tag{7}$$

Since the matrix Σ_s is a symmetric matrix, the equation (7) can be transformed into the following form:

$$U^T \Sigma_s U = S \tag{8}$$

where S is a diagonal matrix and the diagonal elements are singular values, construct matrix E and matrix D, the forms are given as:

$$E = \begin{bmatrix} \Sigma_{s1,1} & 0 & \cdots & 0 \\ 0 & \Sigma_{s2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Sigma_{snX,nX} \end{bmatrix} \tag{9}$$

$$D = \begin{bmatrix} d_{1,1} & 0 & \cdots & 0 \\ 0 & d_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_{nX,nX} \end{bmatrix} \tag{10}$$

where $d_{i,i} = \sqrt{S_{i,i}/\Sigma_{si,i}}$.

Then we get:

$$(D^{-1})^T S D^{-1} = E \tag{11}$$

Combined with formula (8):

$$(D^{-1})^T U^T \Sigma_s U D^{-1} = E \tag{12}$$

Inserting equation (6) into equation (12):

$$\frac{1}{n}(Z_s UD^{-1})^T Z_s UD^{-1} - \frac{1}{n^2}(Z_s UD^{-1})^T HZ_s UD^{-1} = E \tag{13}$$

From formula (13), the covariance matrix of sample space $Z_s^* = Z_s UD^{-1}$ is an unit diagonal matrix which indicates that the parameters in the sample space are completely independent. The correlation coefficient matrix is shown in Fig. 3.

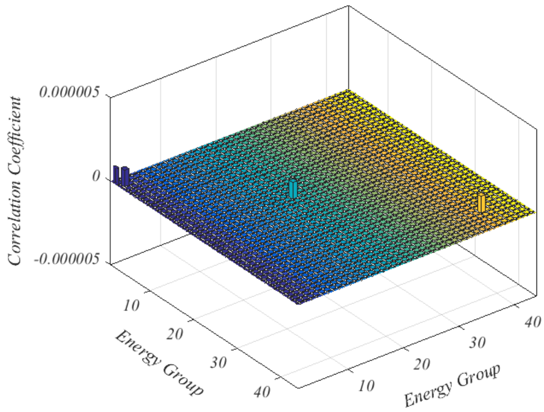

Fig. 3 The correlation information between the parameters in the sample space Z_s^* obtained by LHS-SVDC.

In this way, an independent sample space Z_s^* is generated by using the LHS-SVDC method.

3 Method verification

The distribution characteristics of sample space obtained from the LHS-SVDC method require further testing before it is used to perform uncertainty analysis. Taking multi-group nuclear cross-section covariance matrix for as an example, the sample space is 800 and the Kolmogorov-Smirnov test (referred to as K-S test) [7] is conducted for testing the distribution of samples. Level of significance is shown in Fig. 4.

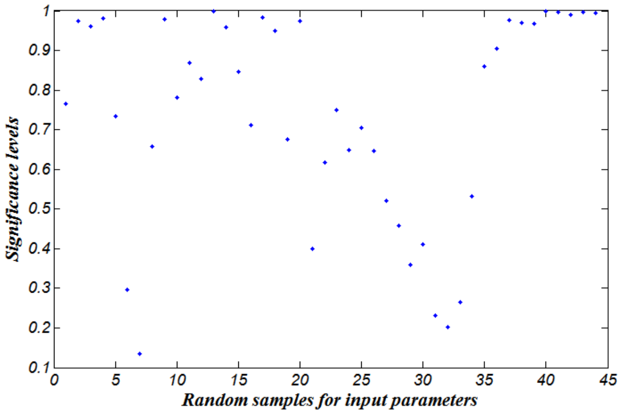

Fig. 4 The K-S test significance level of the parameter identification for random sample Z_s^*.

Where, the number 1-44 represents the associated energy group.

According to Kolmogorov's theorem, the K-S test is performed on sample space of both the hypothetical population distribution and the unknown distribution. If the level of significance is small, the hypothesis will be rejected, that is, the distribution of the random sample space does not satisfy the hypothetical population distribution. If the level of significance is close to 1, the distribution of random samples obeys the hypothetical population distribution. The level of significance can be observed from Fig.4. Among them, the two parameters with the smallest and the largest level of significance in all parameter identifications are chosen to be plotted respectively. The comparison between sample space empirical distribution and the normal distribution of a target are shown in Fig. 5 and Fig. 6.

The K-S test confirms that the sample space of 44 group cross sections for $^{238}U(\mathrm{n},\gamma)$ obtained by the LHS-SVDC method shows good agreement compared to the normal distribution.

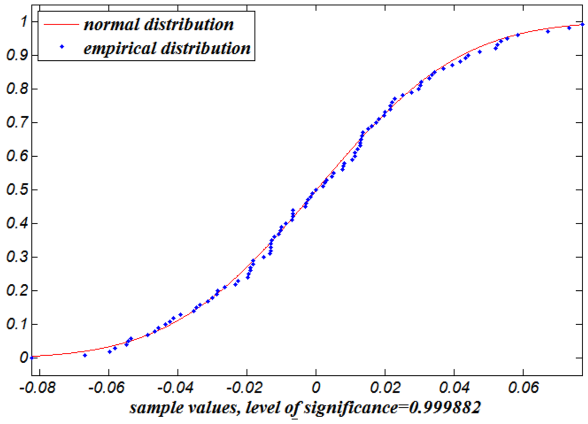

Fig. 5 The distribution of the empirical results with the biggest level of significance is compared with the corresponding target distribution.

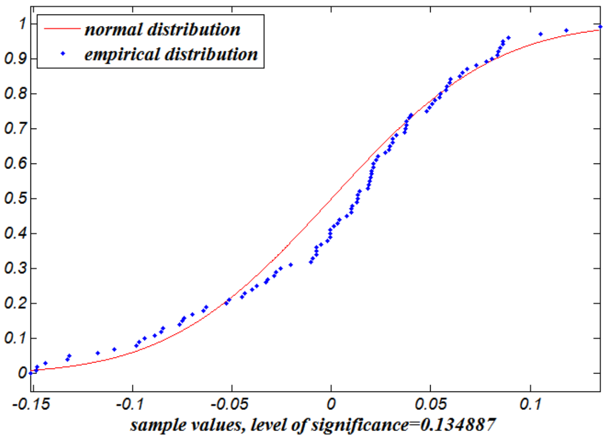

Fig. 6 The distribution of the empirical results with the smallest level of significance is compared with the corresponding target distribution.

The final sample space X which is obtained by the LHS-SVDC method based on the covariance matrix of $^{238}U(\mathrm{n},\gamma)$. The relative covariance matrix and the absolute deviation compared with the original relative covariance matrix are obtained through statistical analysis, as illustrated in Fig. 7 and Fig. 8. Figure 7 indicates that the LHS-SVDC sampling method can generate a desired random sample space, which satisfies the target relative covariance matrix.

From the above analysis, we can observe that the LHS-SVDC sampling method proposed in this paper can efficiently and quickly generate a sample space of multi-group cross sections, which meets the target distribution characteristics and the correlation. The sample space can represent the uncertainty of nuclear data and can be used to propagate nuclear data uncertainty.

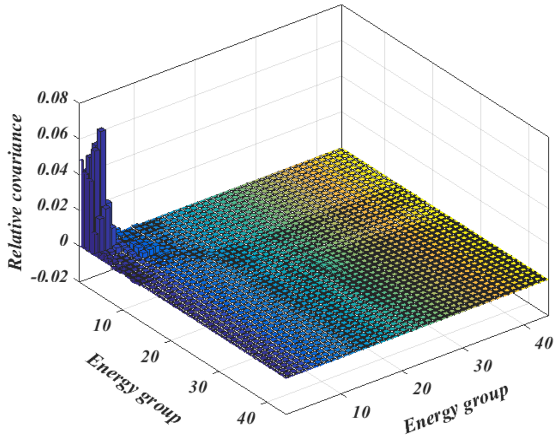

Fig. 7 The Relative Cov Matrix for the sample space obtained by LHS-SVDC.

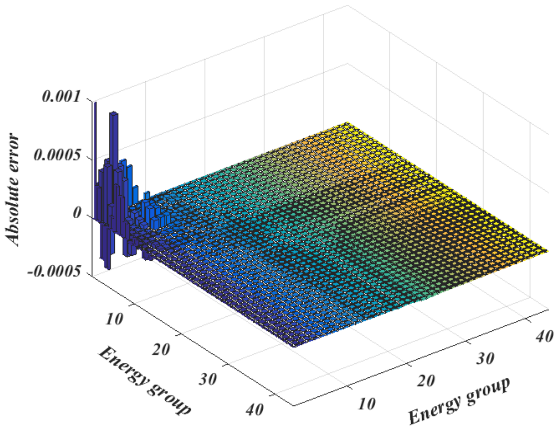

Fig. 8 The absolute deviation of the Relative Cov Matrix between the sample space obtained by LHS-SVDC and the original space for $^{238}U(n,\gamma)$.

4 Numerical analysis

Further verification of the LHS-SVDC sampling method is performed based on TMI-1 fuel cell benchmark in OECD LWR UAM project. The detailed geometry information and material information can be referred in references [8]. This benchmark problem is also conducted by using TSUNAMI-1D module of SCALE6.1 and the resonance self-shielding cross sections are generated by the BONAMI and CENTRM modules [9] based on V6-238 multi-group nuclear cross-section data base. Meanwhile, the NEWT module in SCALE6.1 code is used to perform the transport calculation to obtain k_{eff} for the same problem.

The unperturbed resonance cross sections are used as basic input information for a self-developed MOC transport solver to conduct eigenvalue calculation. The results and reference solution generated by NEWT based on the same set of nuclear cross-section data base are listed in Table 1. The difference between k_{eff} is 27 pcm compared against the reference solution, and this results indicates that the self-developed MOC transport solver can be used to propagate the uncertainty of nuclear data.

Table 1 k_{eff} for TMI-1 Grid element.

Program	Database	k_{eff}
NEWT	V6-238	1.420063
BONAMI/CENTRM +MOC	V6-238	1.419789

In this work, different sampling methods in CUSA code are used to generate the sample space of multi-group cross sections based on the resonance self-shielding cross sections and the relative covariance matrix. By considering the cross-section self-consistency rules, the sample space is chosen as a basic input of a self-developed MOC transport solver for transport calculation, and then some statistical information of k_{eff} can be obtained, which can be used to quantify the contribution to the uncertainty of k_{eff}. At the same time, the sample number is also crucial for nuclear data uncertainty analysis. The contribution to the uncertainty of k_{eff} for different nuclear data under different sample sizes are quantified respectively. The LHS-SVDC sampling method and the LHS-CDC sampling method are used to quantify the contribution to the uncertainty of k_{eff} for two different types of nuclide reactions respectively by using different sample size.

The results for $^{238}U(n,\gamma)$ and $^{235}U(n,f)$ are illustrated in Fig. 9 and Fig. 10. The contribution of nuclear data to the uncertainty in k_{eff} tends to be stable when the sample size is greater than 800. So the sample size is set to 800 in the following uncertainty analysis.

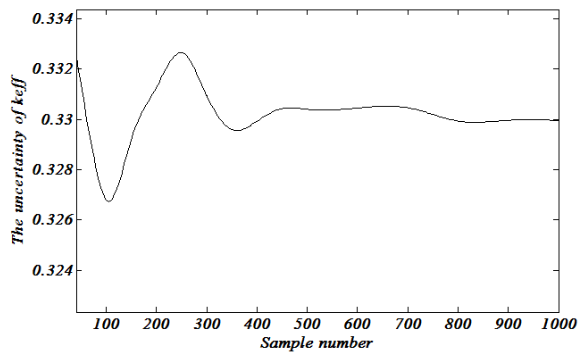

Fig. 9 Uncertainty for $^{238}U(n,\gamma)$ in Calculation of k_{eff} of Grid Element under Different Number of Samples.

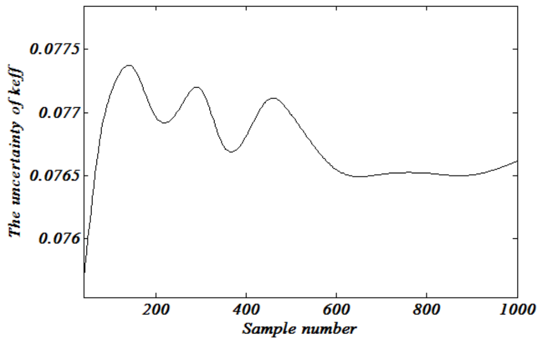

Fig. 10 Uncertainty for $^{235}U(n, f)$ in Calculation of k_{eff} of Grid Element under Different Number of Samples.

Different sampling methods in CUSA code are used to quantify the contribution to the uncertainty of keff for different nuclear cross sections for TMI-1 cell model and those results are compared with the reference solution generated from TSUNAMI-1D which uses the first-order perturbation theory. The numerical results are listed in Table 2.

Table 2 Contribution of Different Nuclear Cross Section to Uncertainty of k_{eff} of Grid Element.

Covariance Matrix		Contributions to uncertainty in k_{eff} (%)			
Nuclide Rea	Nuclide Rea	LHS	LHS-CDC	LHS-SVDC	TSUNAMI-1D
^{238}U(n,γ)	^{238}U(n,γ)	3.665549E-01	3.423566E-01	3.298703E-01	2.7147E-01
^{235}U(nubar)	^{235}U(nubar)	2.640540E-01	2.634789E-01	2.643075E-01	2.6431E-01
^{235}U(n,γ)	^{235}U(n,γ)	2.072330E-01	2.090430E-01	2.094343E-01	2.0997E-01
^{235}U(n,*f*)	^{235}U(n,γ)	5.995201E-02	7.752864E-02	8.302283E-02	1.0384E-01
^{235}U Chi	^{235}U Chi	8.975837E-02	8.858344E-02	8.784752E-02	8.7423E-02
^{235}U(n,*f*)	^{235}U(n,*f*)	7.855359E-02	7.696451E-02	7.652199E-02	7.6399E-02
^{238}U(nubar)	^{238}U(nubar)	7.204624E-02	7.182843E-02	7.158238E-02	7.1212E-02
Zr(n,γ)	Zr(n,γ)	5.413986E-02	5.406682E-02	5.379619E-02	5.0773E-02
^{1}H elastic	^{1}H elastic	2.661902E-02	2.649549E-02	2.623384E-02	2.4856E-02
^{1}H(n,γ)	^{1}H(n,γ)	1.922824E-02	1.932923E-02	1.919137E-02	1.8954E-02
^{238}U(n,2n)	^{238}U(n,2n)	9.713031E-03	9.871362E-03	9.975485E-03	1.4608E-02
^{238}U(n,*f*)	^{238}U(n,*f*)	1.567403E-02	1.521730E-02	1.518329E-02	1.5072E-02
^{238}U Chi	^{238}U Chi	5.301475E-03	5.356751E-03	5.464782E-03	6.7680E-03
total		5.272727E-01	5.153988E-01	5.092430E-01	4.8146E-01

In Table 2, the results obtained by TSUNAMI-1D are calculated using "sandwich rule". The uncertainty results of the statistical sampling method are generated by three different ways: LHS, LHS-CDC and LHS-SVDC method. The total uncertainty of keff is calculated by the root mean square formula. In the previous section, it has been proven that the difference between three sampling methods is the correlation between parameters of sample space, the comparison of the contribution to the uncertainty of keff generated by three methods for different nuclear cross sections shows that the correlation between parameters of sample space has a great effect on the contribution to uncertainty of keff and the effects are distinguishing for different nuclear data cross sections. Meanwhile, as shown in Table 2, analyzing the data of each row, it can be found that the result generated by LHS-SVDC method is closer to the reference solution compared with other two methods, which indicate that the desired sample space generated by using LHS-SVDC method can propagate the uncertainty of nuclear data more accurately, at this point, the correlation between parameters of sample space goes to 0. And the results demonstrate that the method proposed in this paper is a better method and can be used to quantify uncertainty of key parameters of nuclear reactor core propagated from nuclear data.

By comparing the data listed in the Table 2, it is easy to know that the contribution to the uncertainty of keff for calculated by statistical method is much larger than the result of TSUNAMI-1D. It is due to that the sensitivity information of keff for obtained by statistical approach is greater than the corresponding result from TSUNAMI-1D, as shown in Table 3.

Table 3 Sensitivity information of k_{eff} of the grid element for different nuclear reactions.

Nuclide Rea	Statistical Method	TSUNAMI-1D
^{235}U(nubar)	9.3896E-01	9.3925E-01
^{235}U(n,*f*)	2.5399E-01	2.5362E-01
^{238}U(n,γ)	-2.6079E-01	-2.2194E-01
^{1}H elastic	1.9162E-01	1.8633E-01
^{235}U(n,γ)	-1.5425E-01	-1.5394E-01
^{238}U(nubar)	6.1045E-02	6.0752E-02
^{1}H(n,γ)	-3.7115E-02	-3.7959E-02
^{238}U(n,*f*)	2.9181E-02	2.9017E-02

5 Conclusion

In this paper, a new efficient LHS-SVDC method is proposed in order to generate a desired sample space of multi-group cross sections for uncertainty analysis of nuclear data. This new method is derived from strict mathematical derivation and is successful. At the same time, the uncertainty input data generation module 'Guide' in CUSA code system has been updated based on the work presented in this paper.

Numerical results for the TMI-1 pin cell case are presented and compared with the reference solution generated from TSUNAMI-1D. The numerical results indicate that the LHS-SVDC method can generate a desired sample space quickly and effectively, which can be used to propagate the uncertainty of nuclear data to the key parameters and to quantify their uncertainty. Hence, the proposed LHS-SVDC method is an efficient sampling method and will support the uncertainty and sensitivity analysis in the future.

List of Acronyms

LHS:	Hypercube Sampling
LHS-CDC:	LHS combined with Cholesky Decom -position Conversion
LHS-SVDC:	LHS combined with Singular Value Decomposition Conversion
SRS:	Simple Random Sampling
SVD:	Singular Value Decomposition
CUSA:	Code for Uncertainty and Sensitivity Analysis

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