Nuclear data uncertainty for criticality-safety: Monte Carlo *vs.* linear perturbation

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Abstract

This work is presenting a comparison of results for different methods of uncertainty propagation due to nuclear data for 330 criticality-safety benchmarks. Covariance information is propagated to k_{eff} using either Monte Carlo methods (NUSS: based on existing nuclear data covariances, and TMC: based on reaction model parameters) or sensitivity calculations from MCNP6 coupled with nuclear data covariances. We are showing that all three methods are globally equivalent for criticality calculations considering the two first moments of a distribution (average and standard deviation), but the Monte Carlo methods lead to actual probability distributions, where the third moment (skewness) should not be ignored for safety assessments.

1 Introduction and history

The propagation of uncertainties in nuclear simulation is nowadays a field of active research for light water reactors. It includes neutronics fuel and core behavior, damage on reactor vessel, shielding and radio-protection, waste storage or accident simulation. One of the particularities of the nuclear field is the large difference in the scale of interactions: from sub-atomic particles (neutrons, protons) to large installations (reactors, fuel storage): effects at small scales can have an impact on larger ones. The lack of knowledge for the reactions involving these particles (their reaction probabilities are later called nuclear data) can affect our understanding of a reactor core during transients, or can make a facility unexpectedly becoming critical under specific conditions.

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Up to a decade ago, over-designed safety margins were hiding the effect of the nuclear data uncertainties, ensuring safe conditions through high cost. But the new conditions of operations and designs of nuclear facilities (best-estimate calculations, higher burn-up rates, or cost-saving methods for fuel storage) are nowadays putting lights on the degree of knowledge of these nuclear reaction quantities.

These nuclear data (essentially cross sections, emitted spectra and angular distributions) are indeed known to a certain extent, which ranges from a fraction of percent to tens of percent for the isotopes of interest. From the point of view of the nuclear data user, the assessment of the nuclear data uncertainties on specific installations and simulations becomes a must, and the information provided in the nuclear data libraries is used and trusted as the cross sections themselves. With the need of uncertainties on integral quantities, the user can choose between different methods of uncertainty propagation. In the case of k_{eff}, two possibilities exist: Monte Carlo uncertainty propagation, or perturbation/sensitivity coupled with existing covariance information. It is therefore important to make sure that these methods lead to similar uncertainties, and if not, to understand the origin of the differences.

In 2011, a first limited comparison for the propagation of nuclear data uncertainties between the Total Monte Carlo method (TMC) and the use of covariances was presented [1–3], equivalent to the first part of the present study, but for a small number of benchmarks. Alternatively, a first comparison of Monte Carlo methods, between TMC and NUSS was presented in Ref. [4]: the first one based on model parameter covariances, the second one on nuclear data covariances (such as cross sections). In the present work, we are proposing to combine and extend these comparisons, still in the domain of criticality benchmarks. The first comparison consists of calculating k_{eff} uncertainties for criticality benchmarks using existing nuclear data covariance files as given in libraries with two methods: generating random nuclear data based on existing group-averaged covariance files and repeating n times the same calculations (later called NUSS), and using the nuclear data covariances with the perturbation options of MCNP6 sensitivity vectors. For the second comparison, the nuclear data covariances are first produced by sampling reaction model parameters. By sampling these parameters, both random nuclear data and covariances are generated at the same time, containing similar information within the limits of the covariance format and its processing.

Therefore the two presented comparisons are trying to answer two distinct questions: (1) is the Monte Carlo sampling of nuclear data equivalent to the sensitivity/covariance method for k_{eff} ? (2) is enough information stored in the covariance files to assess k_{eff} uncertainties with confidence ?

2 Methodology

This comparative study will be restricted to the calculation of k_{eff} quantities (neutron multiplication factors) for criticality-safety benchmarks as defined in the ICSBEP collection [5]. The information on the comparison of uncertainties on k_{eff} can be useful under very specific conditions: using (1) similar codes, (2) same input data and (3) same measured or calculated quantities. Three different methods are presented in the following, the TMC method (covariance on nuclear physics model parameters), a sensitivity method (covariances for nuclear data such as cross sections plus sensitivity vectors), and the NUSS method (covariances for nuclear data to generate random cross sections in specific energy groups).

2.1 Nuclear data covariances

The information for the uncertainties and correlations on nuclear data can be expressed in at least two manners. The first one is the covariances on pointwise data. Pointwise data can be cross sections (capture, fission), emitted spectra (energy and angle probability distribution of emitted particles), or number of emitted particles (neutron emitted per fission). These covariance information is nowadays usually stored together with the pointwise data, in a format which can easily be processed and used by different codes. The other one is the covariance on resonance model parameters. This is often the case for the cross section information in the thermal and resonance range, from 10^{-5} to a few hundreds of keV. The use of such data is less straightforward compared to the previous case, since these covariances need to be translated into pointwise data information. This action is performed by processing codes, possibly using different formalism than the one intended during the creation of the covariances.
In practice, both types of information are found in the nuclear data libraries: parameter covariances in the resonance range, and pointwise covariances in the fast range. The prospective user needs to combine them to obtain the full uncertainties and correlations for a given isotope.
Another example of such parameter covariances is at the basis of the TENDL library. Model parameters, such as for the TALYS code, are randomly varied following given parameter covariances to produce random nuclear data. These random nuclear data are either averaged to produce a pointwise covariance file, or directly formatted into nuclear data libraries to be used in a Monte Carlo process (leading to the Total Monte Carlo method).

2.2 NJOY processing

In the three types of calculations (perturbation approach, NUSS and TMC), the same MCNP input files are used, together with the same version of MCNP6.1 [6]. Similarly, the same version of NJOY (12.21 [7]) is used to process the ENDF-6 files into the ACE format. The so-called "ENDF-6" format, as defined in Ref. [8], is the basic format used to create and share the nuclear data quantities. In the following, other formats will be used such as the ACE format and the COVERX format. Regarding the processing of the covariance files (to produce the COVERX format or other formats), the new release of NJOY (version 2012 with different updates) could not be successfully used. Instead, the NJOY99 version, update 396 was used for all isotopes.

2.3 Sensitivity approach

For the sensitivity calculations, MCNP6.1 is used together with the same geometry description files as for the two other methods. The only addition to the input files used for sensitivity calculations is the specific "KSEN" card as defined in Ref. [9]. The default options for the "KSEN" card are used (especially for the "BLOCKSIZE" option, set to 5). Sensitivity vectors are calculated for different isotopes using the 187 energy group structure as defined for the NJOY processing code [7]. The generic flowchart of the calculations is presented in Figs. 2 and 3. The number of neutron histories is relatively large, leading to statistical uncertainties for k_{eff} in the order of 20 to 80 pcm, and small uncertainties for the important sensitivities in specific energy groups. An example of calculated sensitivity vectors is presented in Fig 1.

The statistical uncertainties on the sensitivity values can be relatively large (higher than 10 %), but for energy ranges where the specific nuclear data matters, these uncertainties are less than 5 %. These steps are very similar to the work performed in Ref. [1], where instead of the "KSEN" card, the "PERT" card was used with MCNP4 (the main advantage of the "KSEN" card compared to the "PERT" is the use of the adjoint weighting).
Once the sensitivity vectors are obtained (presented as $\overrightarrow{S}$ in Fig. 2), they are used with the covariance matrices V in the simple following formula $S^{\intercal}VS$ to calculate the uncertainty on k_{eff} due to V. This last step is performed by the SUSD3D code [10]. The covariance matrix V is in the "COVERX" format, obtained after processing of the original matrix in the ENDF-6 format. This processing step is realized with NJOY99-396 and the "njoycovx" utility code [7] (integrated in the ERRORR module). The original covariance matrix in the ENDF-6 format can be from any nuclear data library. In the present work, we are using the covariance matrices distributed with the ENDF/B-

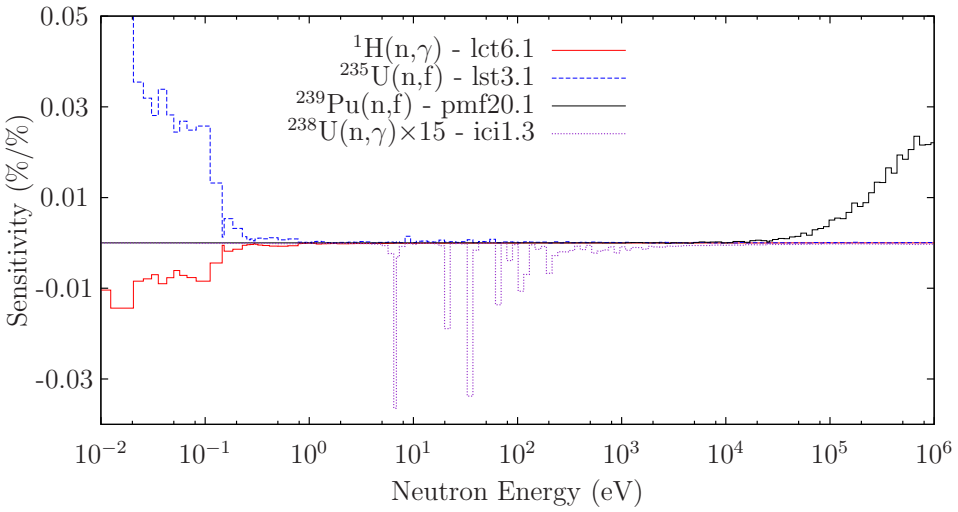

Fig. 1. Sensitivity vectors from MCNP6.1 for four different reactions for four different benchmarks. The three letters followed by numbers are referring to the benchmark case ("l" for low ^{235}U enriched, "c" for compound, "s" for solution, "t" for thermal, "m" for metallic, "f" for fast, and "i" for intermediate.

VII.1 library [11] for the comparison with NUSS and with the TENDL-2014 library [12,13] for the comparison with TMC. The choice of TENDL-2014 allows to use both the covariance files and their equivalent random ENDF and ACE files.

2.4 Total Monte Carlo

The Total Monte Carlo method (or TMC) has been presented in many publications, see for instance Refs. [14,15]. Only the main points will be highlighted here (see Fig. 2). The TMC method is based on the variations of parameters for physical models to produce random nuclear data. The physical models include resonance description (Reich Moore formalism), compound nucleus calculations (Hauser Fechbach), level density representations to cite only a few sources of parameters. All these models are included in a software package which makes use of parameter input files. This software package, called "T6" is extensively developed since 2008 to produce random nuclear data files together with the TENDL libraries [12,13]. One of the advantages of such a method, which is of interest in this work, is the ability to produce both random ENDF-6 nuclear data files with consistent covariance representation, within the limitation of the covariance format. Each random file is completely different from another one: prompt and delayed $\overline{\nu}$, resonance parameters, cross sections, angular and energy distributions, double-differential distributions, photon and isomeric production. In a simplified concept, once the random ENDF-6 files are available, it is relatively easy to apply simple statistical formula to extract averages, standard deviations and correlations and to format them into

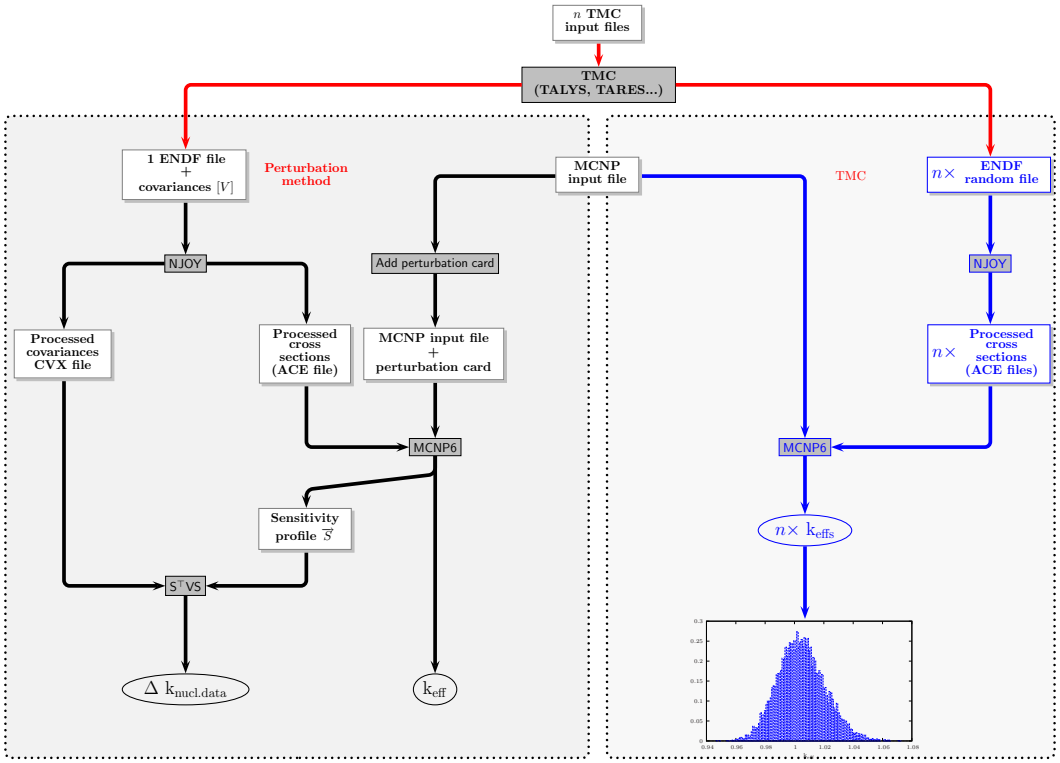

Fig. 2. Principle of the calculation flow for the TMC calculations, compared with the equivalent sensitivity calculation using MCNP6.

an ENDF-6 covariance file (understanding that the covariance ENDF-6 file contains two different quantities: a list of standard deviations and matrices of correlations). Contrary to some previous publications on TMC (see for instance Ref. [16]), the thermal scattering data are not varied in this work, as it is not yet possible to consider their effects using a covariance approach.

2.5 NUSS

The Nuclear data Uncertainty Stochastic Sampling method (or NUSS) was extensively presented in Ref. [17]. Its application in this work is presented in Fig. 3. Implemented to be compatible with MCNP(X) and SERPENT [18], the NUSS scheme applies perturbations to the pointwise nuclear data given in the specific ACE format. The sampling of nuclear data follows the sampling recipe from Ref. [19]. Groupwise perturbation factors as the ratio between the sampled and nominal groupwise nuclear data are applied to the pointwise nuclear data in ACE format. The NUSS module to modify the original ACE file divides the entire length of the nuclear data into G segments where G is the number of energy groups in the given covariance library. In the present work, the 187 energy groups are used, following the same group format as for the processed COVERX files used together with the sensitivity vectors of the perturbation method. Since the pointwise data within each energy group are

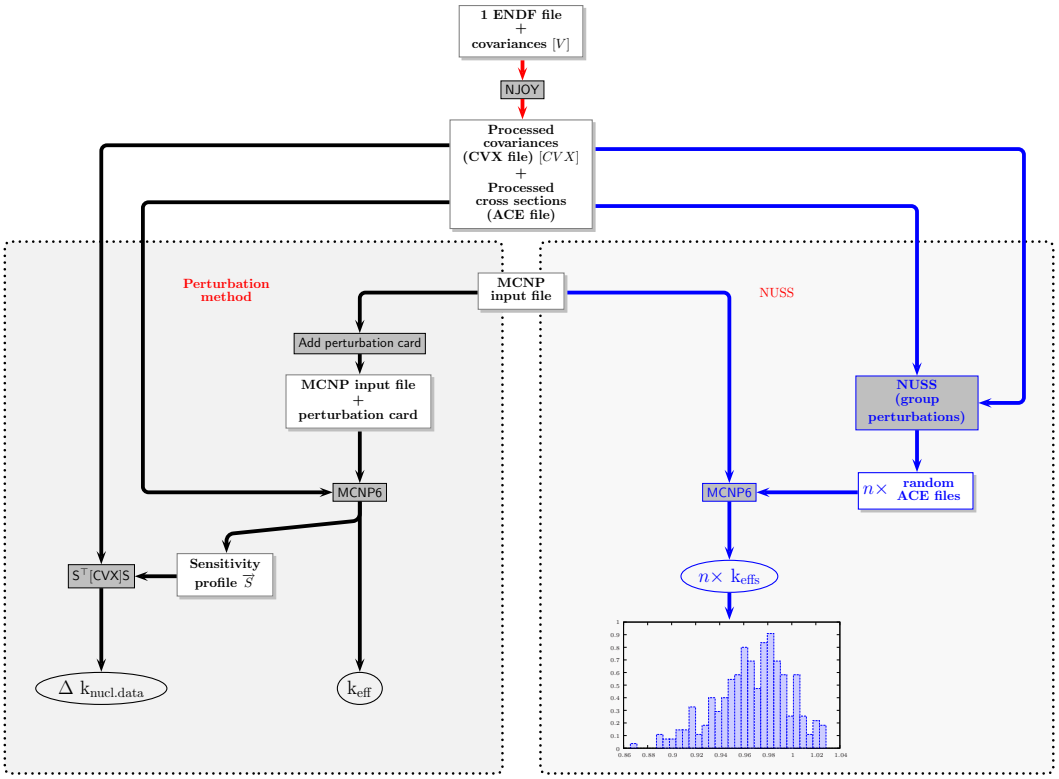

Fig. 3. Principle of the calculation flow for the NUSS calculations, compared with the equivalent sensitivity calculation using MCNP6.

assumed to be fully correlated, they are uniformly varied. Depending on the type of modified cross sections, the total cross section and the reaction cross section are adjusted accordingly to ensure consistency of the ACE file. The following nuclear data can randomly be modified at once: $\overline{\nu}$ (emitted neutron per fission), χ at different neutron incident energy (prompt fission neutron spectra), and cross sections for (n,tot), (n,el), (n,inl), (n,2n), (n,f) and (n,γ), depending on the information given in the COVERX files.

In this work, a limited set of isotopes are randomly varied at the same time, based on the availability of the covariance information given in the ENDF/B-VII.1 library. A total of 66 isotopes are varied, including ^{235}U, ^{238}U, ^{239}Pu, ^{1}H, ^{16}O (and minor actinides such as ^{240}Pu), which are the main sources of uncertainties for k_{eff} calculations. Other structural materials and coolant are also included, such as tungsten, iron, nickel, lead. Depending on the type of considered benchmarks, their impact can be of importance. The same list of 66 isotopes are also considered for the sensitivity calculation using MCNP "KSEN" option, allowing a consistent comparison of uncertainties.

3 Results

3.1 Preliminary remarks

In the following, the uncertainties obtained from these three different methods will be compared, especially between NUSS and the sensitivity method, and between TMC and the sensitivity method. As explained above, the production of these uncertainties, if based on the same sources of information (nuclear data covariances and geometry description) can still differ for a few reasons.

- In the previous comparisons for NUSS and TMC (see Ref. [4]) and for TMC and the perturbation option of MCNP (see Refs. [1–3]), the differences between the uncertainties were within 20 %. The exception was for the comparison of the uncertainties due to $\overline{\nu}$ for ^{239}Pu where a large difference was found. This difference was later resolved by increasing the number of energy groups, leading to similar uncertainties (see Ref. [17]. page 51). These comparisons involved a limited number of benchmarks and not all possible nuclear data reactions were considered.
- Using the random ACE or ENDF-6 files coming from the TMC method, a larger type of nuclear data are varied compared to the information included in the covariance files (such as angular distributions and double-differential spectra). It was shown in Refs. [1,2] that in the case of the criticality benchmarks, the quantities are at best of secondary importance.
- The sensitivity coefficients obtained from MCNP6 are based on linear perturbation theory. Generally speaking, it is believed that the nuclear data uncertainties for core physics applications are in the range for which linear sensitivity theory is accurate enough (not like in the case of shielding calculations). In specific cases nevertheless, calculated uncertainties on k_{eff} can be relatively large (higher than 2000 pcm) and involved nuclear data uncertainties are in the order of tens of percent (*e.g.* for the ^{238}U(n,inl) cross section) which implies a careful interpretation of the validity of the linear-perturbation theory.
- In the use of the covariance matrices for the multiplication with the sensitivity vectors, there is a choice of using either the partial description of the cross sections (elastic, capture, fission, *etc*), or the description of the total cross section. These two options should lead to the same uncertainty, but in practice it depends on the consistency of the cross section covariances which is not always respected. Similar effects can be observed for the covariance file of the $\overline{\nu}$: results will differ strongly depending on the choice of covariance files (covariance information for prompt or total emitted neutron per fission) for ^{235}U in the ENDF/B-VII.1 library. In this work the covariance of the prompt $\overline{\nu}$ (MT-456 in ENDF-6 format) is chosen, since the total covariance (MT-452) leads to unrealistic high uncertainties.

- In the current implementation of the COVERX format, the covariance information for the prompt fission neutron spectrum (pfns) is independent of the neutron incident energy. In practice, only one covariance matrix can be given for the pfns in the COVERX format and the user needs to make an arbitrary choice about which incident neutron energy to consider. Depending on the isotope and on the benchmark, the impact of the pfns covariance matrix can be important. In the comparison between NUSS and the perturbation method, this limitation will not appear as both methods start from the same COVERX file. In the case of the TMC method, the pfns at many incident neutron energies are randomly varied. This can potentially lead to differences in the calculated uncertainties.

3.2 Statistical characteristics of the Monte Carlo methods

In the process of propagating uncertainties by repeating many times the same calculation, care should be given to the convergence of the quantities of interest. These quantities are the different moments of the calculated distribution, such as the average, the standard deviation, but also the skewness or correlation between calculated k_{eff} for different benchmarks. It is difficult to know in advance the number of required iterations, but common practices generally involve more than 300 calculations. Using a Monte Carlo transport code such as MCNP also adds the statistical uncertainty to the effect of nuclear data, and depending on its relative amplitude to the effect of nuclear data, 300 calculations might not be enough (see for instance Ref. [15]). Examples are given in Fig. 4 for two benchmarks, not converging at the same "speed" (the hmf benchmark requires more sampling than the specific hct benchmark).

The average, standard deviation and skewness are calculated using classical statistical formula (for the standard deviation due to nuclear data only, see Ref. [15]). Additionally, these quantities together with the kurtosis and the Kolmogorov Smirnov test are calculated with the GNU PSPP software package [20], for checking purposes and for testing the hypothesis of a Normal distribution. It can be seen in Fig. 4 that starting at 300 iterations, the convergences of the average values and standard deviation are within 100 pcm. In the case of the skewness, 300 iterations corresponds to an uncertainty of 0.14 and for 900, 0.08. In the present work, the main limitation comes from the available computer power. Each benchmark is calculated n times with the NUSS method, m with the TMC method and one time to obtain the sensitivity vectors. Due to the number of available random files, $n \simeq 300$ (varying 66 isotopes at the same time), and $m \simeq 900 - 10^4$ (varying ^{235}U, ^{238}U and ^{239}Pu). In the linear perturbation method, similar question arises for the number of neutron histories, which is solved by taking a relatively large value leading to small statistical uncertainty on k_{eff}.

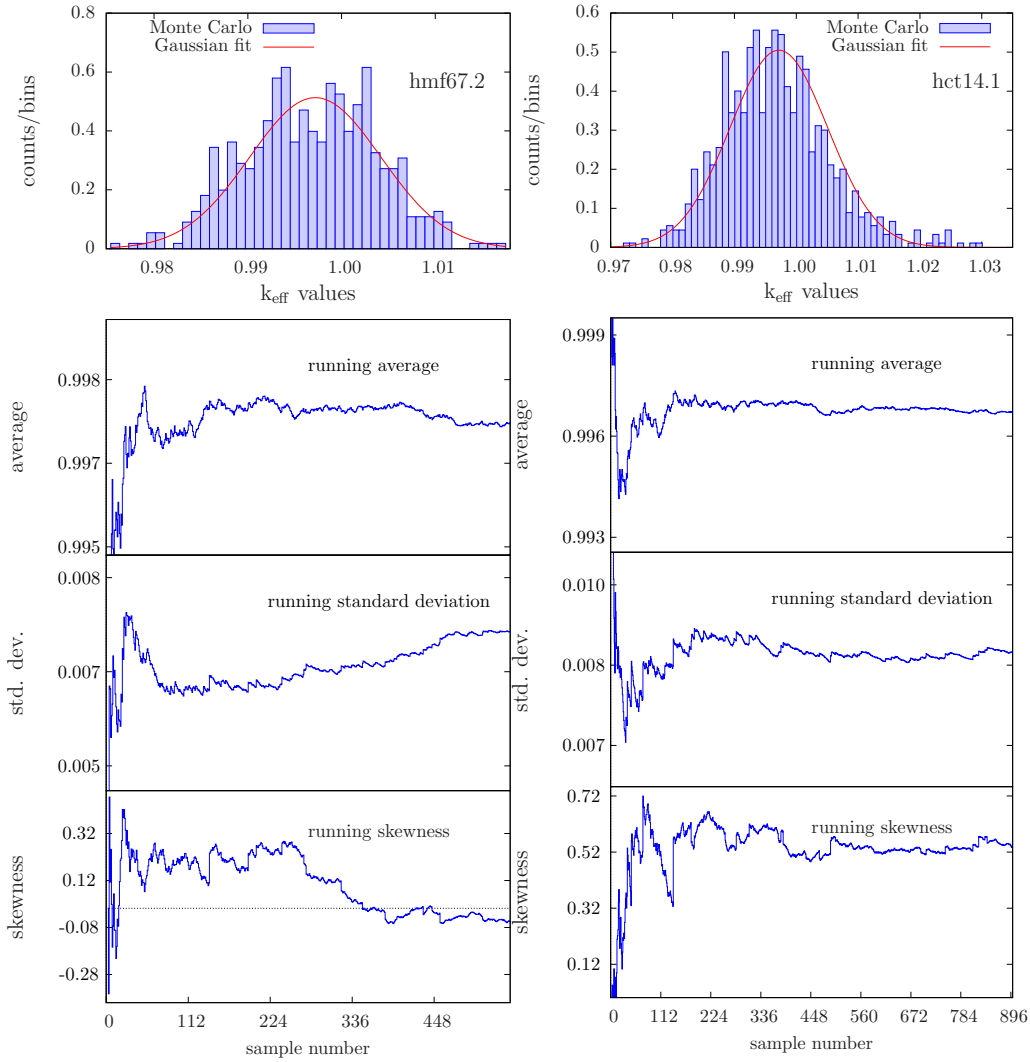

Fig. 4. Probability distributions and convergence of the three first moments for the two benchmarks hmf67 case 2 and hct14 case 1. In both cases uncertainties are obtained varying ^{235}U with the TMC method.

3.3 Comparison of cross section distributions

The comparison of k_{eff} uncertainties heavily relies in the case of NUSS on the agreement between random ACE files and covariance information used by the perturbation method. In the case of the TMC method, the comparison with the perturbation method can be done under the limitations that the COVERX files contain less information than the random ENDF-6 files produced by the TMC method. Fig. 5 presents the comparison of cross sections and uncertainties in the case of NUSS and ENDF/B-VII.1, and in the case of TMC and TENDL-2014. As seen, these comparisons present some good agreements, with some slight constant deviations in the case of TENDL-2014 (less than 2 % relative difference for nu-bar). Additionally, the random ACE files used in the TMC method contains random data which have no equivalent in the

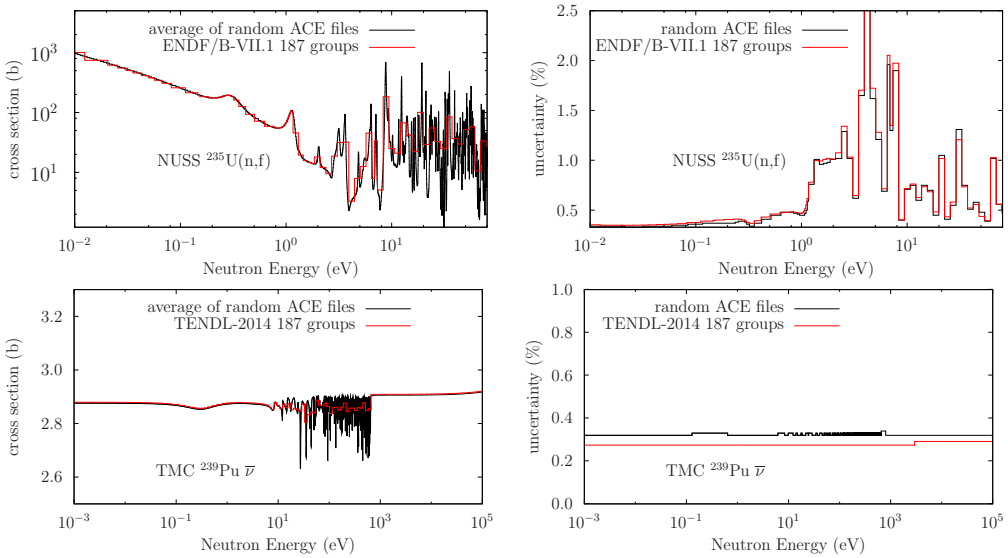

Fig. 5. Top: comparison of cross sections and uncertainties between the random ACE files (used by NUSS) and the ENDF/B-VII.1 covariance information (used by the perturbation method). Below is the same comparison for the TMC method using TENDL-2014 covariances and random ACE files.

covariance files. Such data concerns the angular distributions for elastic and inelastic scattering (see Fig. 6) and are considered to have a small impact on the studied criticality benchmarks. Similarly, the effects of asymmetric distributions produced by the TMC method for cross sections, as well as energy and angular distributions are not reproduced in the covariance files (see examples in Ref. [3]).

3.4 Comparison of k_{eff} uncertainties

In this section, the comparison of k_{eff} uncertainties is presented for about 330 benchmarks. As three methods are used, three different uncertainties are obtained. The comparisons are nevertheless meaningful when comparing the results using same covariance files: (1) NUSS with the MCNP sensitivity method and (2) TMC with the MCNP sensitivity method. Therefore we will present in the following ratios of uncertainties: NUSS/sensitivity and TMC/sensitivity. Concerning the number and types of benchmarks used in this work, different benchmarks were selected: thermal (names ending with a "*t*"), intermediate (names ending with a "*i*"), fast (names ending with a "*f*") or mixed (names ending with a "*m*"). For the full descriptions of the benchmarks, please refer to Ref. [5]. In the case of the TMC method, random ENDF and ACE files are available for ^{235,238}U and ^{239}Pu from the TENDL project [13], whereas in the case of NUSS, random ACE files can be generated for a large number of isotopes (including the main actinides and ^{233}U). Therefore in our comparison, the following isotopes are varied:

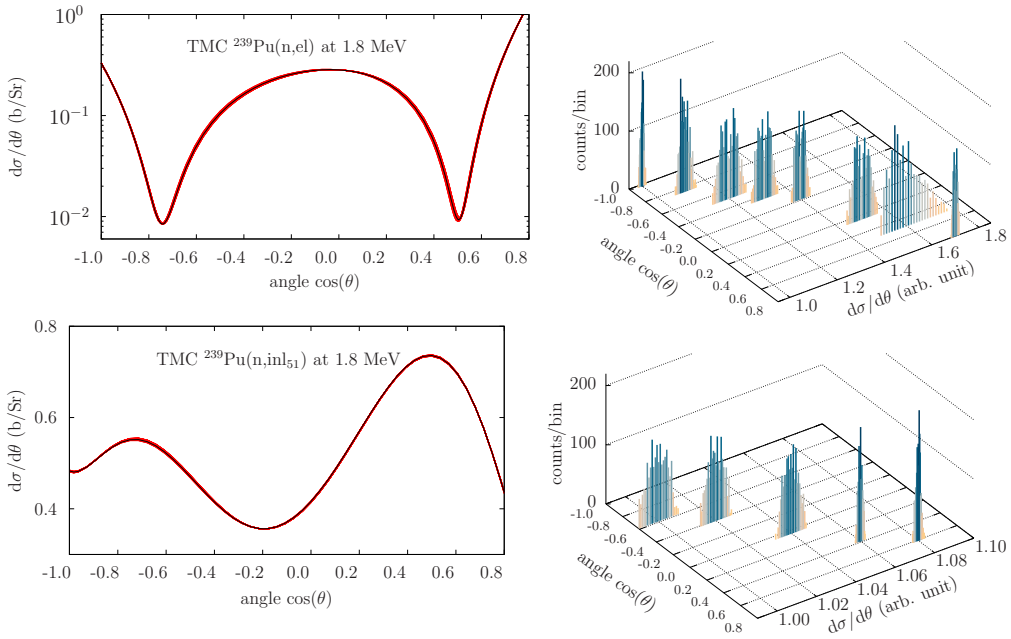

Fig. 6. Example of random angular distributions for the elastic and inelastic cross sections of ^{239}Pu. Left: cases at 1.8 MeV as a function of the scattering angle. Right: histograms if the distributions (at 1.8 MeV). Note that some distributions at specific angles are skewed.

- TMC: 900 to 10^4 random ACE files for ^{235,238}U and ^{239}Pu,
- NUSS: 300 random ACE files for ^{1}H, ^{4}He, ^{6,7}Li, ^{9}Be, ^{10,11}B, ^{12}C, ^{15}N, ^{16}O, ^{19}F, ^{23}Na, $^{24-26}$Mg, ^{27}Al, $^{28-30}$Si,^{41}K, $^{46-50}$Ti, $^{50,52-54}$Cr, ^{54,56,57}Fe, ^{59}Co, ^{58,60}Ni, $^{90-92,94,96}$Zr, $^{92,94-98}$Mo, $^{152,154-158,160}$Gd, $^{204,206-208}$Pb, $^{233-235,238}$U, $^{238-240,242}$Pu, ^{241}Am

3.4.1 Global comparison

Table 1 presents a list of benchmarks for each comparison. For a statistical study of the results, the largest number of benchmarks concerns the pmf and pst types for plutonium benchmarks and the lct and lst types for the uranium benchmarks. The choice of these benchmarks is limited by the availability of the MCNP inputs and of the computer power. Therefore a selection of about 330 benchmarks is presented in this work, still being larger than the limited set presented in the previous works (5 benchmarks in Ref. [1], 33 in Ref. [2]; a larger set was presented in Ref. [3], but the nuclear data were varied in a limited energy range).

From the list of benchmarks presented in Table 1, Fig. 7 presents the ratio of uncertainties for NUSS and TMC over the results from the sensitivity calculations. As the sensitivity method was used with both set of covariance files from ENDF/B-VII.1 (as for NUSS) and TENDL-2014 (produced from the TMC method), these ratios should ideally be 1 if the sensitivity method and

Table 1
Details of the number of considered benchmarks in this work. "*n*" denotes the number of benchmarks and "*ratio*" is the global ratio of either NUSS/sensitivity, of TMC/sensitivity (if the ratio is 1, same uncertainties are obtained between NUSS or TMC and the sensitivity method).

benchmark		ici	imf	ist	pst	pmi	pmf	pcm	pmm	pci	mmf
series		1	1,2,7	2	1-7,9,11	2	1-3,5,6,8-10	1,2	1	1	1,2
					12,14-17		13,15,19,20				11
					22,24,25,34		35,36,44,45				
NUSS	n	3	5	5	55	1	23	3	1	1	5
	ratio	0.97	0.96	1.05	0.99	1.25	1.13	0.80	1.17	0.72	0.98
TMC	n	3	5	5	53	1	35	3	-	-	5
	ratio	0.98	0.72	1.08	1.00	0.85	1.01	0.96	-	-	1.01

benchmark		mcf	mst	lst	lmt	lct	hst	hmt	hct	hmf	hcm
series		3	1,2,6	1,3-7	1,15	1-9	1-4	3,10	13,14	1,5,7,41	2,3
				16-18,20			19,29	22		56,67,69	
				22						72,78-80	
NUSS	n	2	6	45	2	120	18	4	3	15	2
	ratio	1.10	1.00	1.01	0.80	0.99	1.01	0.84	1.28	0.94	0.92
TMC	n	2	6	43	2	124	18	4	3	15	2
	ratio	1.08	1.04	1.13	1.13	1.10	1.06	1.08	1.05	0.88	0.81

benchmark		hci	hmm	uct	umf	ust
series		4,5	5	1	1	1
NUSS	n	2	1	2	1	1
	ratio	1.13	1.03	0.99	1.00	0.95
TMC	n	2	1	-	-	-
	ratio	0.83	0.78	-	-	-

the Monte Carlo methods were equivalent. As shown in this figure, the average values of all the ratios for NUSS and sensitivity method is 1.00, whereas for TMC and the sensitivity method it is 1.05, thus indicating stronger differences between the sensitivity method and TMC, than between the sensitivity method and NUSS.

The agreement between NUSS and the sensitivity method can be considered good, but not perfect as the standard deviation of the ratios is 0.10. Fig. 8 is presenting the probability distribution for these ratios. It is rather peaked around 1, with some extreme results for the hci5-1 benchmark (ratio of 1.3), for pcm2-2 benchmark (ratio of 0.60), or for the pmf44 series. Alternatively, the results are very good for pst, lst, lct and hst benchmarks. As shown in Fig. 8, the TMC method provides larger uncertainties than the sensitivity method (reflected with the ratio of 1.05), and also the standard deviation is larger in this case, being of 0.13 (compared to 0.10 for NUSS/Sensitivity). This shows a larger dispersion, also the extreme values (hci5-1 with 0.65 and lst5-2 with 1.41) are similar as in the NUSS/Sensitivity case.

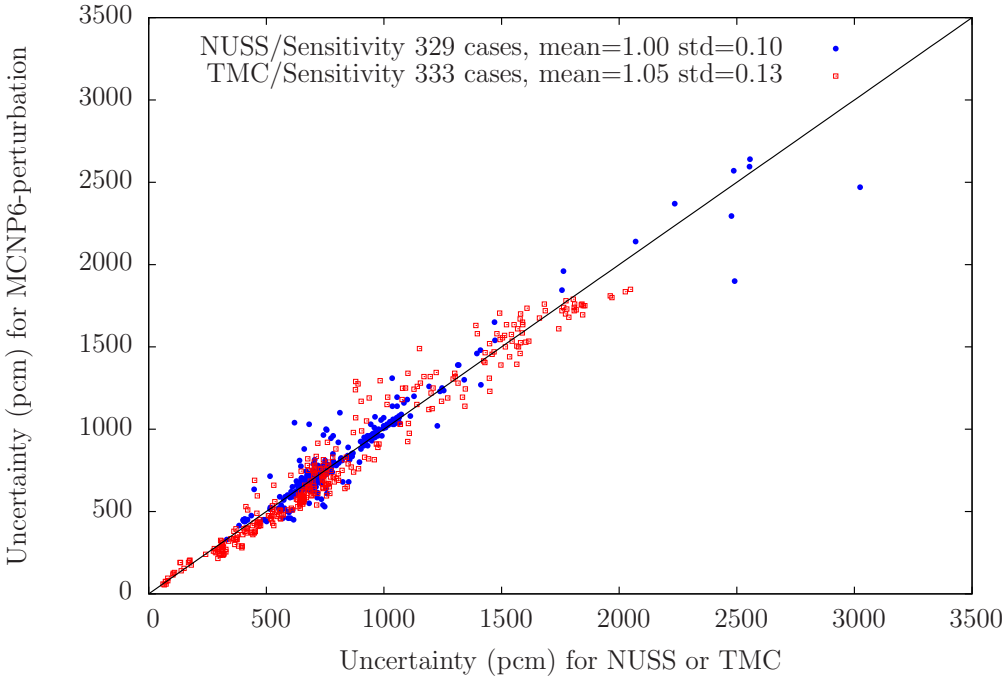

Fig. 7. Comparison of the uncertainties from both Monte Carlo methods compared to the MCNP6 sensitivity method. If the NUSS and sensitivity methods perfectly agree, all full circles would be on the diagonal. Same remark for the TMC and sensitivity methods.

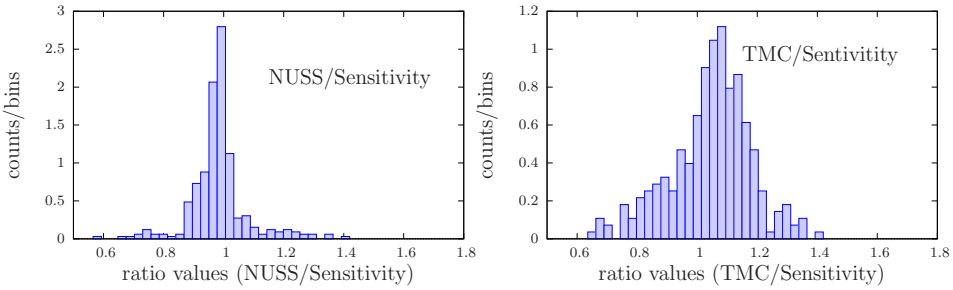

Fig. 8. Histograms of the ratios for NUSS/Sensitivity (left) and TMC/Sensitivity (right) considering about 330 benchmarks in each comparison.

As in the previous studies [1–4], differences can be noticed. As mentioned, the differences in the previous references were within 20 %, whereas this work presents averages for the NUSS/Sensitivity and TMC/Sensitivity of 1.00 ± 0.10 and 1.05 ± 0.13, as presented in Fig. 8. The apparent better agreement obtained in this work can be due to the new sensitivity method used in MCNP6 (linear-perturbation theory using adjoint weighting) compared to MCNP4, which used an approximate method, but also to a larger number of cases studied.

Based on the results presented in Table 1, the ratios can be analyzed as a function of the types of benchmarks. Since differences are obtained between the methods, the reasons can find their origins in (1) the nuclear data and their processing, (2) in the type of benchmarks with particular geometry, reflector, spectrum, or (3) in both the nuclear data and the benchmarks. We will show in this section that there are no clear indications that the characteristics of the benchmarks are a driving reason for the differences in calculated uncertainties.
One of the first distinctions between the benchmarks is related to their neutron spectrum: fast, thermal or intermediate (see Ref. [5] for the exact definition). In the case of NUSS, low and high ratios are obtained for the pmi, hci and pci benchmarks. Unfortunately, only 4 of these benchmarks were used, making the statistical relevance questionable. High ratios are also obtained for the pmf benchmarks (using 23 benchmarks). But relatively good results were observed for the mmf and hmf benchmarks (20 benchmarks). Concerning the thermal benchmarks, good agreements were found for the lst and lct benchmarks (160 benchmarks), and poor agreements were found with the hct, lmt and hmt benchmarks (10 cases). In the case of TMC, poor agreements were found for the lst (43 cases), and the hmf (15 cases). From the present results, there is therefore no clear link between poor ratios of uncertainties (different than 1) and the spectrum of the benchmarks, neither for NUSS nor TMC.
Another distinction between the benchmarks is for the type of fuel: solution, compound or metallic. In the case of NUSS, many metallic benchmarks lead to poor ratios (pmi, pmm, lmt, hmt, and especially pmf) with 30 cases. But the mmf, hmf, hmm and umf cases (for a total of 22 cases) show acceptable ratios. For TMC, the hmt, imf, hmm and hmf benchmarks (23 cases) result in poor ratios, but the pmf, mmf and hmt (44 cases) show good ratios. As in the previous case, there is no clear indication that the type of fuel (solution, compound or metallic) is creating a difference in the results.
Another important difference between the benchmarks lies in the type of fissile materials (^{235}U, ^{238}U or ^{239}Pu). In the case of NUSS, the 23 pmf benchmarks lead to poor ratios, but the 55 pst benchmarks have ratios close to 1. The high or low enriched uranium benchmarks show in general good ratios. In the case of TMC, the hmf benchmarks lead to poor ratios, and the hst benchmarks to good ones. Again, there is no clear indication that the type of fissile material has an impact on the observed ratios.
Other characteristics could be studied such as the type of reflector, or other particularities of some benchmarks. But based on the simple and global assessment, there is no clear indication that the type of benchmarks influences the agreement between the different methods of uncertainty propagation. Following the preliminary remarks given in section 3.1, the differences in the nuclear data, their covariances and their processing have a higher impact on the k_{eff} uncertainty calculation than other factors.

3.4.3 Skewed distributions

Beyond the two first moments of the probability distributions of the random k_{eff}, one can study the third moment, being the skewness. This quantity is not available in the sensitivity approach since it assumes linearity between a k_{eff} change and an input parameter change (such as a cross section). But following a Monte Carlo analysis of the uncertainties for a given calculated quantity, the skewness represents an important factor. In the traditional approach of giving a value with a standard deviation, the implicit assumption is of a symmetric distribution (skewness equals zero), and if one adds the assumption of a Gaussian distribution, about 68 % of the distribution is covered by one standard deviation, and 95 % of the distribution is covered by two standard deviations. In the case of a skewed distribution, these assumptions are not valid anymore, since one side of distribution contains more events than the other. This can have consequences for the calculations of probability of undesired events, such as (in the case of criticality studies) high k_{eff} values.
In the case of the NUSS method, the nuclear data are sampled following a Gaussian distribution, therefore the skewness of the random cross sections is zero. In the TMC approach, the model parameters are sampled, in the present application also following a Gaussian distribution, but the generated random nuclear data (such as cross section) can follow skewed distributions (as presented in Fig. 6). Both Monte Carlo methods can nevertheless lead to non-symmetric (skewed) distributions. To illustrate the skewness distributions, the skewness of the probability distributions for the 330 benchmarks are presented in Fig. 9 for both NUSS and TMC.

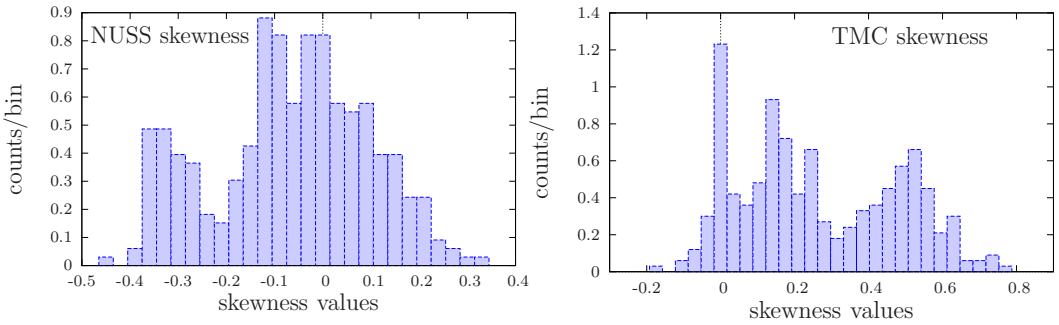

Fig. 9. Left: Distribution of the skewness of the benchmarks from NUSS. Right: same for the TMC method.

As observed in this figure, the skewness for the 330 benchmarks can be different than zero. One needs to keep in mind that for NUSS 300 samples are considered, and for TMC 900, leading to a statistical uncertainty on the skewness of 0.14 and 0.08, respectively.
The first remark is that NUSS and TMC lead to different skewness distributions: one mostly with negative values (NUSS), the other ones with positive values (TMC). From a criticality-safety point-of-view, a positive skewness for a k_{eff} distribution increases the chances of high k_{eff} occurrence, which is not reflected in the value of the standard deviation alone. This should lead to

higher safety constrains, compared to a distribution with similar average k_{eff} and standard deviation and smaller (or negative) skewness.
Also noticeable on Fig. 9, the NUSS distribution contains two peaks, one around skewness of -0.3 and the other one at -0.05. These two peaks come from different benchmarks, but the first one contains pst benchmarks (at about 75 %), meaning that the k_{eff} distributions for the pst benchmarks using NUSS are slightly skewed towards low k_{eff} values. The second peak contains lct, pmf and lst benchmarks. The same structure can be seen for TMC, with one peak around 0.2 and the other one around 0.5. In this case, the lower peak also contains mostly pst and pmf benchmarks at 50 % (pmf benchmarks have a skewness very close to zero) and the higher peak contains lst, lct and hst benchmarks. For both TMC and NUSS, the pst benchmarks have the tendency to induce smaller skewness than other benchmarks such as the lst or lct benchmarks. If the origin of such behaviors lies within the nuclear data, additional calculations can be realized, varying only one type of cross sections at a time. This may indicate the source of the skewness for the k_{eff} distributions. A dedicated study is nevertheless required to better understand these differences and origins and is outside the scope of this paper.

3.5 Specific focus on NUSS and the lct benchmarks

The low enriched uranium (leu) compound (comp) thermal (therm) benchmarks (or lct) are of prime interest for light water reactor (LWR) spent fuel storage and for transport casks. Additionally, they are well-known and accepted benchmarks, still complex systems requiring detailed neutron transport solutions and uncertainty analysis, for instance due to nuclear data. At PSI, a subset of the lct benchmarks is selected based on their similarity to designs found in todays Swiss LWR compact dry storage pools and transport casks. They are then used for criticality safety assessment within a validated computer code system. Due to their importance for the PSI criticality safety assessment methodology, a dedicated study with the ENDF/B-VII.1 nuclear data (from NUSS) is extracted from the previous global results.
A total of 120 lct benchmarks (not necessary the same as in the subset for the PSI criticality safety assessment methodology) were studied and the ratio of the calculated nuclear data uncertainties from NUSS over the MCNP6 sensitivity method is 0.99 ± 0.08 (1σ).

Fig. 10 presents the ratios of uncertainties between NUSS and the sensitivity method from MCNP6 and the skewness distributions for these lct benchmarks. The x-scales are intentionally kept the same as in Figs. 8 and 9. As mentioned, the distribution average is 0.99 and the spread in the ratio of uncertainties is rather limited, showing the global good agreement between both methods. About 86 % of the ratios are included in the 1σ band interval (93 % in the

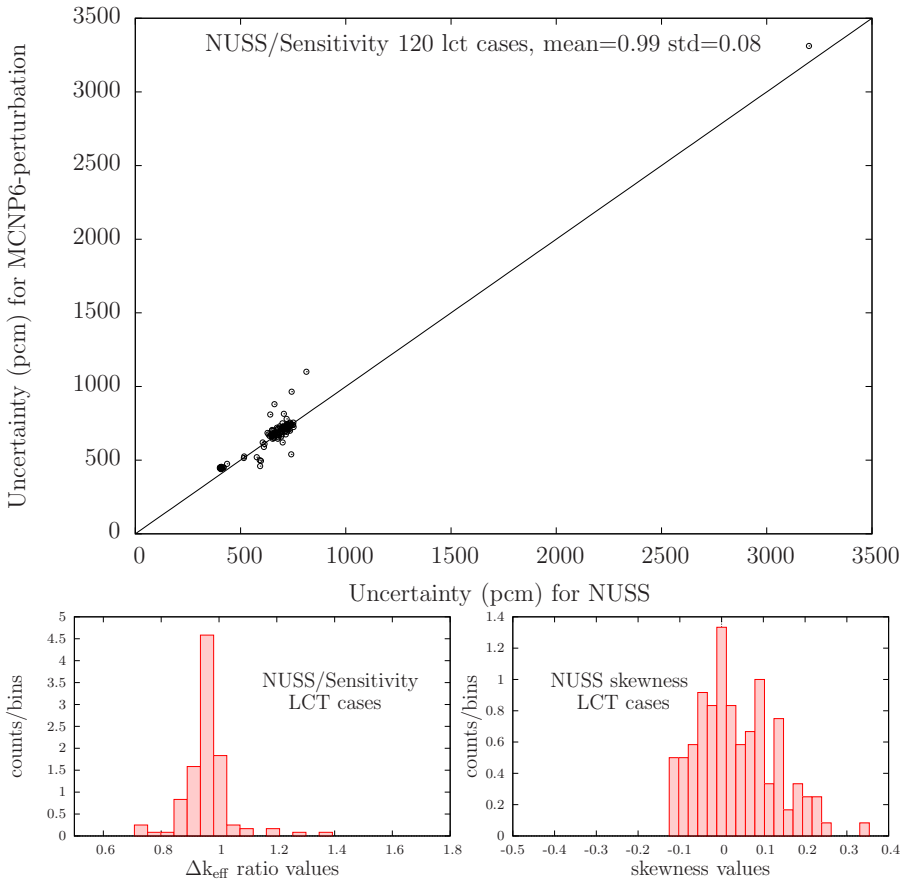

Fig. 10. Top: Same as Fig. 7, but for the selected lct benchmarks. Bottom left: ratios of uncertainties for NUSS over the sensitivity method for the 120 lct benchmarks. Bottom right: skewness distribution from NUSS sampling for the same benchmarks.

2σ band interval). Regarding the skewness distribution, the majority of the lct benchmarks presents a weak skewness, indicating a rather symmetric distribution of random k_{eff}, minimizing the risk of occurrence of unexpected high k_{eff} values, for instance compared to the pst cases (as indicated in Fig. 9 left). Additionally, the ratio distribution is rather peaked (high kurtosis), showing that many ratios are very close to the average (0.99).

As a conclusion, the nuclear data uncertainties for k_{eff} in the case of the selected lct benchmarks show a rather good agreement between NUSS and the MCNP6 sensitivity method. The dispersion of results gives confidence that the NUSS method is adequate to correctly estimate the k_{eff} uncertainties for a given set of nuclear data covariances.

Alternatively, it can be noticed that the TMC method, using a different set of nuclear data covariances, suggests higher skewnesses (0.34 on average). This does not undermine the capability of the NUSS method, but indicates that the choice of nuclear data covariances can sensibly modify the shape of the k_{eff} probability distributions.

As presented in the introduction, this work tried to answer two questions: (1) is the Monte Carlo sampling equivalent to the sensitivity/covariance method regarding the uncertainty propagation for k_{eff} ? and (2) is the information stored in the covariance files (following the ENDF-6 format) enough to correctly assess the k_{eff} uncertainties ?
To the first question, the present work seems to globally confirm the agreement of results. In some cases, differences can appear. One needs nevertheless to keep in mind that for the largest differences found (for the pcm2-2 benchmark), one method leads to 600 pcm, the other one to 1000 pcm. These 400 pcm difference is still very small compared to the calculated k_{eff} and the benchmark value (1.03095 and 0.9990 $\pm$ 0.00460, respectively). Similar remark can be done for the other extreme case, the hci5-1 benchmark (600 pcm difference), where the benchmark value is 1.0320 $\pm$ 0.00400, and the calculated value is 1.00807 (with the JENDL-4.0 library, one finds 0.98477 [21]). In perspective to the possible differences between the nuclear data libraries (ENDF/B-VII.1, JENDL-4.0, TENDL-2014) and between the calculated and benchmark k_{eff} values, the apparent discrepancies of uncertainties is small.
To the second question, the present comparison between TMC and the sensitivity/covariance methods is showing a larger spread of results, compared to the previous comparison. These differences of results indicate indeed that the TMC method, by varying more nuclear data, leads to higher uncertainties. The differences are nevertheless not drastically important and seem small compared to the differences induced by simply changing libraries.
One of the advantages of the Monte Carlo methods, if one is ready to pay the additional computational time, is the access to the probability distribution of the calculated quantity, which cannot only be represented by an average and a standard deviation, as in the case of the sensitivity/covariance method(s).

4 Conclusion

In this work, the comparison between different methods for the nuclear data uncertainty propagation on k_{eff} is presented for a large selection of criticality-safety benchmarks. Two Monte Carlo methods are compared with the sensitivity method as developed in MCNP6. One of these Monte Carlo methods (NUSS) is based on nuclear data covariances (cross sections, particle emissions) and the other method (TMC) is based on model parameter covariances. It was shown that for the k_{eff} uncertainties, the average of NUSS results over the sensitivity results for 330 benchmarks is 1.00 with a standard deviation of 0.10. In the case of TMC results over the sensitivity results, a value of 1.05 was obtained for the average and 0.13 for the standard deviation. First studies

show that the origin of these discrepancies are linked to the nuclear data and their processing. Finally, the Monte Carlo methods give access to the full probability distributions, including the third moment or skewness. This moment, when not equal to zero needs to be taken into account for a more complete uncertainty assessment.

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