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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. 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 (Rochman et al., 2011; Rochman, 2011, 2009), 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 reference Zhu et al. (2014): 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

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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 (International Handbook of evaluated criticality-safety benchmark experiments, 2010). 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 (MCNP6 Users manual-Code version 6.1.1beta, 2014). Similarly, the same version of NJOY (12.21 MacFarlane and Kahler, 2010) is used to process the ENDF-6 files into the ACE format. The so-called "ENDF-6" format, as defined in reference Trkov et al. (2012), 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 reference Kiedrowski (2013). 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 (MacFarlane and Kahler, 2010). 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 20–80 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 reference Rochman et al. (2011), 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 $\vec{S}$ in Fig. 2), they are used with the covariance matrices V in the simple following formula $S^T V S$ to calculate the uncertainty on k_{eff} due to V. This last step is performed by the SUSD3D code (SUSD3D, 2008). 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

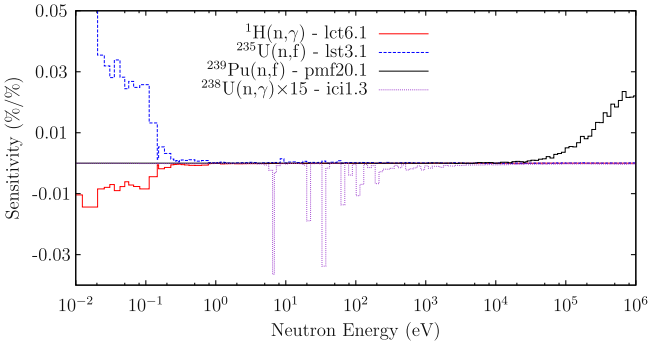

Fig. 1. Sensitivity vectors from MCNP6.1 for four different reactions for four different benchmarks. The three letters followed by numbers are referring to the benchmark case ("l" for low ^{235}U enriched, "c" for compound, "s" for solution, "t" for thermal, "m" for metallic, "f" for fast, and "i" for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