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Cross-sections Generation using TXT2NTAB code for Uncertainty Propagation with Burnup Dependence

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One of the challenges of study the neutronics of reactor is to generate reliable parameterized libraries, which contains information to simulate the core in all possible operational and transient conditions. These libraries must include tables of cross-sections and other neutronics and kinetics parameters and are obtained by simulating all the assemblies in a transport code. At lattice level, one can use branch calculations to change "instantaneously" the feedback parameters as a function of burnup. When using random sampling for the lattice calculations, one can obtain statistical information of the output parameters and use it in a core simulation to characterize the accuracy of the data estimating uncertainties when simulating a heterogeneous system at different scales of detail.

This work presents the methodology to generate NEMTAB libraries from data obtained in SCALE code system to be used in PARCS simulations. The code TXT2NTAB is used to reorder the cross-sections tables in NEMTAB format and generate another NEMTAB of standard deviation. With these libraries, the authors perform a steady state calculation for an LWR to propagate several uncertainties at the core level. The methodology allows to obtain statistical information of the most important output parameters: multiplication factor (k_{eff}), axial power peak (P_z) and axial peak node (N_z).

I. Introduction

To establish the accuracy of codes that simulate a heterogeneous system with a different level of details is one of the most important issues in modeling and can be applied to any area of engineering. The new tendency is to perform Best Estimate Plus Uncertainty (BEPU) calculations to evaluate the confidence of results.

This is the approach to be followed for many nuclear reactor fields, like research, industry, regulation and safety.[1] In fact, many international benchmarks have been launched in the past decade to develop and assess the uncertainty quantification (UQ) in an integrated framework. This has allowed the development of BEPU approach to be applied to multi-physics simulations, for standalone or coupled codes, during normal and transient conditions.[2]

In this work, the authors have developed a methodology to propagate uncertainties of nuclear data, along a Best Estimate hierarchical steady-state model of LWR core.

The first step is to simulate all the assemblies and reflectors of the core configuration at the lattice level. To do so, the authors have chosen a deterministic code to solve the transport equation and generate cross-sections tables with burnup dependence. In these simulations, branch calculations allow changing conditions of feedback parameters that represent fuel temperature, moderator density, moderator temperature, control rod presence, and changes in soluble boron.

A stochastic approach can be used for the uncertainty propagation. According to this approach, one can determine the uncertainty in the output parameters by sampling the value for each input parameter, considering its Probability Density Function (PDF) and the covariance data of the input parameters.[3] For the second step, the authors apply the Simple Random Sampling (SRS) technique at the lattice level, thus perturbing the nuclear data library to propagate the uncertainties from the problem-independent nuclear data up to the problem-dependent cross-sections library (homogenized and collapsed).

Afterward, the obtained macroscopic cross-sections are converted in a parameterized format to use these multidimensional tables in the core simulator. To accomplish this third step, the authors have developed the TXT2NTAB code.[4] TXT2NTAB stores the average values of cross-sections data corresponding to the unrodded configuration in a *nemtab* file, while cross-sections average values corresponding to the rodded configuration are kept within a *nemtabr* file.

Moreover, TXT2NTAB saves the standard deviation values obtained from the lattice calculations using the stochastic approach and writes them in a NEMTAB format creating two additional libraries (one unrodded and one rodded) to be read by the nodal code. This approach does not consider directly the correlations between few-group cross-sections obtained from the lattice calculations but, a perturbation factor to the standard deviation values is applied, as explained in next section."

Once the NEMTAB libraries are obtained, the use of a statistical tool is needed to provide the perturbation factors to be used in the core simulations. The nodal code needs to have the capability to read the perturbation factors and the NEMTAB libraries containing the cross-sections average values and standard deviations. Then, running the input many times, one achieves the propagation of the neutronic parameters uncertainties from the problem-dependent cross-sections library to the core level.

With the entire methodology, one obtains the k_{eff} value and the power distributions (radial and axial), with additional information about PDF, standard deviation, and the correlation coefficients of chosen output parameters. Therefore, the methodology is advisable to provide realistic results with safety margins and determine which input parameters have a stronger impact on output uncertainties.[5]

The outline of this paper is as follows: Section 1 is the introduction. Section 2 describes the codes employed in this work and the model of the simulated LWR. Section 3 emphasizes the use of TXT2NTAB, a code developed by the authors to generate the NEMTAB libraries that include uncertainties information. In Section 4 all the relevant results are presented and discussed and, finally, Section 5 summarizes the conclusion.

II. Methodology

The Nuclear Data Libraries (NDLs) are considered to be the primary source of uncertainties for the neutronic calculation. These libraries are used to solve the transport equation consequently, the data uncertainty is propagated starting at pin level, then lattice and finally core level.

However, the evaluation of nuclear data induced uncertainties is possible by using nuclear data covariance information usually kept in covariance library, available in major NDLs.

In this work the nuclear data library ENDF/B-VII.1 is used, discretized in 56 energy groups with the 56-group covariance library provided by SCALE6.2.3 code system.[6] The collapsed cross-sections generation is discretized into two energy groups using the standard 0.625 eV as energy cutoff.

For the assembly simulations, the authors have employed the TRITON/NEWT modules in SCALE6.2.3 code system.[7] SCALE solves the transport equation in 2D for a small zone of the core with good detail. It produces collapsed and homogenized cross sections for fresh and depleted states.[8]

SCALE uses the ORIGEN module for the depletion and isotopic transmutation tracking, with the CENTRM option for the cross-sections processing in the resolved energy range and BONAMI in the unresolved energy range.[9] [10] That allows to update the cross-sections and create the multi-group problem-dependent tables.

Based on the nominal case defined in the lattice model, branches calculations are performed to solve the transport problem with the feedback parameters modified one at a time. In addition, in SCALE the burnup calculation is not repeated for the branches set but the resulting of the nominal case is used instead.[11] This means that all branches calculations follow the same depletion steps, resulting in a more efficient calculation. Branches calculation allows to simulate different conditions for feedback parameters to cover the expected range of core operating conditions. In this study, the combination of feedback parameters results in 40 state points. An explanation of them is provided in the next section.

For the probabilistic approach, as mentioned in the previous section, nuclear data are sampled using the Simple Random Sampling (SRS) technique, which generates each sample randomly according to the PDF of the input parameters, which are expected to be normally distributed.[12] According to the Nonparametric Sampling, it is possible to sample all parameters at the same time and assume that the number of samples is not dependent on the number of input parameters.

The UQ in SCALE6.2.3 code system is carried out with Sampler module.[13] This module generates a set of perturbation factors for the multi-group cross-sections tables using the SRS technique.[14]

The perturbations are defined as multiplicative factors for each nuclide *i*, nuclear reaction *x* and energy group *g*.

$$Q_{x,g}^{i} = 1 + \frac{\Delta\sigma_{x,g}^{i}}{\sigma_{x,g}^{i}} \tag{1}$$

Where

$Q_{x,g}^{i}$ is the perturbation factor for a specific isotope, reaction, and energy group, and

$\frac{\Delta\sigma_{x,g}^{i}}{\sigma_{x,g}^{i}}$ is the relative covariance obtained from the covariance library.

Due to the high number of feedback parameters and the depletion set (many steps up to 365 days of burnup), the calculation in SCALE takes several days to complete (around seven days in a server composed by 72 nodes, each of them with two processors Intel Xeon E5-2450 8c/16T and 64 GB/RAM DDR3). Because of that, a limited number of 60 samples have been run as a first deployment of the methodology. However, the stochastic sampling methodology can produce meaningful and reliable UQ results with a number of runs between 15 and 100.[15]

After the lattice simulations in SCALE, the authors employ DAKOTA6.3 code to generate the perturbation sets to be used in the core simulation to expand the UQ process.[16] 1000 random numbers are generated for each neutronic composition and main parameters contained in the neutronic library. Assuming the perturbation factors normally distributed and taking into account 0 as average values and an upper/lower limit of ±1. Table 1 lists the main parameters chosen from the simulation in SCALE at the lattice level to expand the UQ process.

For the neutronic calculation at the core level, the authors use PARCSv3.2 code to solve the diffusion equation with the multi-group approximation.[17] This 3D nodal code involves the initial eigenvalue problem to solve the subsequent spatial kinetics calculation, introducing k_{eff} into diffusion equation to determine how far from steady conditions the system is.

Table I. Parameters considered in DAKOTA pre-process.

<table>
<tr><td colspan="2">Multiplication factor k_{eff}</td></tr>
<tr><td colspan="2">Scattering Fast to Thermal (down-scattering)</td></tr>
<tr><td>Diffusion Coefficient</td><td rowspan="3">Fast and
Thermal group</td></tr>
<tr><td>Absorption cross-section</td></tr>
<tr><td>Fission cross-sections
(average neutrons per fission time)</td></tr>
</table>

PARCS uses the homogenized and collapsed cross-sections obtained by SCALE, in terms of average values and standard deviations, ordered in NEMTAB format by

TXT2NTAB code. The NEMTAB generation process by TXT2NTAB code will be explained in the next section. PARCS source code was modified to read the random factors generated by DAKOTA, thus the input was run 1000 times applying different perturbations. Besides, for the steady-state simulations PARCS can interpolate the cross-sections according to the thermal-hydraulics conditions. These are given by 3D distributions moderator density and fuel temperature stored in DENS and TFUS files.

Finally, the Sensitivity Analysis (SA) is performed using DAKOTA, to analyze the output parameters of the core simulation: multiplication factor k_{eff}, axial power peak P_z, and peak node location N_z. These output parameters are chosen because they are related to the reactor safety.[18]

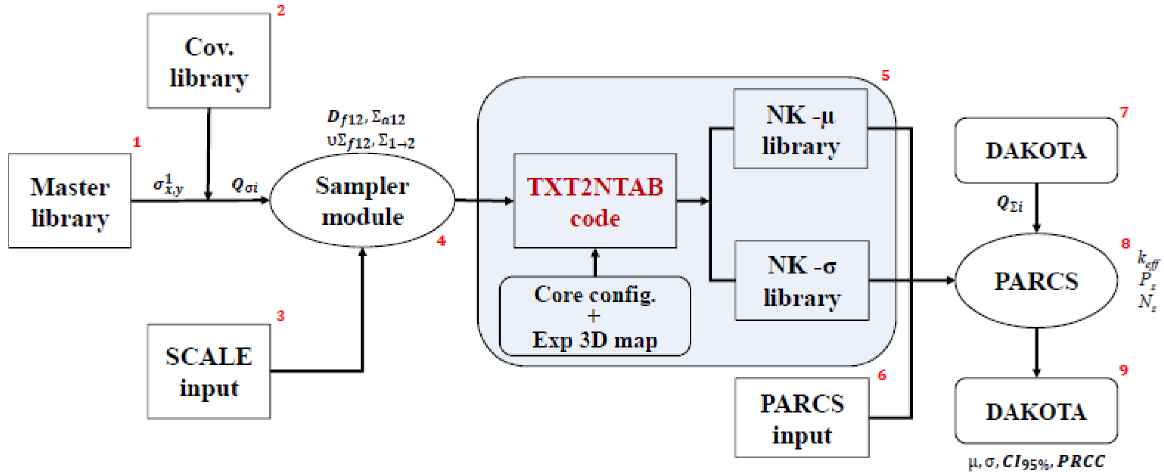

Figure 1. Diagram showing the neutronic parameters propagation.

Figure 1 shows a flow diagram of the methodology. With the master library (1) and the covariance library (2), one can run the same SCALE input (3) applying different perturbations to the master cross-sections library using Sampler module (step 4). Then, with TXT2NTAB two Neutronic-Kinetic (NK) libraries are created, one with average values and the other with standard deviation values (step 5). For this step, the core configuration and the burnup distribution must be considered to calculate the number of compositions resulting in the NEMTAB libraries. Next, with the PARCS input (6), the random perturbation factors generated with DAKOTA (7), and the NEMTAB libraries from the previous step, one can run many PARCS simulations (step 8). Finally, the Sensitivity and Uncertainty (S&U) analysis is performed by DAKOTA to study the most important output parameters (9).

II.A. PARCS model

In this work, the authors choose a BWR-GE6 for the simulations. There are 4 types of fuel assemblies with various enrichment and configuration regarding gadolinia pins (GdO_2+UO_2), and 3 reflectors (top, bottom, and radial). Figure 2 shows the fuel type radial mapping and the control rod bank distribution.

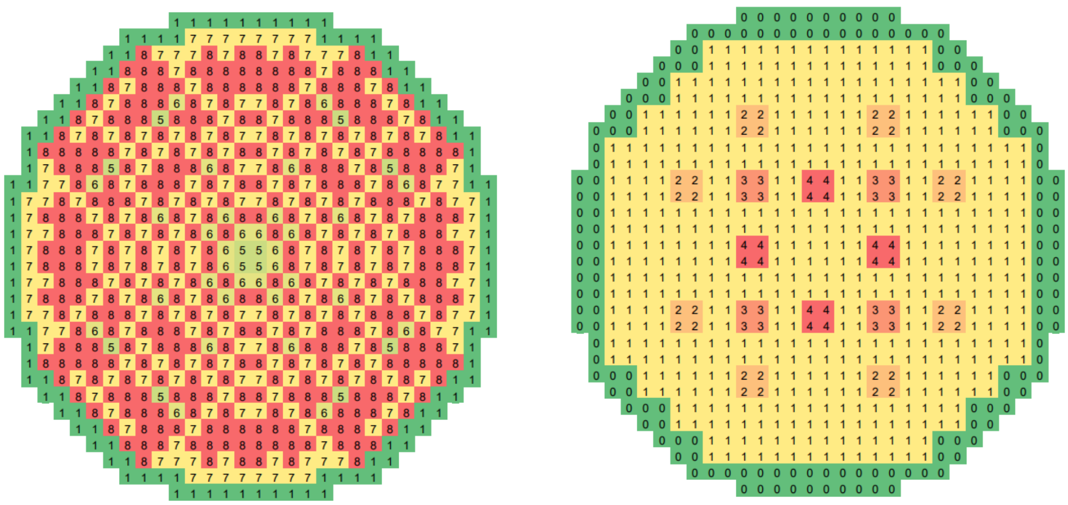

Figure 2. BWR-GE6 core configuration. Fuel type radial mapping (left) and control rod bank distribution (right).

The neutronic behavior is modeled in PARCS3.2 dividing the core in 25+2 axial nodes, with dimension 15.24 cm x 15.24 cm, and based on the one-node-per-assembly configuration. All boundary conditions are set to zero flux. The decay heat model is activated (considering the fission products and transuranic elements) and the diffusion equation solver is HYBRID. The thermal-hydraulics 3D boundary conditions used for the BWR are between 900 and 1500 K for the fuel temperature, and moderator density between 100 and 700 kg/m^3. These data are given to PARCS as 3D radial maps, in the TFUE and DENS files, respectively.

III. NEMTAB libraries generation

TXT2NTAB is a set of MATLAB® scripts developed to fill the gap between the lattice physics code system SCALE and any core simulator that uses NEMTAB-formatted libraries (such as PARCS). Moreover, TXT2NTAB can process the results of TRITON-NEWT or Polaris modules to generate NEMTAB libraries and, additionally, it can also process Sampler results to include uncertainty information. Optionally, TXT2NTAB can generate the GEOM file needed by PARCS.

The nodal core simulator must have data for all changing conditions that the expert needs to model. This is accomplished, in lattice physics calculation, using branch calculations where the feedback parameters are instantaneously changed.

There are three important features to take into account:

(1) Feedback parameters to be included. Fuel temperature and moderator density are necessary (besides control rod condition).

(2) The number of points for each feedback parameter. With an increasing number of points, more accuracy is obtained, but more computational time is needed.

(3) The range for the feedback parameters. The range must be enough to simulate all desired operating and transient conditions using the core physics code.

Since the core physics code interpolates the cross-sections based on the feedback parameters for each node, is not necessary to specify branches for every possible operational condition, reducing significantly the computational time. On the other hand, the envelope formed by the chosen feedback parameters should cover the range of all possible conditions because the extrapolation of nodal parameters (in case operating condition lies outside the envelope of feedback parameters) can be particularly risky.[19]

The feedback parameters chosen in this work are listed in Table 2 and Table 3. There are 7 different data points of fuel temperatures and 4 different moderator densities points. The moderator temperature is not included as a state variable, because its effect is treated implicitly in the moderator density assuming single phase at constant pressure which is a common assumption under normal operation.

Table II. Fuel temperature data and history points.

T_{fuel} (K)			
1	293.0	**5**	1396.5
2	561.4	**6**	1764.3
3	870.0	**7**	2132.2
4	1142.2	**Hist.**	870.0

Table III. Moderator density data and history points.

D_{mod} (kg/m^3)	
1	38.01
2	456.34
3	735.22
4	998.19
Hist.	735.22

The control rod is not taken as a state variable, but the same branch calculations performed without control rod are made with the control rod inserted. The segments representing the reflector do not require simulations with control rods, thus they have half of the feedback state points. The mesh formed by the feedback parameters can be seen in Figure 3, with 20 feedback combinations simulated in the lattice code for each assembly.

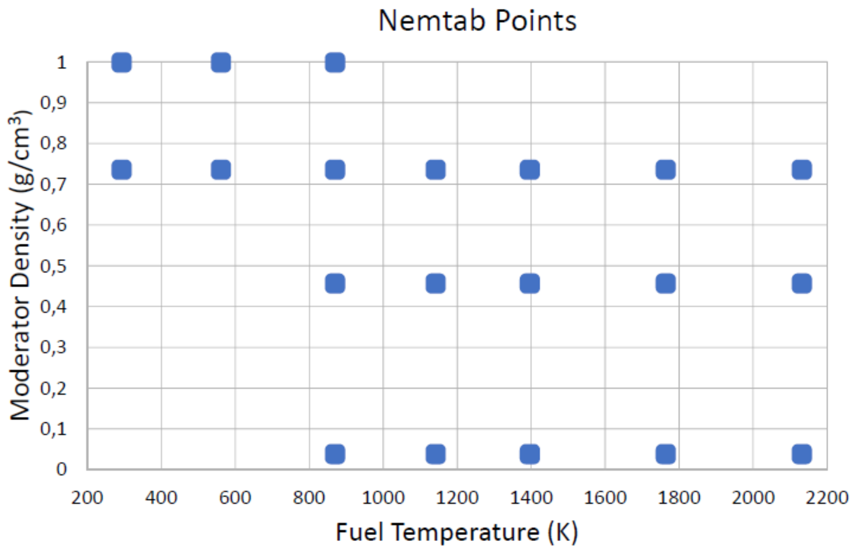

Figure 3. Feedback combinations in NEMTAB library.

Additionally, a 3D burnup map is used to associate each burnup with its corresponding node of the core. The 3D burnup map is read by TXT2NTAB code which selects (in the *txtfile16* files) the cross-sections tables for the feedback parameters of interest, taking into account the distribution of segments in the core and the corresponding depletion. If a particular burnup value from the 3D map is not included in the burnup steps simulated at lattice level, then TXT2NTAB can interpolate cross-sections between the two nearest burnup steps.

The neutronic compositions resulting in the NEMTAB library are determined considering the core configuration and the 3D burnup map. In case of having a very heterogeneous depletion distribution, the 3D map can be slightly simplified, combine similar depletions that correspond to the same fuel type in the core.[20]

In this work, according to the core configuration (see Figure 2) there are 4 fuel assembly types. Considering the 3D burnup map, one gets many different neutronic compositions belonging to the same fuel type. To simplify the compositions, the burnups that differ 0.1 MWd/KgU, for the same fuel type, are interpolated and considered as the same neutronic composition. This results in 1003 different neutronic compositions in the core, including reflectors.

Figure 4 shows a 2D average burnup map obtained by collapsing the axial burnup of the core, although the real information used in this work is a 3D nodal map.

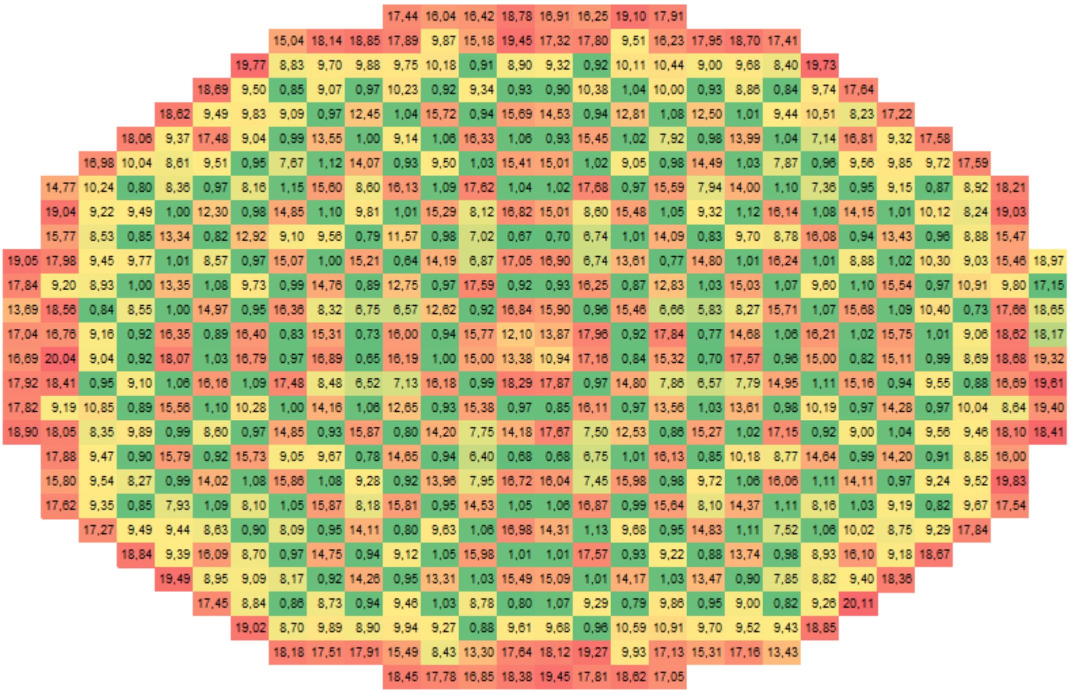

Figure 4. 2D burnup map (average axial values).

If Sampler module is used for the lattice simulations, TXT2NTAB is capable to generate a library with cross-sections average responses and a second library with the responses' standard deviations, both in NEMTAB format.

Considering the unrodded and rodded configuration, TXT2NTAB generates four files: *nemtab*, *nemtab_sd*, *nemtabr*, and *nemtab_sd*. These libraries are tabulated for each neutronic compositions as a function of feedback parameters (fuel temperature and moderator density) and the collapsed energy group.

IV. Results

Once obtained within the NEMTAB libraries, the cross-sections uncertainties are propagated through PARCS using the statistical tool DAKOTA. The main results of the standalone neutronics simulation with the nodal code are presented in this section, considering the main output responses: multiplication factor k_{eff}, axial power peak P_z, and peak power node location N_z.

Table 4 shows the average responses and standard deviations, both with lower and upper limits, and the normality parameters skewness and kurtosis. A value of zero for the kurtosis indicates a normal distribution, while a value of zero for the skewness indicates a symmetric distribution.

Table IV. Statistical information of the output responses.

	Average	Standard deviation	Skewness	Kurtosis
k_{eff}	1.02902 ± 4.154E-5	6.693E-4 ± 3.070E-5	-0.0389	0.0966
P_z	3.86379 ± 0.03569	0.57521 ± 0.02638	0.5095	0.44916
N_z	4.949 ± 0.077	1.243 ± 0.057	0.5736	0.090

From Table 4 one can summarize that the uncertainty in the k_{eff} is low, and its distribution is normal. The peak node location is in node 5, but its standard deviation of 1 indicates that the peak has some chances to be located in node 4 and 6 too. This can be also seen in the axial power profile in Figure 5 where the standard deviation (dashed-red lines) is wider around the power peak. Moreover, Figure 6 represents the average normalized radial power profile and its standard deviation.

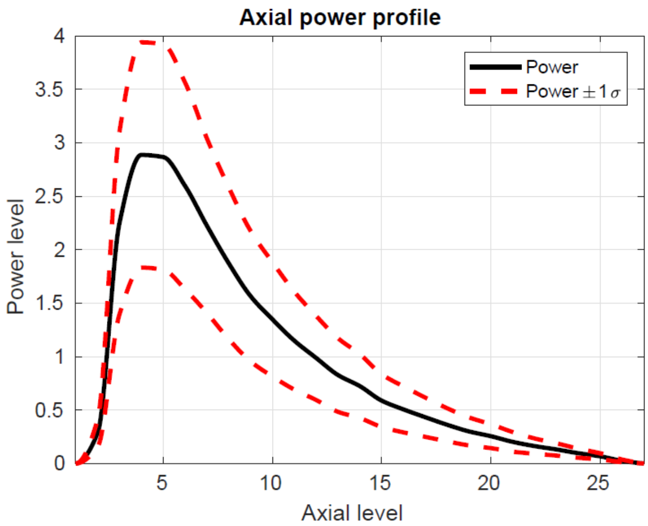

Figure 5. Normalized axial power profile with its ±σ zone.

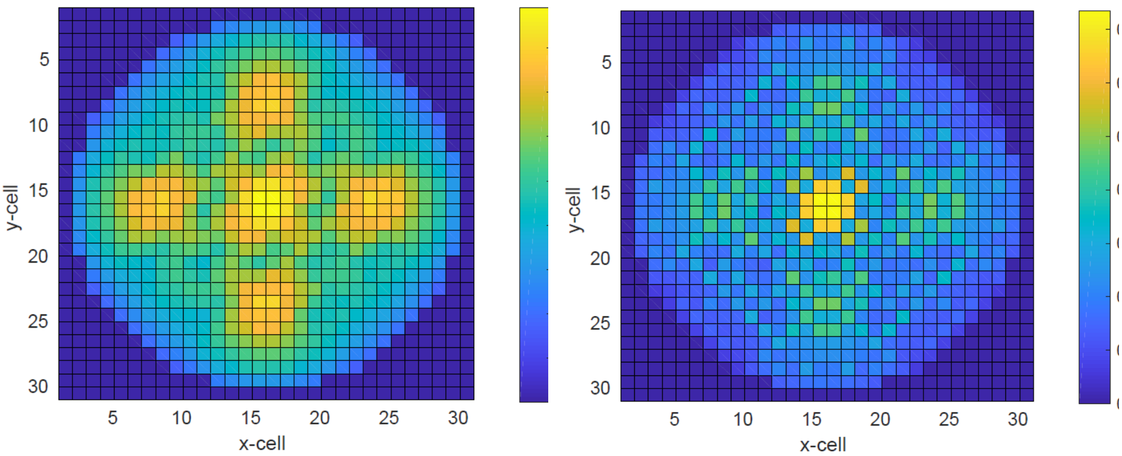

Figure 6. Normalized and collapsed radial power profile, average (left) and standard deviation (right).

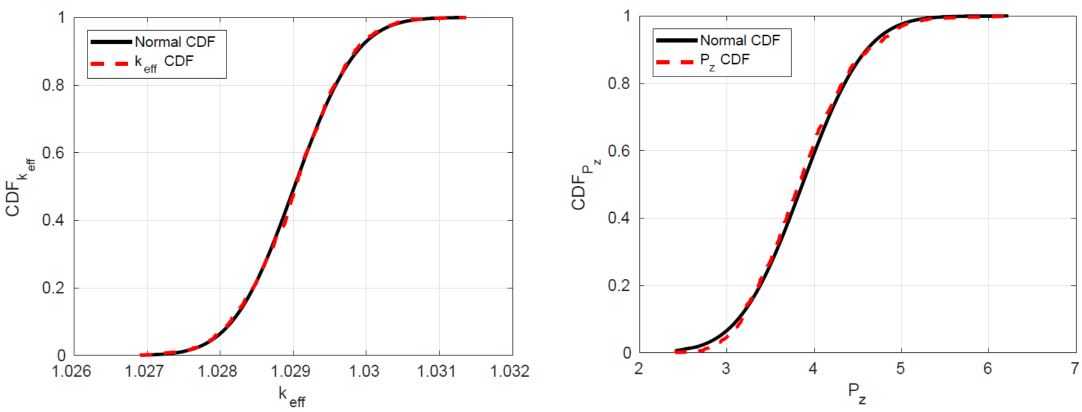

Figure 7. Cumulative Distribution Functions of k_{eff} (left) and P_z (right).

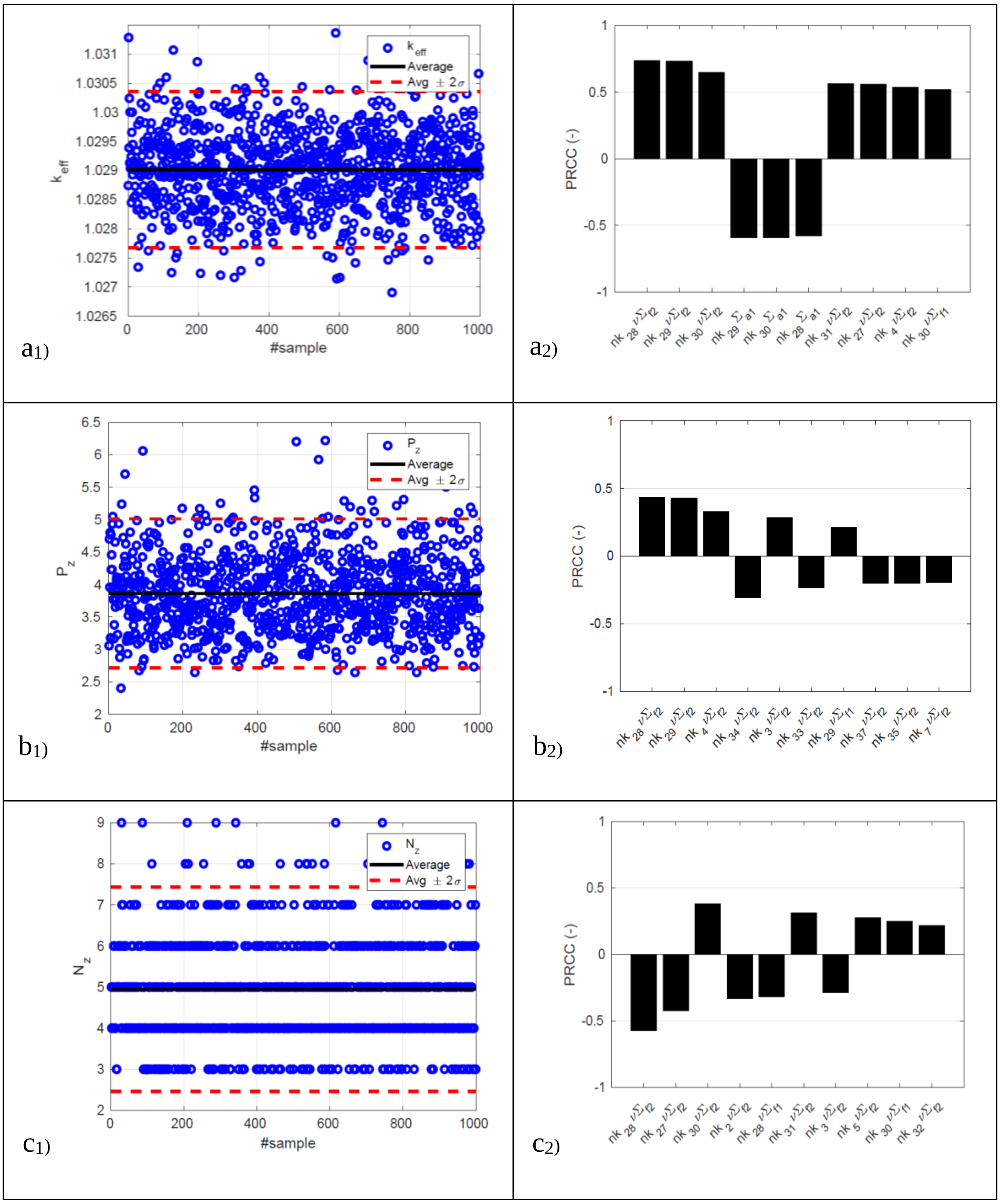

Figure 8. Scatter plots and partial rank correlation coefficients of the output parameters. k_{eff} (a_1 and a_2), P_z (b_1 and b_2) and peak power node location N_z (c_1 and c_2).

Figure 7 shows the Cumulative Distribution Functions (CDFs) compared with the standard normal CDF (obtained using the same average and standard deviation). The CDF for the N_z response is not shown because it is a discrete function. Looking at these functions can be said that the output responses can be represented with normal distributions. Figure 8 represents the scatter plots and Partial Rank Correlation Coefficients (PRCC) for the same variables. The PRCC provides a measure of the strength of a linear association between an input parameter and an output parameter. From Figure 8 it can be seen that the absorption and fission cross-sections are the most sensitive parameters for all referred variables. Similar statistical results have been found studying a BWR in for fresh fuel conditions.[21]

V. Conclusions

This work provides a methodology to propagate uncertainties from basic nuclear data library to the few-group nodal homogenized cross-sections and core calculations through SCALE and PARCS simulation, including neutronic and kinetics parameters and taking into account the uncertainties due to the energy collapse and spatial homogenization process. The Sampler stochastic module in SCALE is used with NEWT lattice physics sequence to obtain cross-sections tables with statistical information.

To accomplish the purpose of this work the authors developed TXT2NTAB code, a computer program able to read statistical information achieved by Sampler and re-order cross-sections libraries in NEMTAB format as a function of feedback parameters. TXT2NTAB code generates two libraries with average cross-sections values (for the rodded and unrodded configuration), and other two libraries with their standard deviations.

To propagate the uncertainties at core level, thousand PARCS simulations are run using the parametrized cross-sections tables, each simulation with a different set of random perturbation factors generated by DAKOTA. PARCS source code is modified for this purpose. Finally, a sensitivity analysis is carried out with DAKOTA to study the main

PARCS output parameters: multiplication factor k_{eff}, axial power peak P_z, and peak power node location N_z.

The methodology can be applied to propagate uncertainty for any neutronic and kinetic parameter at different levels of detail. Moreover, the code TXT2NTAB allows to reorder cross-sections obtained in SCALE in NEMTAB format, to be used in a core simulator with no limitations on the type of reactor and its configuration. At this point, the correlations between few-group cross-sections obtained from the lattice calculations are not considered in the core simulation, a perturbation factor to the standard deviation values is applied instead. The possibility to take into account the few-group cross-sections correlations is part of further development of this work.

Acknowledgments

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