Nuclear data uncertainty quantification in the ARC fusion reactor

NUCLEAR DATA UNCERTAINTY QUANTIFICATION IN THE ARC FUSION REACTOR

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ABSTRACT

It is widely recognized that the design of a nuclear reactor requires also an uncertainty quantification (UQ) analysis, in the spirit of the Best Estimate Plus Uncertainty (BEPU) approach. The evaluation of uncertainties is especially important in the case of a nuclear fusion machine such as the Affordable Robust Compact (ARC) reactor, where the uncertainties of the nuclear data of uncommon nuclides in the nuclear field, like fluorine, beryllium and lithium, can have a significant impact on fundamental design parameters, such as the achievable Tritium Breeding Ratio (TBR). In this work, three different methods, namely the fast Total Monte Carlo (fTMC), the GRS and the Unscented Transform (UT), have been employed for the neutronic UQ analysis of ARC, with the use of the Monte Carlo code Serpent. These methods lead to similar values in terms of relative standard deviation on the TBR due to nuclear data, and can be considered as fast alternatives to brute-force sampling methods. The paper also provides suggestions to select the best approach according to the kind of analysis performed and to the nuclides considered in the study. The main outcome of these analyses suggests that the uncertainties in nuclear data of fluorine, beryllium and lithium is sufficiently small to prevent the TBR to assume values below the design constraints.

KEYWORDS: Nuclear Fusion, Uncertainty Quantification, Fast Total Monte Carlo, GRS, Unscented Transform

1. INTRODUCTION

The Affordable Robust Compact (ARC) reactor [1] , see fig. 1, is a small D-T based tokamak design aimed at the production of electric power, with a significant size reduction with respect to other next-generation machines, such as DEMO (DEMOnstration Power Plant) [2], with an electrical output of $200\,\mathrm{MWe}$. In the ARC design the size minimisation and, as a consequence, its cost and complexity reduction, will be achieved by increasing the magnetic field intensity, thanks to high-temperature superconductors.

In the current design of ARC, the vacuum vessel is submerged in a breeding blanket filled with a molten salt, i.e. FLiBe (76.79% fluorine, 9.09% beryllium and 14.12% lithium). The FLiBe salt works simultaneously as neutron multiplier, neutron moderator, shield, heat transfer fluid, breeder, and tritium carrier, and it is continuously circulated. In order to achieve a Tritium Breeding Ratio (TBR) larger than one, thus ensuring the reactor self-sustainability of the fuel production, the lithium in the salt is isotopically enriched in ^{6}Li up to 90%. In this reactor, the neutron multiplier for the enhancement of the neutron economy is beryllium, present both in the molten salt composition and in a layer inside the vacuum vessel.

The preliminary neutronic modelling of ARC has been performed with the Monte Carlo particle transport code Serpent 2 (v. 2.1.31) [3] in a previous work [4], for the evaluation of the tritium breeding ratio and the power deposition by neutrons and photons inside the breeding blanket, proving the capability of Serpent

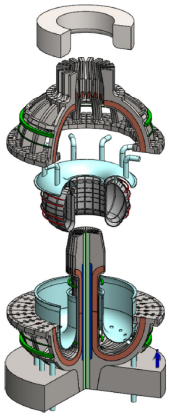


Figure 1: ARC assembling scheme (reproduced from [1]).

to suitably simulate fusion reactors, leading to an estimated TBR>1. In this work, the same ARC reactor model, sketched in figure 2, is used with a focus on the nuclear data uncertainty quantification.

The usual approach to evaluate the uncertainty when the number of uncertain input and output parameters is large is based on perturbation methods. Specifically, the nuclear data uncertainty evaluation relies on the well-known sandwich rule [5],

$$\mathrm{var}[r] = \vec{\mathrm{S}}_p^r \mathrm{cov}[p] \vec{\mathrm{S}}_p^{r^T}, \tag{1}$$

where $\mathrm{var}[r]$ is the variance of the response, $\vec{\mathrm{S}}_p^r$ is the relative sensitivity of r with respect to a variation in the input p, and $\mathrm{cov}[p]$ is the relative covariance matrix associated to p. The calculation of the relative sensitivity is usually performed using the Generalised Perturbation Theory (GPT) [6], which is also available in Serpent [7]. Despite the implementation of this approach in Serpent has been recently assessed for fast reactors [8,9] GPT cannot be currently employed for source-driven system, as the case of ARC. Therefore, this paper presents three sampling-based, non-intrusive UQ methods as an alternative to GPT: the fast Total Monte Carlo [10], the GRS [11] and the Unscented Transform [12]. These techniques do not require any modification to the original model, allowing to consider it as a "black-box", but, as a drawback, they require a number of model simulations somehow proportional to the dimensionality of the uncertain input, meaning that their use is efficient when the number of input parameters is relatively low compared to the number of output quantities. In this case, it is physically reasonable to assume that the output responses of interest, i.e. the TBR and the power deposited, are mostly influenced by the nuclides composing the salt, i.e. ^{6}Li, ^{9}Be and ^{19}F. Therefore, the UQ study will deal with these isotopes, aiming at verifying whether the combination of the uncertainty due to the nuclear data and the statistical one associated to the Monte Carlo method, could yield a TBR <1, which is the reference design target. Here, the ^{7}Li has not been considered because it has been proven to have a negligible impact on the TBR of ARC in a previous work [4], even if it represents a significant percentage of the FLiBe composition.

2. UNCERTAINTY QUANTIFICATION METHODS

In this section, the uncertainty quantification methods employed in the present work are briefly described. As mentioned, the choice of non-intrusive methods requires no need for modifications of the original model, but only the generation of a set of perturbed nuclear data to be employed in a set of neutronic Monte Carlo simulations.

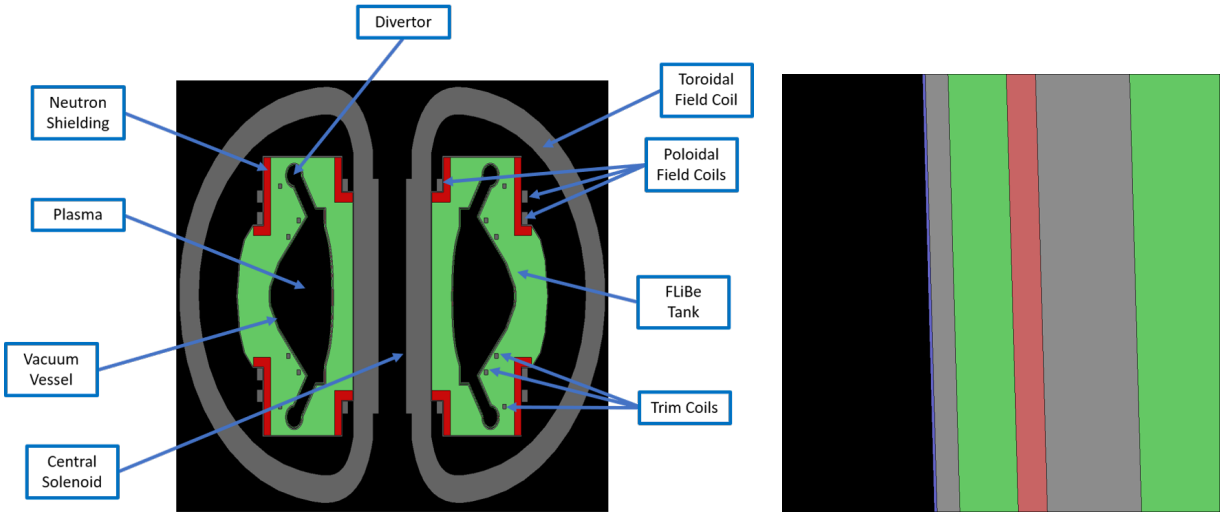


Figure 2: Poloidal section of the ARC model implemented in Serpent (a), and detail of the radial build of the vacuum vessel (b). From the left to the right: plasma chamber (black), first wall (blue), inner vacuum vessel (gray), cooling channel (green), neutron multiplier (red), outer vacuum vessel (gray) and FLiBe blanket (green).

In this work, the tool used for the generation of the perturbed data is the SANDY Python package [13], as it allows to produce perturbed files starting from the evaluated nuclear data covariances, meaning that the perturbed data distribution is supposed to be normally distributed. All the nuclear data and the corresponding covariances used for the UQ analysis are taken from the ENDF-B/VIII.0 library. This choice was made to be consistent with the Serpent simulations presented in [4], performed using this library. However, considering that the covariance data depend also on the data library, future work should investigate also the impact induced by the choice of other libraries, like the FENDL-3.2 and the JEFF-3.3.

2.1. Fast Total Monte Carlo

The fast Total Monte Carlo (fTMC) [10] is a faster alternative to the reference Total Monte Carlo (TMC) method [14]. The fTMC performs the same number of Monte Carlo simulations of TMC, but each one with a number of neutron histories reduced by a factor of n, a different seed for the random number generator and a different perturbed nuclear data library. Consequently, the total run time is reduced by a factor of n neutron histories. Of course, the factor n cannot be too large to avoid significant statistical uncertainty in the results. In fact, considering that the nuclear data variance is obtained with the expression:

$$\sigma^2_{ND} = \sigma^2_{obv} - \overline{\sigma}^2_{stat}, \tag{2}$$

where $\overline{\sigma}^2_{stat}$ is the average of the statistical variances of the simulations, while σ^2_{obv} is the variance of the vector of observables, it is of course possible that, if the statistical error on the estimations is too large, the resulting nuclear data uncertainty can be negative, which is an unphysical result.

At the end of the fast Total Monte Carlo simulations, the result is a vector of observables (e.g a vector of TBR values) and a vector of statistical errors.

2.2. GRS Method

Another fast alternative to the TMC is the GRS method [11], which requires two different set of simulations, each simulation with a different perturbed nuclear data library and a number of neutron histories *n* times smaller than the TMC, reducing the computational time by a factor of *n/2*. The simulations belonging to one set share the same seed, which is different from the one of the other set. After the two sets of simulations are completed, computing the covariance of the corresponding two vectors of observables, it is possible to evaluate the nuclear data variance as:

$$\sigma_{ND}^2 = \mathrm{cov}(\vec{k_1}, \vec{k_2}), \tag{3}$$

where $\vec{k_1}$ and $\vec{k_2}$ are the vector of observables of the first and of the second sets of simulations, respectively.

2.3. Unscented Transform

The Unscented Transform (UT) [12] is based on the idea that approximating the input distribution should yield better results than approximating the output distribution, especially when the model is non-linear. This approximation is realised generating a set of sigma points that represent the probability distribution of the input data, independently on its nature. Usually, $2n+1$ sigma points are sufficient to get a good approximation of the input, where *n* represents the dimensions of the input perturbed data. In this case, *n* can be large, as it is given by the product of the MT cross section reaction numbers associated to the specific nuclide and the number of energy groups upon which the covariance matrix is defined. Therefore, to overcome this issue, a suitable reduction technique will be employed.

At first, the components of the sigma points vector χ are computed according to the following equations [15]:

$$\begin{aligned} \chi^{[0]} &= \mu \\ \chi^{[i]} &= \mu + \left(\sqrt{(n+\lambda)\Sigma}\right)_i \quad \text{for } i = 1, ..., n \\ \chi^{[i]} &= \mu - \left(\sqrt{(n+\lambda)\Sigma}\right)_{i-n} \quad \text{for } i = n+1, ..., 2n, \end{aligned} \tag{4}$$

where μ is the mean vector of the input (in our case, the mean nominal cross sections from the nuclear data library), λ is an arbitrary spreading parameter (see below), and Σ the corresponding covariance matrix. Once the sigma points have been obtained, each one of them is assigned to a weight calculated as follows:

$$\begin{aligned} \omega^{[0]} &= \frac{\lambda}{n+\lambda} \\ \omega^{[i]} &= \frac{1}{2(n+\lambda)} \quad \text{for } i = 1, ..., 2n. \end{aligned} \tag{5}$$

The sigma points are generated so that their mean and covariance is calculated as follows,

$$\mu = \sum_{i=0}^{2n} \omega^{[i]} \chi^{[i]} \tag{6}$$

$$\Sigma = \sum_{i=0}^{2n} \omega^{[i]} \left(\chi^{[i]} - \mu\right) \left(\chi^{[i]} - \mu\right)^T. \tag{7}$$

Finally, the sigma points are passed as an input to the non-linear function *g* (i.e the Serpent simulations) and the mean and covariance of the transformed distribution are calculated as:

$$\mu' = \sum_{i=0}^{2n} \omega^{[i]} g\left(\chi^{[i]}\right) \tag{8}$$

$$\Sigma' = \sum_{i=0}^{2n} \omega^{[i]} \left(g\left(\chi^{[i]}\right) - \mu'\right)\left(g\left(\chi^{[i]}\right) - \mu'\right)^T, \tag{9}$$

where the index *i* represents the *i-th* sigma point and weight. The value of Σ' represents the uncertainty on the output results of the model, obtained propagating the nuclear data uncertainties through the neutronic model itself.

The definition of the sigma points and of the weights depend on an arbitrary spreading parameter λ, which represents the spreading of the sigma points. Since we are assuming a Gaussian distribution for the input, the best choice is to select $n + \lambda = 3$ [12]. However, in case *n* is large, as here, this could lead to a set of negative weights $\omega^{[i]}$. This is not an issue for deterministic models, but it could jeopardise the UT approach in case a stochastic model is employed, as discussed later.

The main drawback of this method is the computation of the square root of the perturbed data input covariance matrix, necessary to calculate the sigma points. In the case of a symmetric and positive semi-definite covariance matrix, this problem can be handled with the Singular Value Decomposition (SVD) [15] as follows:

$$\Sigma = VDV^T, \tag{10}$$

where the matrix D is a diagonal matrix composed by the singular values. However, it may happen that the covariance matrices extracted from the ENDF/B-VIII.0 nuclear data library are non-positive semi-definite. Thus, before applying the UT, the *statsmodels* Python package [16] is used to evaluate the closest semi-positive definite matrix to the original one, following the procedure given in [17].

At this point, it is possible to maintain a satisfactory accuracy in the computation of Σ reducing the number of active singular values obtained with the SVD, thanks to the redundancies due to the strong correlation among the nuclear data reactions. As a consequence of this reduction, the final number of active singular values *k* is smaller than the number of non-zero singular values *r*. The matrix that is obtained in this way is an approximation of the actual one and the truncation coefficient *k* is evaluated computing the so called energy of the singular values:

$$E_k = \frac{\sum_{l=1}^{k} \sigma_{ll}}{\sum_{l=1}^{r} \sigma_{ll}}. \tag{11}$$

In this study, the truncation criterion for the selection of the *k* active singular values is $E_k < 99.997\%$. This truncation allows to decrease the number of sample points from $2n$+1 to $2k$+1 and the computational time of the uncertainty quantification.

3. RESULTS

In this section, the most significant results obtained with the different methods are presented. In subsection 3.1, fTMC and GRS results are presented together, due to the similarities between these two fast alternatives of the TMC. The results of the UT are shown in a dedicated subsection 3.2, since they require a more in-depth analysis.

3.1. Fast Total Monte Carlo and GRS

Initially, the fast Total Monte Carlo has been employed since it is the easiest method to be implemented and it is faster than the GRS. We performed 500 simulations, each one with a different perturbed library generated with SANDY, using 50 batches, each one with 10^4 neutron histories, for the ^{9}Be and the ^{19}F,

which has been considered a sufficiently high number in order to obtain a statistical uncertainty smaller than the nuclear data one. In the case of ^{6}Li, this number of neutron histories was not sufficient to obtain a positive nuclear data uncertainty from Eq. 2. This was a first sign of the fact that the influence of the uncertainty on ^{6}Li is not significant, however for this nuclide the number of neutron histories per batch has been increased to 3×10^4 in order to reduce the statistical error and obtain a positive nuclear data uncertainty.

The results with the fTMC for the TBR are shown in Table I. The contribution of the ^{6}Li on the final uncertainty is negligible, being one order of magnitude smaller than those of the other two nuclides. On the other hand, the nuclear data relative standard deviation (RSD) of ^{9}Be and ^{19}F is larger than the statistical one and it is independent of the number of neutron histories simulated, meaning that it is not possible to reduce it.

Table I: Nuclear data uncertainty for the TBR evaluated with the fast Total Monte Carlo method. The number in parenthesis has to be applied as a $\pm$ on the last digit of the result.

	^{6}Li	^{9}Be	^{19}F
TBR [-]	1.085(2)	1.086(3)	1.086(6)
Statistical RSD [%]	0.106 3	0.182 9	0.182 5
Nuclear data RSD [%]	0.016 7	0.263 1	0.524 5

The same type of analysis has been performed with the GRS method, doubling computational time (see section 2.2 above). Since a result of the fTMC was that the nuclear data uncertainty of ^{6}Li can be disregarded, this nuclide has not been taken into account during this analysis.

Comparing the results of the GRS method in Table II with the ones of the fast Total Monte Carlo, it is possible to observe a perfect agreement, suggesting, in this case, the preferable use of the fTMC due to its lower computational time.

Table II: Nuclear data uncertainty for the TBR evaluated with the GRS method The number in parenthesis has to be applied as a $\pm$ on the last digit of the result.

	^{9}Be	^{19}F
TBR [-]	1.083(3)	1.086(6)
Statistical RSD [%]	0.182 9	0.182 5
Nuclear data RSD [%]	0.264 9	0.523 2

Another quantity of interest is the volumetric power deposited by the neutrons in the main components of the ARC reactor. The results for fluorine and beryllium are shown in Table III and Table IV respectively. Again, the results obtained with the two methods are comparable, even if the discrepancy is larger with respect to the TBR results. Moreover, in this case the nuclear data uncertainty depends on the amount of the specific nuclide present in the different components. In fact, the largest uncertainty with fluorine is in the cooling channel (CC) and the breeding blanket (BB), as they are made of FLiBe, while for the beryllium the highest contribution is in the neutron multiplier (NM) layer.

Table III: Nuclear data uncertainty of ^{19}F for the volumetric power deposition. The number in parenthesis has to be applied as a $\pm$ on the last digit of the result. (FW: first wall; VV1: inner vacuum vessel; CC: cooling channel; NM: neutron multiplier; VV2: outer vacuum vessel; BB: breeding blanket).

Fast Total Monte Carlo						
	FW	VV1	CC	NM	VV2	BB
Volumetric power deposition [$\mathrm{MW/m^3}$]	0.910(6)	4.45(3)	10.8(2)	5.55(4)	2.34(2)	0.714(6)
Nuclear data RSD [%]	0.434 5	0.520 0	1.541 6	0.626 7	0.819 8	0.887 2
GRS						
Volumetric power deposition [$\mathrm{MW/m^3}$]	0.905(7)	4.44(3)	10.7(2)	5.54(4)	2.33(2)	0.713(7)
Nuclear data RSD [%]	0.521 6	0.548 1	1.568 3	0.605 1	0.824 4	0.902 4

Table IV: Nuclear data uncertainty of ^{9}Be for the volumetric power deposition. The number in parenthesis has to be applied as a $\pm$ on the last digit of the result. (FW: first wall; VV1: inner vacuum vessel; CC: cooling channel; NM: neutron multiplier; VV2: outer vacuum vessel; BB: breeding blanket).

Fast Total Monte Carlo						
	FW	VV1	CC	NM	VV2	BB
Volumetric power deposition [$\mathrm{MW/m^3}$]	0.911(5)	4.46(1)	10.79(4)	5.55(9)	2.336(6)	0.714(2)
Nuclear data RSD [%]	0.146 1	0.102 2	0.329 2	1.603 1	0.149 0	0.160 4
GRS						
Volumetric power deposition [$\mathrm{MW/m^3}$]	0.906(5)	4.45(1)	10.75(4)	5.51(9)	2.333(6)	0.714(1)
Nuclear data RSD [%]	0.113 7	0.104 2	0.324 8	1.629	0.188 4	0.140 2

3.2. Unscented Transform

Concerning the Unscented Transform method, we have considered a larger neutron population, in order to further reduce the statistical error. In fact, the fTMC and the GRS are specifically developed for Monte Carlo applications, thus they manage to provide meaningful results even with non-negligible statistical errors (indeed, they are studied in order to obtain similar results to TMC but simulating less neutron histories). On the other hand, the UT should theoretically require a null statistical error. To reduce the impact of this aspect, the total neutron population has been increased to 6×10^6, meaning 1.2×10^5 neutron histories per batch, leading to a statistical error smaller than 1 %.

At first, the UT has been applied to beryllium. Figure 3 shows the covariance matrices of the two most important cross sections of the beryllium, the elastic scattering (MT=2) and the radiative capture (MT=102), obtained with SANDY. The aim of the UT is to produce a sufficient number of sigma points generated according to Eq. 4 in order to reconstruct these matrices. Using the SVD and truncating at an energy of 99.997% (value chosen according to [18]), the resulting covariance matrices obtained using the sigma points are displayed in figure 4, showing that the pattern of the covariance has been preserved, even using only 40 singular values over 3133. Moreover, we have also numerically verified that this truncation energy

guarantees that the relative difference with respect to the original covariance matrix is smaller than 1%. For these reasons, it is possible to say that the reduced covariance matrix reconstructed from the sigma points is in good agreement with the original one. The main consequence of this truncation, considering that the reconstructed matrices are similar to the initial ones, is a dramatic reduction of the computational cost (i.e., 81 simulations instead of 6267).

The sigma points and the results for the beryllium (shown in Table V) have been obtained with $\lambda = 0.5$. This choice avoid the presence of negative weights and generates weights featured by the same value. This choice has been made to avoid the appearance of negative variances, as for the case where $n + \lambda = 3$. Further analyses are currently under way to investigate whether this is a general issue associated to negative λ values for Monte Carlo codes, or if it is due to the fact that, with $\lambda < 0$, the results with Serpent are less spread and, thus, partially blurred by the statistical error. In fact, the standard deviation of the vector of TBRs is comparable with the difference between two values of TBR obtained with two different Serpent simulation and using the nominal nuclear data. A possible solution in this sense can be to further increase the number of neutron histories with negative λ.

Another set of simulation has been performed with $\lambda = 0$: in this case the weight associated to the nominal nuclear data is 0, meaning that they are not taken into account in the UT. The results are comparable with those obtained with $\lambda = 0.5$ and with the fTMC and GRS.

Table V: Nuclear data uncertainty of ^{9}Be with UT for the TBR and the volumetric power deposition. The number in parenthesis has to be applied as a $\pm$ on the last digit of the result. (FW: first wall; VV1: inner vacuum vessel; CC: cooling channel; NM: neutron multiplier; VV2: outer vacuum vessel; BB: breeding blanket).

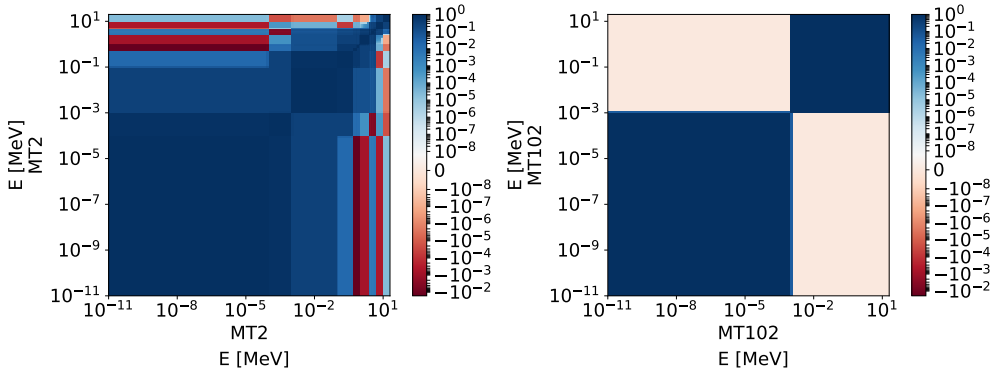
Fast Total Monte Carlo						
	FW	VV1	CC	NM	VV2	BB
Volumetric power deposition [$\mathrm{MW/m^3}$]	0.911(1)	4.46(6)	10.79(4)	5.55(9)	2.336(4)	0.714(1)
Nuclear data RSD [%]	0.1574	0.1268	0.3297	1.5916	0.1762	0.1742
TBR			1.086(3)			
Nuclear data RSD [%]			0.2689			

4. CONCLUSIONS

The results of the uncertainty quantification analysis in the ARC reactor obtained with the three methods employed in this work (fast Total Monte Carlo, GRS and Unscented Transform) are comparable in terms of nuclear data relative standard deviation. From the point of view of the computational time, the UT is the preferable choice when the number of singular values necessary to reproduce the covariance matrix is smaller than the number of simulation required for the fTMC and the GRS (generally larger than 500), as in the case of beryllium. For other nuclides, like fluorine and fissile elements, featured by many resonances, it is expected that the UT is not the most suitable choice.

The results show that the contribution of each specific nuclide is not sufficient to reduce the TBR of ARC below one. However, it is possible that the combination of the nuclear data uncertainties of all the nuclides present in ARC could lead to a TBR smaller than one.

As a future work, the UT method will be applied to fluorine too, in order to complete the present comparison. Then, a deeper investigation on the appearance of a negative variance with negative values of λ will



(a) (b)

Figure 3: Covariance matrices for elastic scattering (a, MT=2) and radiative capture (b, MT=102) for the ^{9}Be taken from ENDF-B/VIII.0 library.

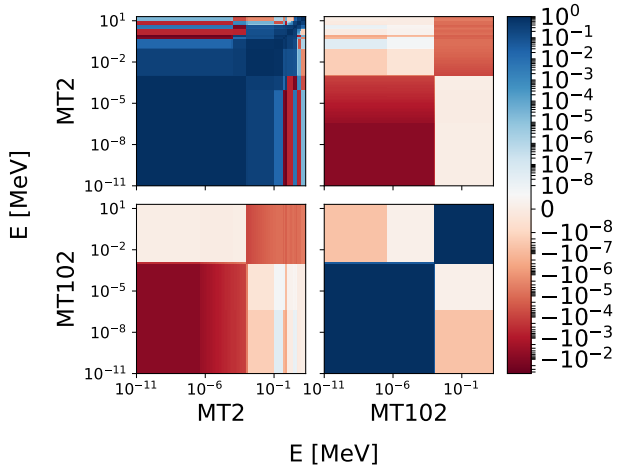


Figure 4: Covariance matrices for the ^{9}Be reconstructed from the sigma points, considering a truncation energy of 99.997%.

be carried out. Finally, the same methods are going to be adopted also for other important nuclides present in ARC, like nickel, the main component of the vacuum vessel.

- conto libreria diversa $\longrightarrow$ o intera libreria (JEFF 3.3.) oppure solo covarianza
- conto struttura energetica diversa
- sezione PCE in cui si mostrano i nodi necessari per ordini 1 e 2 (e 3)

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