# Incorporating experimental information in the TMC methodology using file weights

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Some criticism has been directed towards the Total Monte Carlo method because experimental information has not been taken into account in a statistically well-founded manner. In this work, a Bayesian calibration method is implemented by assigning weights to the random nuclear data files and the method is illustratively applied to a few applications. In most of the considered cases, the estimated nuclear data uncertainty is reduced and the central values are significantly shifted. The study suggests that the method can be applied both to estimate uncertainties in a more justified way and in the search for better central values. Some improvements are however necessary; for example, the treatment of outliers and cross-experimental correlations should be more rigorous and random files that are intended to be prior files should be generated.

## I. INTRODUCTION

Total Monte Carlo (TMC) [1, 2] is a method for propagating nuclear data (ND) uncertainties based on sampling of nuclear model parameters, *e.g.* input parameters to TALYS [3]. It is easy to implement using the publicly available random ND files from the TENDL project [2] and it has been applied to a wide range of applications, see *e.g.* Refs. [4–6]. However, since the introduction of the method, some criticism has been directed towards it because experimental data have not been taken into account in a statistically well-founded manner, see *e.g.* Ref. [7].

The inclusion of experimental information makes up a substantial part of ND evaluation and large efforts towards general methodologies has been made, see for example Refs. [7–11]. In Ref. [9], the authors present UMC-B and mention an "augmented version" of TMC, where weights and ND libraries would be combined. A similar method, UMC+TMC, is applied to prompt fission neutron spectra in Ref. [7] but details on the methodology are not provided. In this paper, it is briefly described how Bayes' theorem is implemented by assigning weights to the random ND files used in TMC, and this is used to calibrate the propagated ND uncertainties in a set of applications.

## II. METHODOLOGY

In TMC, nuclear model parameters $\mathbf{p}$ are randomly sampled a number of times, yielding $n$ random ND files which can be used in simulations to propagate uncertainties. In this work, experimental information is included by assigning each random file a weight which is proportional to the likelihood function

$$L\left(\mathbf{p}^{(k)};\mathbf{x}\right) \propto e^{-\chi_k^2/2}, \tag{1}$$

where $\mathbf{p}^{(k)}$ is the parameter set giving the $k^{\text{th}}$ random file, $\mathbf{x}$ is a vector of experimental values and

$$\chi_k^2 = \left(\mathbf{x} - \boldsymbol{\tau}\left(\mathbf{p}^{(k)}\right)\right)^{\mathrm{T}} \mathbf{C}_{\mathrm{E}}^{-1} \left(\mathbf{x} - \boldsymbol{\tau}\left(\mathbf{p}^{(k)}\right)\right), \tag{2}$$

where $\boldsymbol{\tau}\left(\mathbf{p}^{(k)}\right)$ is a vector of theoretical values found in the $k^{\text{th}}$ random file and $\mathbf{C}_{\mathrm{E}}$ is "the experimental covariance matrix".

More details on Eqs. (1) and (2) and on how to practically make use of the weights are found in Secs. II A and II B while Secs. II C and II D describe how $\mathbf{x}$ and $\mathbf{C}_{\mathrm{E}}$ are obtained from the EXFOR [12] database.

### A. Using file weights – mathematical formalism

Our nuclear model (T6 [2]) depends on a set of parameters $\mathbf{p} = (p_1, p_2, ..., p_N)^{\mathrm{T}}$. The experimental values $\mathbf{x} = (x_1, x_2, ..., x_m)^{\mathrm{T}}$ are observations of corresponding random variables $\mathbf{X} = (X_1, X_2, ..., X_m)^{\mathrm{T}}$, *i.e.* $\mathbf{X}$ has the distribution of the possible experimental outcomes. The index $m$ can span over different quantities, reaction channels, nuclides and energies. Corresponding theoretical values, $\boldsymbol{\tau}(\mathbf{p}) = (\tau_1(\mathbf{p}), \tau_2(\mathbf{p}), ..., \tau_m(\mathbf{p}))^{\mathrm{T}}$, can be computed for each $\mathbf{p}$.

If $f_0(\mathbf{p})$ is the prior probability density for the parameters, Bayes' theorem states that the probability density

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for $\mathbf{p}$ given the experimental data $\mathbf{x}$ is

$$f(\mathbf{p}|\mathbf{x}) \propto L(\mathbf{p};\mathbf{x}) f_0(\mathbf{p}), \tag{3}$$

where $L(\mathbf{p};\mathbf{x}) = f_{\mathbf{X}}(\mathbf{x}|\mathbf{p})$ is the likelihood function, *i.e.* the probability density of $\mathbf{X}$ evaluated at $\mathbf{x}$ given that $\mathbf{p}$ is the true set of parameters [13]. Assuming that $\mathbf{X}$ is multivariate Gaussian yields Eqs. (1) and (2) where $\mathbf{C}_{\mathrm{E}}$ is the covariance matrix of $\mathbf{X}$.

By sampling $\mathbf{p}^{(k)}$ from $f_0(\mathbf{p})$ for $k \in \{1, 2, ..., n\}$, it is now theoretically possible to explicitly estimate $f(\mathbf{p}|\mathbf{x})$ using Eqs. (1) and (2) in Eq. (3). Sampling from a general multivariate distribution is however computationally demanding and we suggest to instead assign weights $w_k \propto L(\mathbf{p}^{(k)}, \mathbf{x})$ to each set of parameters $\mathbf{p}^{(k)}$; in this way correlations as well as higher order moments are included without any assumption on the distribution of $f(\mathbf{p}|\mathbf{x})$. If $q$ is some integral quantity, *e.g.* $k_{\mathrm{eff}}$, it can easily be shown that

$$\widehat{q^j(\mathbf{p})} = \frac{\sum_{k=1}^{n} w_k q^j\left(\mathbf{p}^{(k)}\right)}{\sum_{k=1}^{n} w_k} \tag{4}$$

is a consistent estimate of the $j^{\mathrm{th}}$ moment of $q$ given $\mathbf{x}$. The variance of $q$ is consequently estimated by

$$\sigma^2_{\mathrm{observed}}(q) = \widehat{q^2(\mathbf{p})} - \left(\widehat{q(\mathbf{p})}\right)^2. \tag{5}$$

In this work, Monte Carlo codes are used for uncertainty propagation and therefore a part of the variance arises from code statistics. This part, $\sigma^2_{\mathrm{stat}}$, can be estimated either using the Monte Carlo codes' uncertainty estimates or by performing another TMC-run with fixed nuclear data [14]. As in Refs. [4, 14], the standard deviation due to nuclear data can be estimated using

$$\sigma_{\mathrm{ND}}(q) = \sqrt{\sigma^2_{\mathrm{observed}}(q) - \sigma^2_{\mathrm{stat}}(q)}. \tag{6}$$

The uncertainty of the uncertainty is estimated by repeatedly dividing the files into two sets as described in Ref. [4]. This estimate should be interpreted with care if the average file weight $\overline{w} \ll 1$, since the derivation assumes $n \gg 1$.

In practice, a prior distribution $f_0(\mathbf{p})$ completely disregarding experimental information is hard to imagine. A practical solution to this is to use a prior distribution which covers all reasonable values in such a way that a modification of the prior has insignificant impact. In this first study, available random files from the TENDL project [2] were used for practical reasons. These are not intended to be "prior files" but rather to quantify the uncertainty *including* the experimental information. This is undesired since the same experimental information is used twice and the results should be interpreted with this in mind. Moreover, the random files do not represent the physics as well as desired for some reaction channels in some energy zones and therefore, some such zones are discarded as described in Sec. II D.

### B. Russian Roulette (RuR)

A downside with the use of file weighting to propagate uncertainties is that time-consuming simulations of the considered system will be performed for $\mathbf{p}^{(k)}$ although $w_k \ll 1$. A way to reduce this problem is to randomly discard files with a survival probability proportional to $w_k$, similar to the Russian Roulette used in non-analogue Monte Carlo transport codes [15]. There are several ways to perform this in a correct way; here, a simple method ensuring that all surviving files obtain the same weight is used:

For each file, generate a random number $u$ from a uniform distribution on $[0, 1]$ and

**if** $w_k < u \cdot \max(w_k)$, set $w_k = 0$ (the file is discarded),
**otherwise**, set $w_k = \max(w_k)$ (the file survives).

### C. Interpreting the EXFOR database

In this study, experimental cross section data from the EXFOR database [12] in both `x4` and `c4` format has been used. As of today, estimates of experimental covariance matrices are rarely available in EXFOR [16], and the *full* experimental covariance matrix $\mathbf{C}_{\mathrm{E}}$ (*i.e.* including cross-experimental correlations) is certainly not available. However, in the `x4` format the uncertainties are often divided into statistical and systematic parts which can be used in a simplified construction of $\mathbf{C}_{\mathrm{E}}$. Preliminarily, it is done according to the following scheme (each EXFOR *entry* is considered an experiment):

1. Experiments with a root-mean-square uncertainty of less than 0.1 % are considered unrealistic and are discarded.

2. If only one uncertainty estimate is given for each experimental point, the point is assigned with both a statistical and a systematic uncertainty of this magnitude. Otherwise, uncertainties denoted `ERR-S` are interpreted as statistical and all others are considered systematic. In this way, experiments with a less rigorous uncertainty treatment are conservatively penalized. If no uncertainty denoted `ERR-S` is found, the uncertainty according to the `c4` format is used as statistical.

3. Each systematic uncertainty is assumed to be fully correlated for the whole experiment, however uncorrelated to other systematic uncertainties. The statistical uncertainties are considered uncorrelated.

4. The energy resolution $\Delta E$ is obtained from the `c4` format and is "translated" into an additional statistical variance in $X$ according to

$$V_{\Delta E}(X) = (\Delta E)^2 \overline{\int f_E(E) \left(\frac{\mathrm{d}\tau(E;\mathbf{p})}{\mathrm{d}E}\right)^2 \mathrm{d}E}, \tag{7}$$

where $f_E$ is an assumed Gaussian probability density function for $E$ with a variance of $(\Delta E)^2$ about the experiment's central value $\langle E \rangle$, $\tau(E;\mathbf{p})$ is the theoretical values at $E$ using parameter set $\mathbf{p}$ and the mean is taken

over the $\mathbf{p}^{(k)}$. The expression is based on linear uncertainty propagation [13] but estimating the expected value of the squared derivative instead of evaluating it at $\langle E \rangle$. If no $\Delta E$ is given, the experiment is penalized with a 10 % energy resolution before Eq. (7) is applied.

5. If the total systematic uncertainty is less than 5 % (relative to the average *theoretical* value), it is increased until this value is reached. The same procedure but with 10 % is used for the statistical uncertainty.

6. Extra uncertainties of 5 mb are added to both the systematic and statistical uncertainty for each experimental point as well as an extra statistical uncertainty of 20 % relative to the statistical uncertainty and an extra systematic uncertainty of 0.5 % relative to the average theoretical value. These additions are due to a belief that experimental uncertainties often are underestimated, *e.g.* only counting statistics may be reported. Also, adding an absolute uncertainty decreases the importance of smaller cross sections.

7. An uncertainty of 1 % which is fully correlated for all experimental points within the same reaction channel is used. This is a temporary attempt to take cross-experimental correlations, arising from *e.g.* relative measurements, into account.

### D. Treating outliers and discarding energy zones

A simplified treatment of outliers is used in this study, and it should be replaced with more sophisticated techniques in future studies. For the $j^{\text{th}}$ experiment, $\chi^2_{j,\text{central}}$ is computed for the average theoretical values according to Eq. (2), giving an estimate of a $p$-value according to

$$P_{1,j} = 1 - F_{\chi^2(m_j)}\left(\chi^2_{j,\text{central}}\right), \tag{8}$$

where $m_j$ is the number of experimental points in experiment $j$ and $F_{\chi^2(m_j)}$ is the distribution function for a $\chi^2$-distributed random variable with $m_j$ degrees of freedom. Finally, if $P_{1,j} < 5\,\%$, experiment $j$ is discarded.

Independently of the outlier treatment, the experiments are also divided into a number of energy zones (details in Sec. III). A common $p$-value $P_{1,\ell r}$ is then computed for the experimental points in each energy zone $\ell$ and reaction channel $r$ according to Eq. (8). Moreover, another $p$-value $P_{2,\ell r}$ is computed as the $p$-value assuming that the probability for each experiment to exceed the theoretical prediction is 1/2. One $P_{2,\ell r}$-value is obtained for each random file, and the least of the top 5 % is used, $P^{5\,\%}_{2,\ell r}$. Finally, all experiments in the zone are discarded if $\min(P_{1,\ell r}, P^{5\,\%}_{2,\ell r}) < 2.5\,\%$ for reasons discussed at the end of Sec. II A. In this way, the two $p$-values are conservatively combined using Bonferroni's procedure [17] and applied with a significance level of 5 %.

The computation of $P_{2,\ell r}$ neglects knowledge of correlated uncertainties and should be avoided in future studies; in fact, the rejection of energy zones should be abandoned as more purposive random files are generated and a more sophisticated treatment of outliers is applied.

## III. STUDIED APPLICATIONS

Files with transport and activation data for $^{235}$U, $^{239}$Pu and $^{56}$Fe from the TENDL random files have been calibrated according to Sec. II using the (n,tot), (n,el), (n,2n), (n,f) and (n,$\gamma$) cross sections, and the uncertainties have been propagated through a few examples of applications:

- Data for $^{235}$U in a PWR pin cell with $UO_2$ fuel modeled in Serpent [18] as in Ref. [4], with burnup up to 61 MWd/kgU. The results are only reported at the End Of Life (EOL).
- $^{239}$Pu data in the conceptual reactor ELECTRA (European LEad Cooled Training ReActor) modeled in Serpent [18] as in Ref. [5, 19].
- $^{56}$Fe data in a computation of the dose rate from a 14 MeV neutron source shielded with iron-rich concrete modeled in MCNPX [15] as in Ref. [6]. The modeled shielding is part of a Uppsala Univeristy facility named FREIA, a name which is referred to in the following.

$^{235}$U and $^{239}$Pu have been calibrated using experiments with neutron energies $E < 5$ eV (referred to as "thermal" or "Th.") and $E \geq 1$ MeV (referred to as "fast"), while only experiments with $E \geq 1$ MeV have been used for $^{56}$Fe. The two energy regions are studied separately. For the discarding of energy zones (see Sec. II D), the thermal region has zone limits at 0.1 and 1 eV and the fast region at 5 and 10 MeV. For the calibration, the theoretical values are obtained from linear interpolation between energy grid points in `ace`-files processed for 300 K using NJOY [20], while other processing temperatures are used in the applications when applicable.

## IV. RESULTS

### A. Surviving experiments and weight distribution

TABLE I. *Above*: Number of experimental points within each energy region before (total) and after rejecting outliers (−outliers) and energy zones (final). *Below*: the distribution of the file weights summarized as the fraction (%) of weights greater than or equal to 1 %, 10 % and 50 %, respectively.

| | | $E < 5$ eV | | $E \in [1, 20)$ MeV | | |
|---|---|---|---|---|---|---|
| | | $^{239}$Pu | $^{235}$U | $^{239}$Pu | $^{235}$U | $^{56}$Fe |
| | total | 5252 | 9636 | 2850 | 4370 | 6390 |
| | −outliers | 3689 | 9636 | 2817 | 4370 | 6387 |
| | final | 2075 | 5251 | 784 | 1838 | 1080 |
| Fraction [%] of $w_k$ | $\geq 1\,\%$ | 3.1 | 29 | 55 | 7.6 | 100 |
| | $\geq 10\,\%$ | 1.5 | 13 | 11 | 1.2 | 95 |
| | $\geq 50\,\%$ | 0.59 | 2.8 | 0.44 | 0.27 | 24 |
| Average weight $\overline{w}$ [%] | | 0.75 | 4.7 | 3.9 | 0.72 | 37 |

For the studied nuclides, the upper part of Tab. I views the number of experimental points that are treated at all, *i.e.* that survive step 1 in Sec. II C, as well as how many files that survive the rejection of outliers and of energy zones according to Sec. II D. Relatively few experimen-

tal points are rejected as outliers while about half of the points or more are discarded in the rejection of energy zones. The rejected zones are listed in Tab. II.

The distributions for the weights obtained according to Sec. II A (normalized such that $\max(w_i) = 1$) are briefly summarized in the second part of Tab. I. For $^{239}$Pu and $^{235}$U, most files get low weights – the average weights are on the order of percent and a few or several percent have weights greater than 10 %. For $^{56}$Fe, the weights are considerably greater – this is also the case with the highest fraction of rejected experimental points.

TABLE II. Energy zones rejected according to Sec. II D.

| | $^{239}$Pu | $^{235}$U | $^{56}$Fe |
|---|---|---|---|
| (n,tot) | [0.1, 5) eV<br>[1, 10) MeV | [0, 0.1) eV<br>[1, 5) MeV | [1, 5) MeV<br>[10, 20) MeV |
| (n,el) | - | [0.1, 1) eV<br>[1, 5) MeV | - |
| (n,2n) | [5, 10) MeV | - | [10, 20) MeV |
| (n,f) | [0, 0.1) eV | [0, 1) eV | - |
| (n,$\gamma$) | [0, 0.1) eV<br>[1, 5) MeV | [1, 5) MeV | [10, 20) MeV |

### B. Propagated to applications

Tab. III summarizes the impact of the calibration on the nuclear data (ND) uncertainty and central values of the applications briefly described in Sec. III. Values without the use of weights are compared to values using weights from experiments in the fast and thermal regions, respectively, with and without the use of RuR (see Sec. II B). The central values are also compared to what is obtained using more established ND libraries.

Considering the results without the use of RuR, the weighting gives at least somewhat significant shifts in the central values in all cases, and the ND uncertainty is significantly reduced in all cases but for FREIA; the greatest difference is however seen for the central values. The most significant shift in the central value is obtained for the PWR with weights for $^{235}$U obtained using thermal region experiments and this case is illustrated in Fig. 1. As can be seen, the files resulting in a low $k_\infty$ are consistently given a very low weight and vice versa. It can be interesting to note that in this case, the weighted central value is much closer to the value using the more established ND library JEFF 3.1. This also holds for ELECTRA, but the shift is far less significant. For FREIA, the weighted central value is further from the value obtained using ENDF.B-VI.1 – both the unweighted and weighted results are however substantially different from the result using ENDF.B-VI.1. The barely significant shifts using fast region experiments for the PWR also result in values further away from the results using JEFF 3.1.

The results using RuR are consistent with the results not using RuR – the only difference is that the uncertainties, both on the central values and on the ND uncertainty, typically are greater with RuR which is expected since less information is used. However, much less simulations are performed as seen in the second last column of the table.

Some precision is lost for the weighted results, both for the ND uncertainty and on the central values. This is also expected since the weights effectively yield less random files.

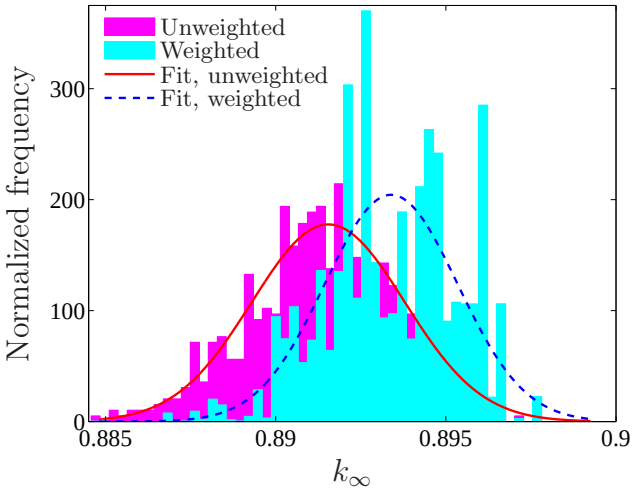


FIG. 1. The distribution of $k_\infty$ for the PWR pin cell at EOL varying $^{235}$U using weights from experiments with $E < 5$ eV.

## V. DISCUSSION

As noted already in Sec. II A, the used random files are not intended to be prior files, implying that all results should be interpreted with care; the reduction of uncertainties can possibly be unjustified since more likely regions of the parameter space may be uncovered. For example, one may query what the effect would be if there were random files resulting in greater $k_\infty$-values for the PWR pin cell, see Fig. 1; perhaps the ND uncertainty would be *increased* and the central value even more shifted. Also, a lot of experimental information was disregarded because the theoretical values did not agree well with these experiments. This is an undesired approach since it suffers the risk of confirming erroneous parameters in a self-fulfilling way. Instead, the distribution of the prior random files should be adjusted to cover these experiments better.

To use a default uncertainty to include cross-experimental correlations is clearly rather arbitrary and, as has been noted by several authors before [7, 10], the assessment of proper experimental covariances including cross-experimental dependencies is of high importance.

Generally, the rules for the construction of experimental covariance matrices in Sec. II C can be discussed but the rules are transparent, easy to overview and with an attempt to make conservative assumptions when necessary. There are other alternatives as for example the EXFOR web tool [21]; this however includes arbitrary choices

TABLE III. Central values and propagated nuclear data uncertainties using Eq. (6) with or without different weights or using Russian Roulette (RuR). The central values are also compared to values obtained with more established libraries ("J3.1/E.B-VI.1", JEFF 3.1 for the former two and ENDF-B.VI.1 for FREIA) and their uncertainties refer to those of the mean. The fraction of files surviving the RuR is also included (RuR surv/tot) as well as the expected number of surviving files (RuR $\langle$surv$\rangle$).

| | Varied data | Exp. energies | Central values Unw. | Weighted | RuR | J3.1/E.B-VI.1 | ND uncertainty $\sigma_{\text{ND}}$ [%] Unw. | Weighted | RuR | RuR surv/tot | RuR $\langle$surv$\rangle$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| PWR at EOL, $k_\infty$ | $^{235}$U | Th. | 0.8913(1) | 0.8934(2) | 0.8939(3) | 0.8949(2) | 0.28(2) | 0.20(1) | 0.19(2) | 32/739 | 35 |
| | | Fast | | 0.8905(5) | 0.8915(9) | | | 0.19(4) | 0.24(6) | 6/739 | 5.3 |
| ELECTRA, $k_{\text{eff}}$ | $^{239}$Pu | Fast | 1.0010(3) | 0.9998(6) | 1.000(1) | 1.00006(7) | 0.74(2) | 0.67(3) | 0.66(7) | 25/683 | 26 |
| FREIA, dose [pSv/n] | $^{56}$Fe | Fast | 1.221(2) | 1.208(3) | 1.209(4) | 1.362(4) | 4.3(4) | 4.3(4) | 4.5(7) | 324/896 | 329 |

as well, for instance the correlation length. Hopefully, experimenters and EXFOR compilers will start to provide carefully evaluated experimental covariance matrices.

In principle, more experimental information and several nuclides could be treated simultaneously. Given experimental information which is detailed enough, this gives the possibility to properly include cross-nuclide correlations but it will also give rise to larger experimental covariance matrices $\mathbf{C}_{\text{E}}$. In the case that the matrices become so large that the matrix inversion necessary for Eq. (2) becomes problematic, *sampling of systematic errors* may be an option. This has been implemented by the authors and gives results that are consistent with those obtained with matrix inversion but the method is less efficient for the matrix dimensions in this study.

Experiments in the resonance region are left out in this study since resonance parameters are given for each resonance, meaning that it becomes inefficient to assign weights to complete files based on resonance data. To infer differential experimental information from the resonance region into the TENDL random files will thus need some special treatment. This is however of high importance since the resonance parameters seem to dominate the propagated uncertainty in some applications [22].

Differential experiments are used in this work but the method could equally well be applied using integral experiments, or a combination of both. This could also give an alternative treatment of the resonance region, giving a distribution of parameters well describing the "overall behavior" of the resonance region without really covering the parameter space.

Any effects of model defects, *i.e.* that the physical models are imperfect irrespective of the parameters, are disregarded in this work. The impact of this simplification should be subject to future studies and it can possibly be treated, *e.g.* along the lines suggested in Ref. [23].

## VI. CONCLUSIONS

The suggested technique of calibrating nuclear model parameters by assigning weights to random nuclear data files has been seen to be practically feasible and to have impact on a number of applications, both with respect to propagated nuclear data uncertainty and, more significantly, on the central values. The method is founded on well established mathematics and a limited set of assumptions, giving it potential for reliable, transparent and reproducible results. Before achieving this goal some improvements are necessary, *e.g.* more purposive prior files, a more rigorous treatment of outliers and better motivated cross-experimental correlations.


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