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Nuclear data uncertainties and adjustments using deterministic and Monte-Carlo methods along with PWR measurements

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ABSTRACT

Nuclear power plants safety relies partly on predictions from numerical simulations. Their uncertainties must therefore be evaluated. In PWR reactor physics, the simulations' uncertainties are nowadays estimated on the basis of the differences between existing measurements and the corresponding simulations. This approach leads to weaknesses in the estimation of uncertainties. For example, a novelty can induce more deviations than those seen in the past. Moreover, in some (common) cases, these uncertainties are based on differences between measurements and *adjusted* simulations, i.e. carried out *after* the measurements and by *forcing* the simulations as close as possible to the measurements. The residual deviation thus leads to consider compressed uncertainties. This method of evaluating uncertainties can therefore be improved. To further increase robustness, the approach proposed in a recently published Ph.D. thesis is to return to the fundamentals : the sources of errors in the simulations. The two main types discussed in this paper are the following. On the one hand, physical and numerical approximations introduce deterministic biases, which can be evaluated as the difference with Monte-Carlo. On the other hand, the nuclear data uncertainties, that arise from the limited human understanding of nuclear physics, are propagated in this article with a Total Monte-Carlo approach.

KEYWORDS: Total Monte-Carlo, BFMC adjustment

1. DETERMINISTIC SIMULATIONS AND THEIR BIASES

For the purpose of this demonstration, we developed DRAKKAR, a deterministic calculation scheme covering from nuclear data processing up to 3D diffusion. It was designed to be representative of standard industrial schemes, but open source [1] and provided to the research community for further scientific advances. It is built around DRAGON5, TRIVAC5 and DONJON5 codes ; its main characteristics are the following [2].

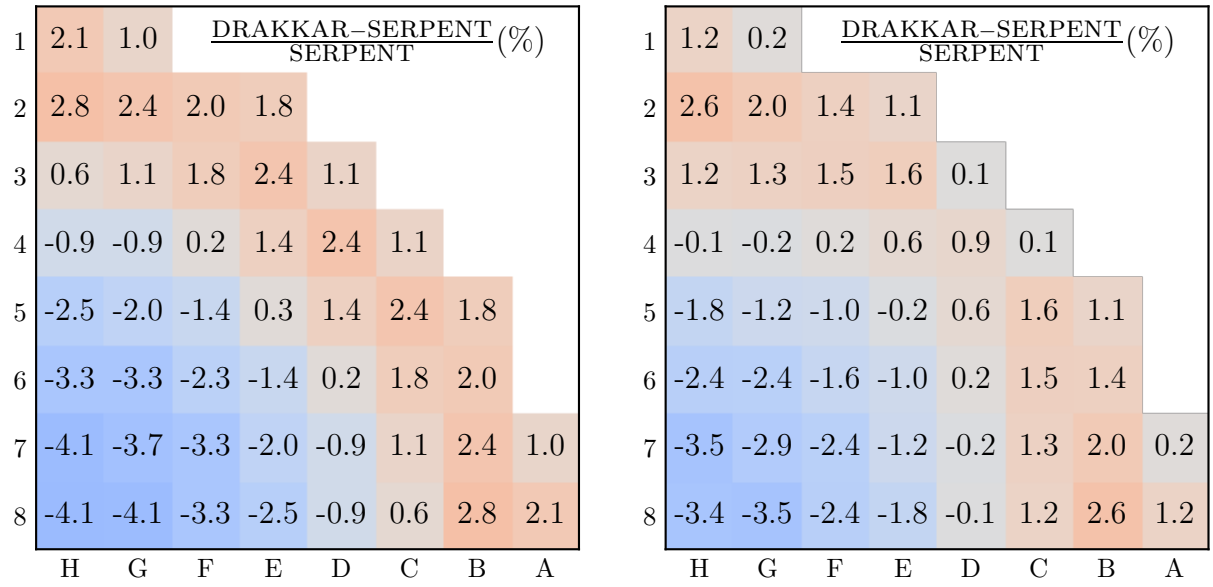
— A 295-groups cross section library is produced from the selected nuclear data with PyNjoy2016 [3].

— To account for the skin effects, the fuel and AIC absorbing rods are divided into four rings [4].

— $^{235,238}\mathrm{U}$, $^{107,109}\mathrm{Ag}$ and $^{90,91,92,94,96}\mathrm{Zr}$ are self-shielded with a subgroub method [5]. It relies on probability tables that are mathematical [6] from 4.63 eV to 11.1 keV and physical beyond [5]. Only $^{238}\mathrm{U}$ is self-shielded in a spatially-differentiated manner, on the same four rings.

— After transport correction, the neutron transport equation is solved with an interface current first collision probability (P_{ij}) method, considering a linearly anisotropic current (UP1) at the cell interfaces [2].

— The leakage is modeled according to the fundamental mode approximation, with a homogeneous B_1 model. The leakage rates are reincluded in the heterogeneous transport with the Diffon method [2].



(a) First start-up of Tihange-1 [9], all rods out.

(b) First start-ups of Bugey-2, Fessenheim-1 and 2 [10], all rods out.

FIGURE 1 – Relative differences in power distributions between (deterministic) DRAKKAR and (Monte-Carlo) SERPENT2.1.32. Available plotting instructions [11,12], relying on serpentTools [13].

— A two-group condensation is followed by an SPH equivalence with Selengut [2] normalization. For this, the fluxes at the assembly edge are obtained from the outgoing currents of the assembly.

— A heterogeneous 1D reflector model (from the core center to the vessel) is solved in S_{16}. Then, the equivalent homogeneous reflector is determined with the Lefebvre-Lebigot method [7].

— The 3D full core two-group diffusion is solved by a Raviart-Thomas quadratic superconvergent finite elements method. The assemblies are divided into four (two by two) radial meshes and 50 axial meshes.

A few first PWR start-ups were calculated with JEFF-3.3 and this calculation scheme. The difference with Monte-Carlo, shown on Figure 1, corresponds to its deterministic bias, reaching 4% on assembly power. Note that the nuclear data processing are highly consistent between deterministic and Monte-Carlo route – see the companion paper [3] – so that the only difference is the deterministic bias. Also, the assembly power Monte-Carlo 1σ statistical standard errors have been estimated [8] to 0.16% (at most), with 50 independent simulations from different random seeds, each with 100 000 neutrons per generation, 1 200 generations and 200 inactive ones. These high numbers are selected to avoid a statistical bias in the Monte-Carlo results.

2. A REFERENCE PROPAGATION OF NUCLEAR DATA UNCERTAINTIES

In the previous section, only the best estimate of the nuclear data is considered. In this case, an obtained power distribution is also the best estimate. However, a robust nuclear safety approach considers the envelope case, within the estimated uncertainty. This envelope case rarely coincides with the best estimate.

Here, the nuclear data uncertainties, stemming from nuclear physics, are propagated with a reference method, the Total Monte-Carlo method [15], through reactor physics simulations. A sampling of hydrogen nuclear data within its uncertainties [3], through the deterministic calculation scheme described in the previous section, produces a probability distribution for the power of each assembly, shown in blue in Figure 2. From the previous section, we know that this probability density is affected by the deterministic bias. For example, for the central assembly, the best estimate is shifted by -4% (see Figure 1, bottom left corner). But beyond this expected shift, it is interesting to investigate whether this distribution is also distorted by the deterministic bias. To this purpose, the same exercise was conducted in Monte-Carlo (orange in Figure 2). It can be observed that both deterministic and Monte-Carlo lead to the same standard deviations (i.e. to the same nuclear data uncertainty). A Kolmogorov-Smirnov statistic confirms that the two distributions are similar, *not* distorted. Therefore, the deterministic bias can be considered constant for variations in

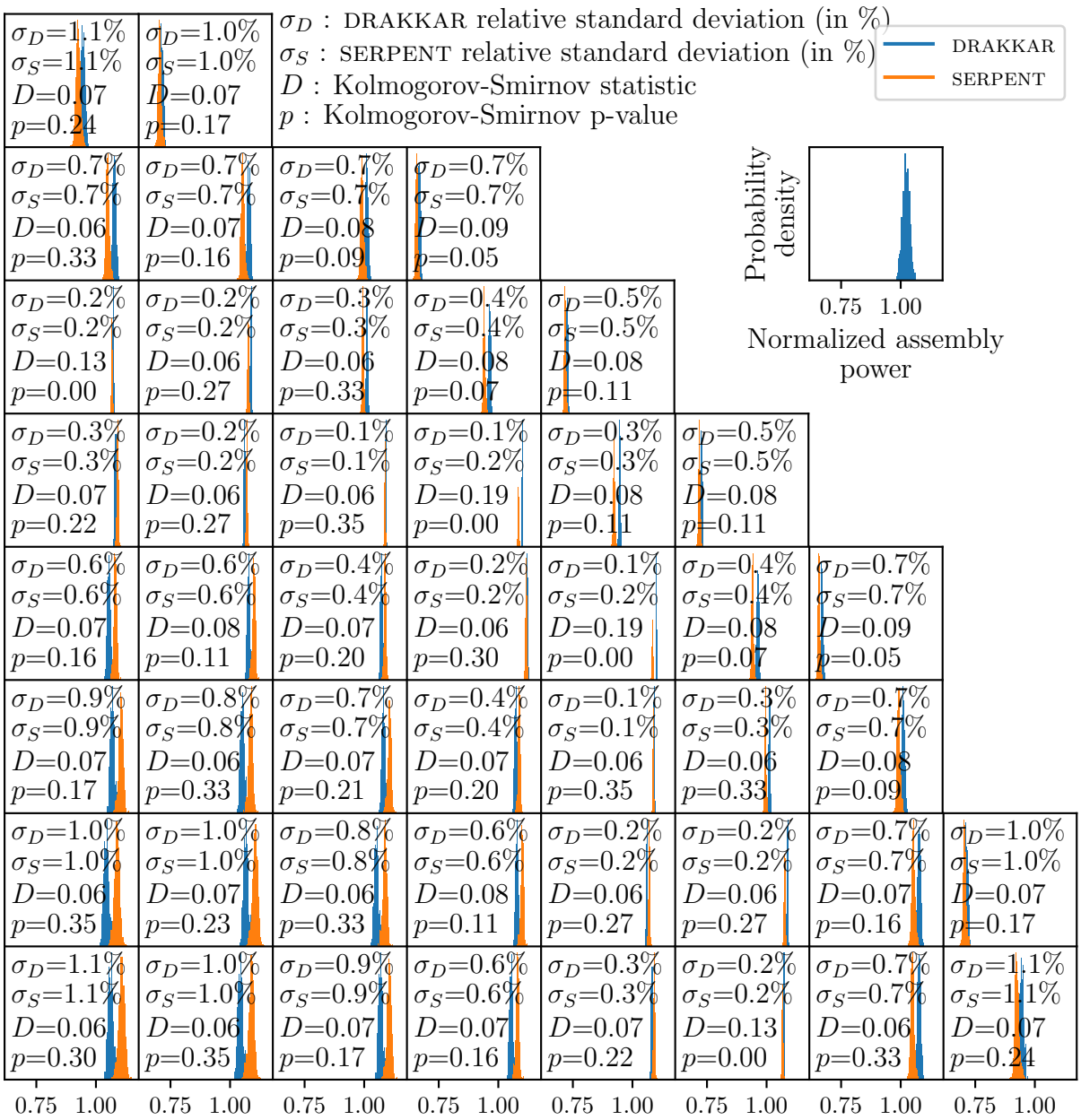


FIGURE 2 – Probability density of the assembly power, with (deterministic) DRAKKAR, SERPENT and the best estimate of JEFF-3.3, except for hydrogen bound to light water (300 samples in JEFF-3.3, sampled with SANDY code) on the first start-up of Tihange-1 [9]. Each nuclear data sample is simulated 4 times (with 4 different random seeds), 200 000 neutrons per generation, 2 000 active generations and 100 inactive ones. Plotting instruction are available [14].

nuclear data typically corresponding to their uncertainties. Although seemingly insignificant, this excellent agreement opens new perspectives. Indeed, all the different samples of nuclear data can be propagated with approximate deterministic methods, and then corrected at once with one single reference solution; graphically, as a translation of the deterministic peak on the Monte-Carlo best estimate. This original dual approach allows to benefit from the *best of both worlds* :

— The Monte-Carlo method is the preferred choice for computing an unbiased response, which is perfect for the mean (i.e. best estimate). But for higher orders, it is very much affected by statistical noise; higher orders are much harder to converge and often unreachable.

— Conversely, deterministic methods are systematically biased, providing a biased mean, which cannot be taken for granted. But this deterministic bias being almost identical for adjacent cases, the nuclear data uncertainty becomes accessible for a low computational cost for any moment order (starting with the standard deviation). Deterministic methods excel in their absence of statistical noise.

This very central discovery, which has been checked [1,8] on many isotopes (^{235,238}U, ^{1}H, ^{56}Fe, ^{16}O, ^{90}Zr and ^{107}Ag) in many control rod insertions, will find particular applications in the remainder of this work.

3. RANKING OF NUCLEAR DATA UNCERTAINTIES

Since the propagated uncertainties are identical between the Monte-Carlo and deterministic methods, it becomes possible to explore a much larger space with the inexpensive deterministic methods, while maintaining good confidence in the result. On this basis, a ranking of nuclear data uncertainties is proposed on Figure 3. The top three is occupied by uranium 238, hydrogen and iron 56, with an impact that remarkably does not vary according to the control rod insertion for iron 56 only. The omnipresent oxygen 16, the fissile uranium 235 and the transparent zirconium 90 are relegated further down, together in a surprising group. This time, only uranium 235 is not sensitive to the control rod insertion.

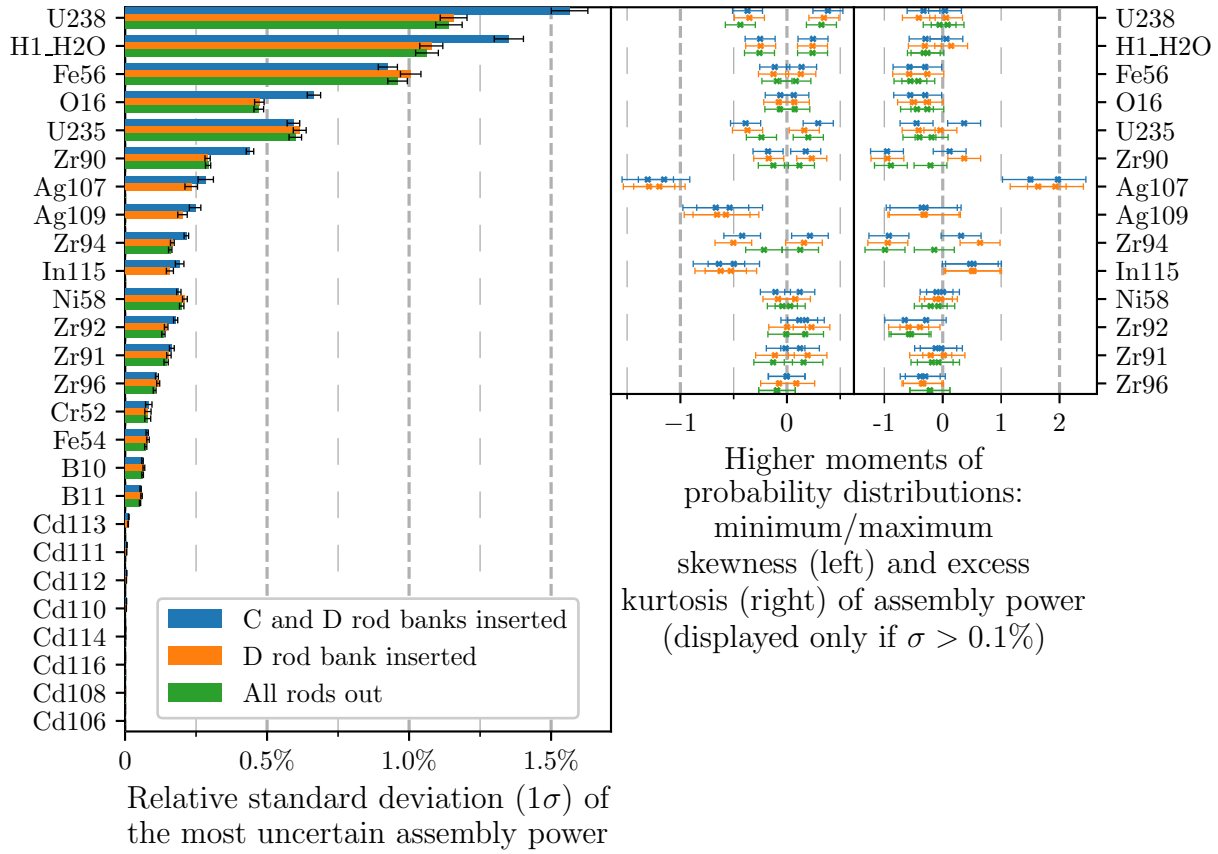


FIGURE 3 – Ranking of nuclear data uncertainties computed with DRAKKAR on the first start-up of Tihange-1 [9]. Generally, the assembly with the most uncertain power (left frame) is located in the core periphery or in the core center, sometimes equally (see Figure 2). All error bars correspond to statistical standard errors (1σ). TENDL-2019 continuous uncertainties are used in most cases. When TENDL does not provide uncertainties, JEFF-3.3 covariance matrices are used instead.

4. A BALANCED, BAYESIAN NUCLEAR DATA ADJUSTEMENT ON MEASUREMENTS

It is legitimate to consider that simulations should reproduce trusted experimental measurements. However, the D_1 reflector adjustment, standard in France [10,16,17,18], is based on fragile foundations, i.e. on compensations between errors of different natures (various detetermistic biases, nuclear data errors...). Consequently, these compensations are not universal, as pointed out by Muller [19]. Extrapolation is therefore

not ideal, either for introducing industrial innovations or for accident simulations. Moreover, these standard adjustments do not assess uncertainties ; the question of uncertainties is absent in these adjustments.

In order to address these two issues, we rely on a more complete paradigm. All nuclear data uncertainties are propagated with deterministic methods, but eliminating the deterministic bias (see Figure 1b and section 2). Afterwards, the BFMC method [20] is brought to bear, as illustred on Figure 4. Among the plausible nuclear data, a sample k in better agreement with PWR detector measurements [10], i.e. with a low [20]

$$\chi_k^2 = \sum_{i=1}^{n_{\text{exp}}} \frac{(C_{i,k} - E_i)^2}{\sigma_{E_i}^2} \tag{1}$$

is considered more likely and attributed a higher weight [21]

$$w_k \propto \exp\left(-\chi_k^2/\chi_{\text{min}}^2\right). \tag{2}$$

Figures 5 and 6 show that the nuclear data uncertainties are reduced in a balanced way, from 1.8% to 1.3% in maximum uncertainty of detector response. As can be seen in figure 7 for the most affected isotope, no signs of overfitting appear : the adjustment is very moderate, appearing even small compared to the reduction of the detector response uncertainty. The apparition of correlations between the 26 present isotopes, illustrated in figure 8, contributes to reduce efficiently the uncertainty on the detector responses, without affecting the uncertainties of each isotope to any great extent. New correlations are normal and even desirable, because the contribution of the different isotopes cannot be separated in an integral experiment. Moreover, on figure 7, the uncertainty is reduced on only one side, discarding the side less in agreement with the experiment, which is also desirable. Finally, this adjustment does not rely on experimental power distributions [9], as those are actually not measured but *inferred* from experiments using biased deterministic methods. Instead, as recommended by Askew [22], it relies on *measured* detector responses [10].

5. CONCLUSION

Nuclear data uncertainties have been propagated with the reference Total Monte-Carlo method. This technique proves to be industrializable as it is. Moreover, uncertainty propagations have been performed through standard deterministic methods, affected by deterministic biases, and with Monte-Carlo transport. Comparison of the two led to this central finding : for variations in nuclear data typically corresponding to their uncertainties, the deterministic biases can be considered constant, i.e. identical between different samples. Although seemingly insignificant, this excellent agreement brings the evaluation of all sources of errors within reach. Indeed, the different samples of nuclear data can be propagated with approximate methods, and then corrected at once with a single reference solution. This dual approach benefits from the best of both deterministic and Monte-Carlo worlds, by retaining the order moments on which each excels.

Beyond this first theme concerning the propagation of uncertainties, a second theme – closely related – is covered : adjustments to measurements. It is legitimate to consider that simulations should reproduce measurements performed experimentally on real PWR reactors. However, the most common adjustment methods are based on non-universal error compensations, which affects their extrapolation capabilities. Moreover, the question of uncertainties is absent in these adjustments. These two issues are addressed with nuclear data uncertainty propagation, elimination of the deterministic bias and the BFMC method. Among the plausible nuclear data, those in better agreement with experimental measurements are considered most likely. The nuclear data uncertainties are reduced in a balanced way, without showing signs of overfitting.

By mobilizing a physical and universal knowledge of the root causes of errors (nuclear data, deterministic bias), the ensemble of methods exploited in this work [8] present strong arguments, that can claim a better extrapolation capability than standard methods of uncertainty evaluation and adjustment, thus improving nuclear power plants safety.

Furthermore, this research leads to the following three recommendations :

(1) to renounce deriving, from measurements, non-measurable quantities (such as assembly power) when comparing simulations and measurements, but rather to directly simulate and compare the quantities actually measured by the detectors [22] ;

(2) to systematically evaluate the technological and measurement uncertainties affecting power nuclear reactor cores, with particular attention to their very first start-ups ;

(3) to carry out a decennial reassessment of the simulations' uncertainties, similar to the French periodic (decennial) reviews of nuclear installations, to account for the evolution of knowledge, as also done for public health and environmental hazards.

Finally, this work is carried out with particular attention to its reproducibility, by providing openly the software developed and the data produced [1]. The data release includes plotting instructions, DRAGLIB and ACE libraries, DRAKKAR and SERPENT inputs and outputs.

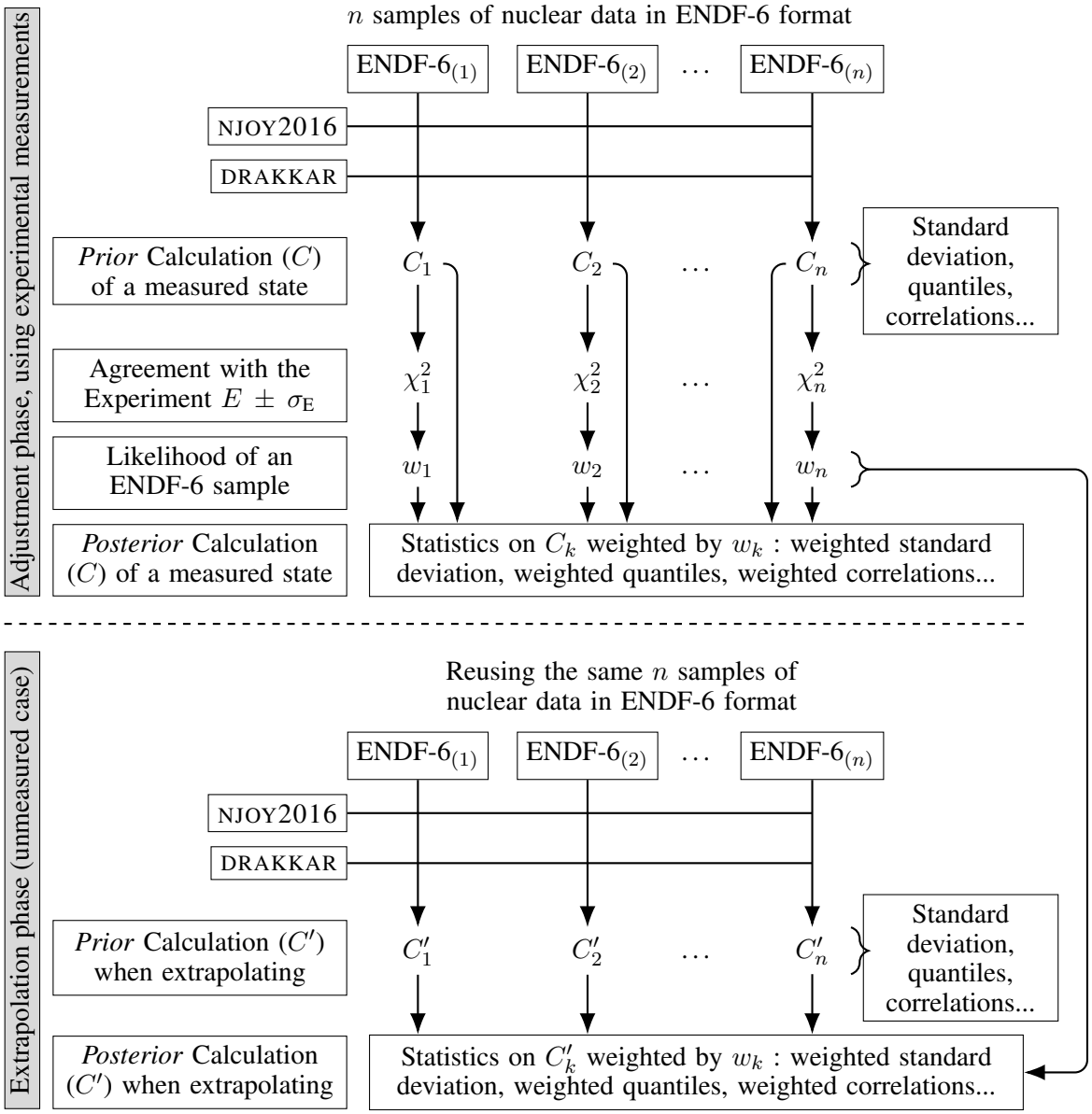


FIGURE 4 – Data flow of the BFMC method (also applicable to the BMC method [23]), from adjustment to extrapolation. This scheme is simplified : the removal of deterministic biases with SERPENT is not shown. C_k and E must correspond to the same type of data (here, a detector response), but C'_k can be a very different computational output (the power of an assembly…). Similarly, the codes used for the adjustment and for the extrapolation can be identical, as in this diagram, or very different (deterministic and Monte-Carlo, for example), provided that their biases are negligible.

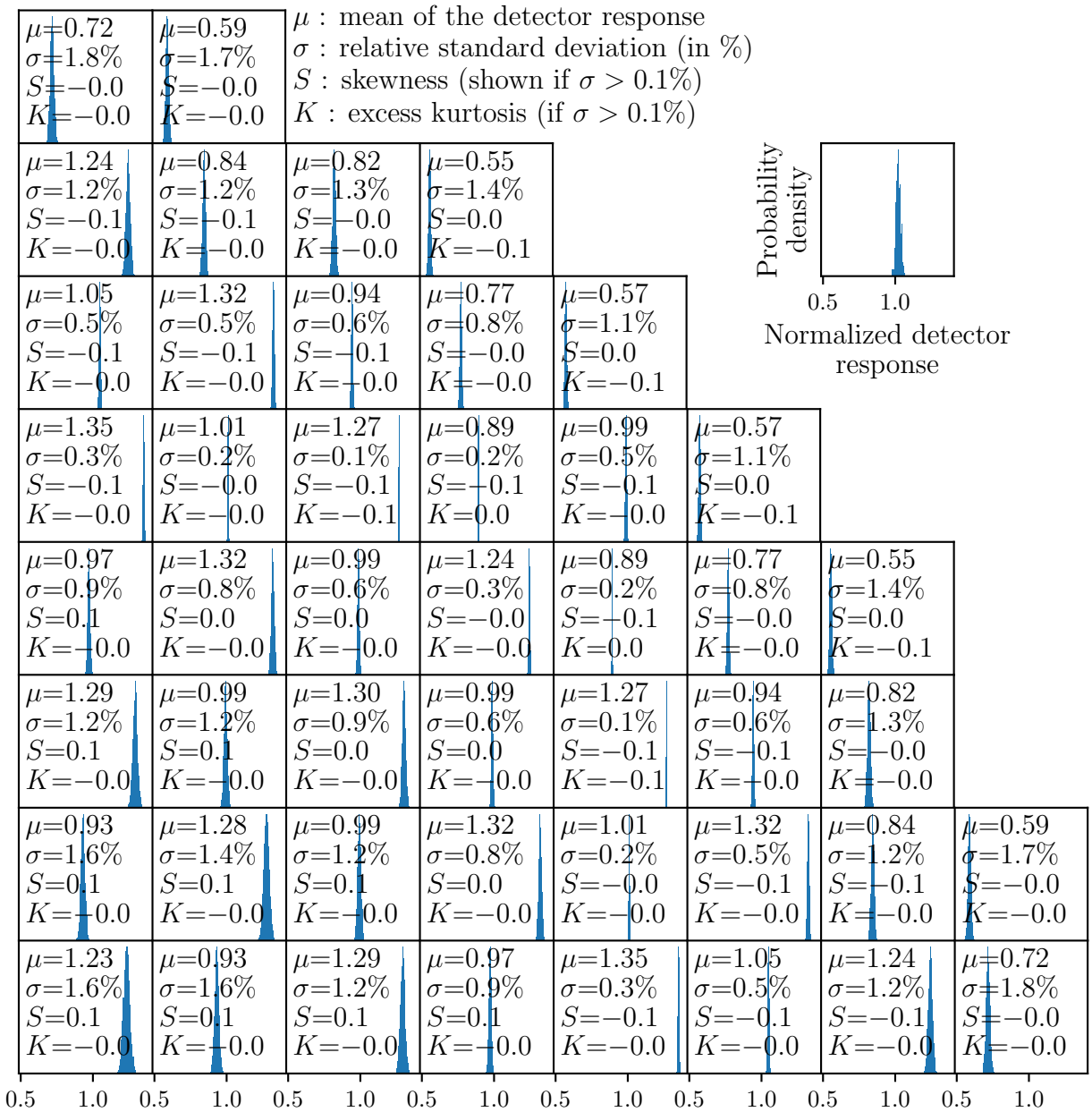


FIGURE 5 – Prior probability density of the detector responses, with SERPENT (mean) and DRAKKAR (higher order moments) for nuclear data sampled simultaneously for all isotopes, on the first start-up of Bugey-2, Fessenheim-1 and 2. Plotting instructions are available [24].

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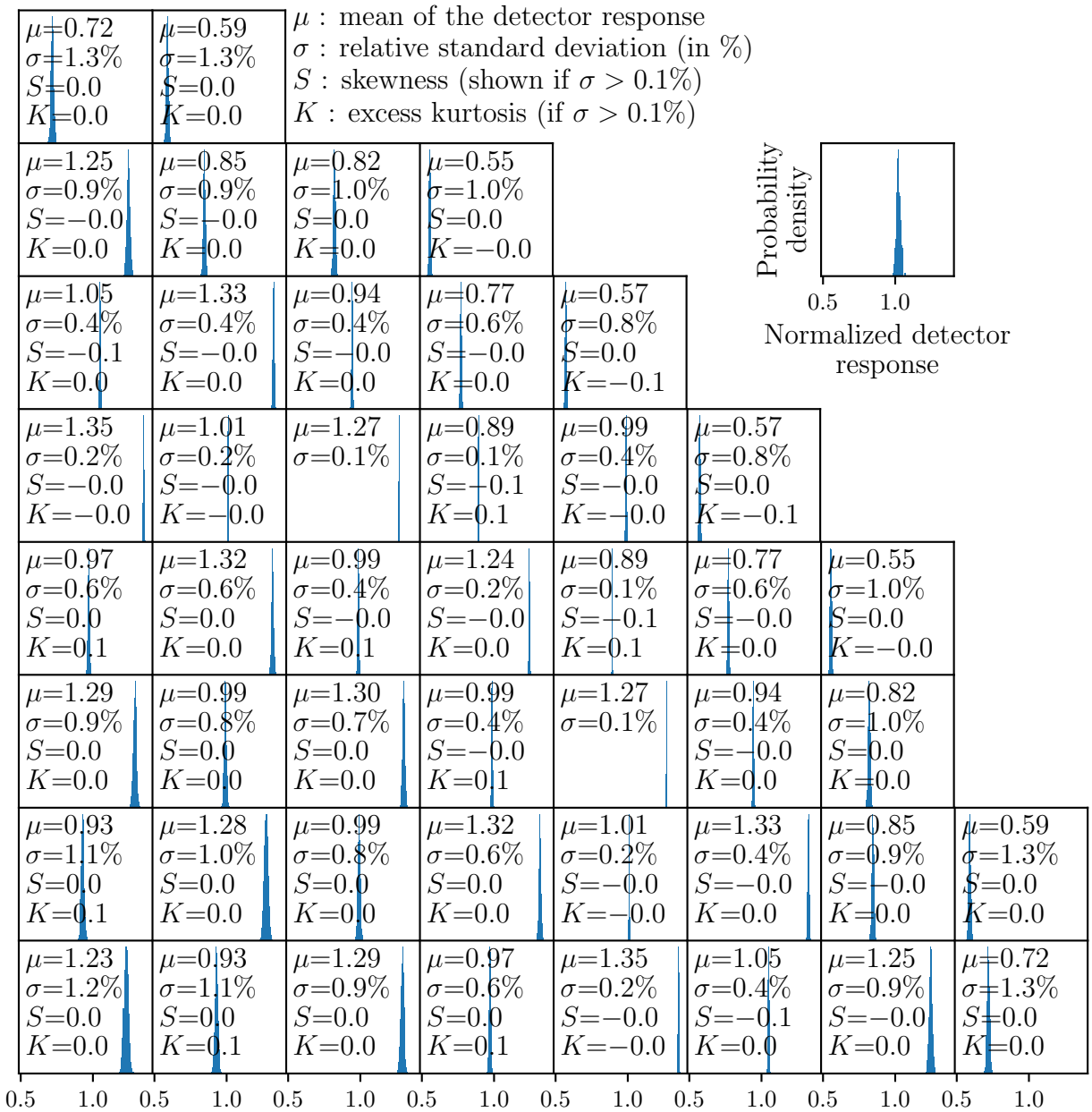

FIGURE 6 – BFMC posterior probability density of the detector responses, with SERPENT (mean) and DRAKKAR (higher order moments) for nuclear data sampled simultaneously for all isotopes, on the first start-up of Bugey-2, Fessenheim-1 and 2. Plotting instructions are available [24].

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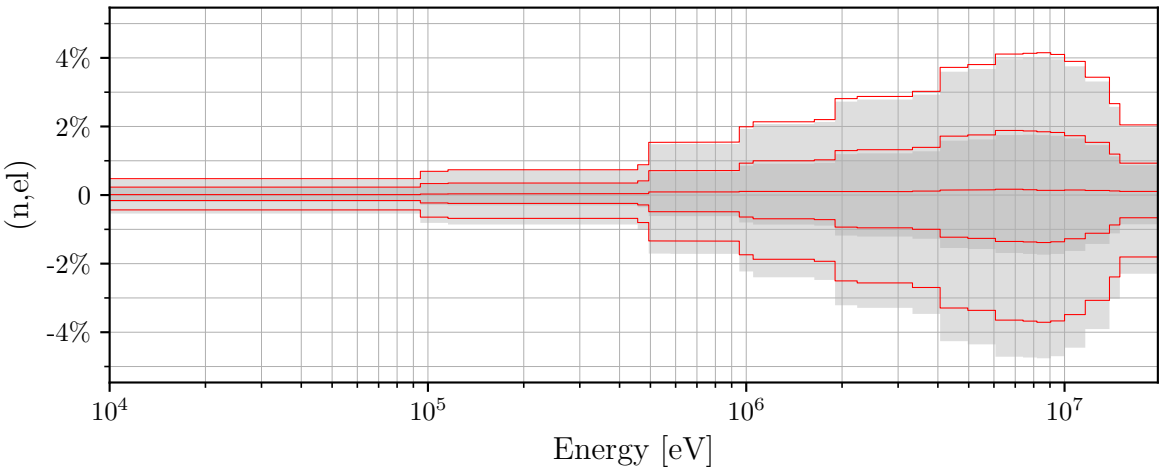

FIGURE 7 – Deviations relative to the prior median of hydrogen cross sections, for five prior quantiles (gray) and five posterior quantiles (red). The five quantiles are those at 5%, 25%, 50% (median), 75% and 95%. For example, the central red line corresponds to the posterior median, while the dark gray area corresponds to [25% ; 75%] prior. Plotting instructions are available [24].

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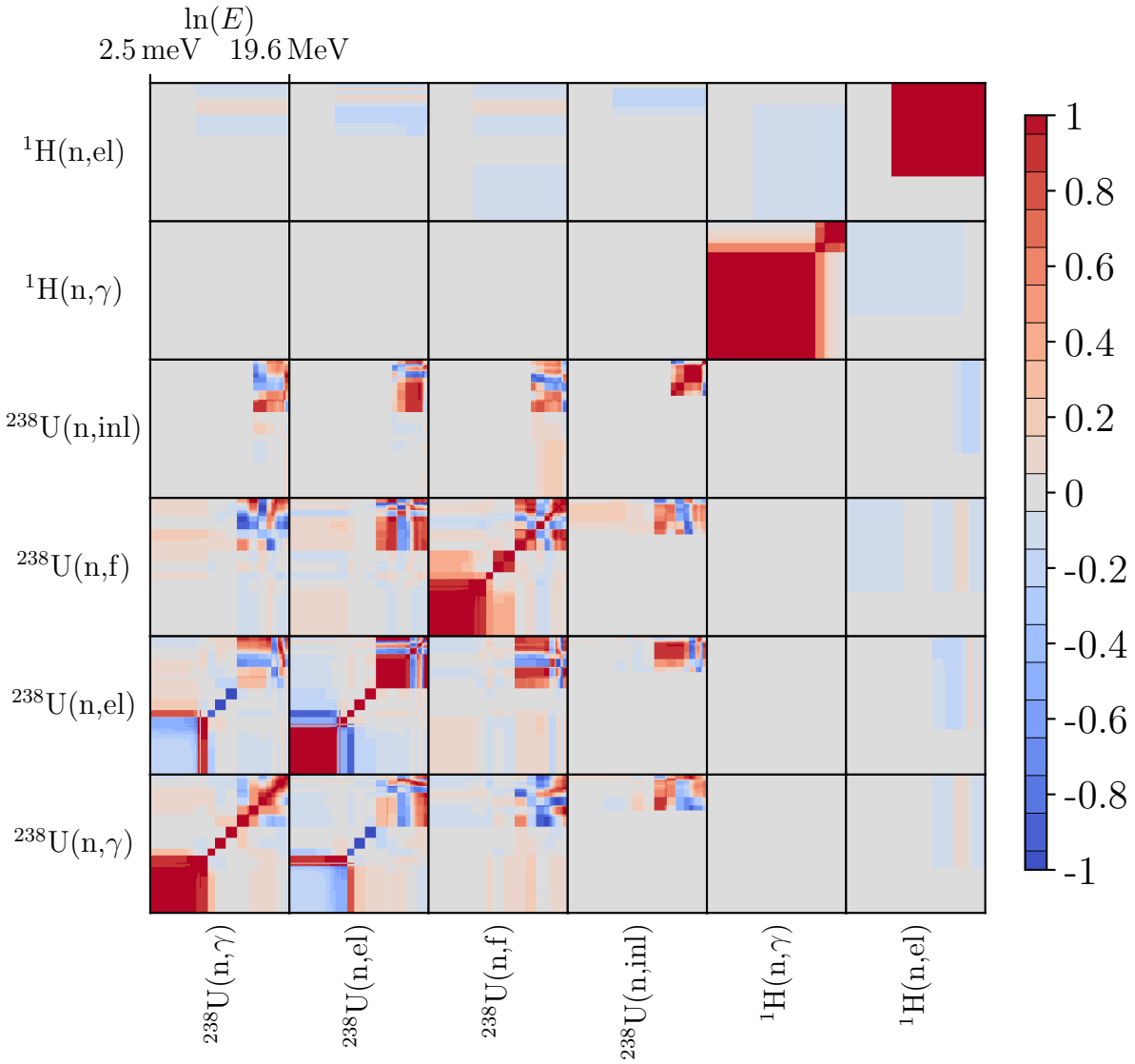

FIGURE 8 – BFMC posterior correlation matrix, zoomed in on uranium 238 and hydrogen, for their main reactions and for the whole energy range. Plotting instructions are available [24].

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