Building bridges between nuclear reactions and statistical models

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Abstract. In modern nuclear data evaluations, nuclear reactions and statistical methods cannot be separated. Whereas the first one is continuously improved for many decades, the second one is now benefiting from large computer power. Ahead of its time, our colleague Eric Bauge had understood the advantage of linking them together. He developed modern Bayesian methods, and helped many of us to move in this direction. This short paper will present two examples of the work that we did together, following his vision: the application of BFMC, and the evidence of correlation between nubar, chi and fission cross section. Finally, he was not only a bridge builder, he was also able to jump from fundamental physics to very applied aspects, making him a frontier crosser.

1 Introduction

Eric was one of my estimated colleagues and we will miss him very much. His last visit at my institute in 2017 resulted in a home diner, as well as a number a specific publications, following his vision. This vision was developed for many years, and one its descriptions was presented in 2017 in a paper entitled "*Connecting the dots, or nuclear data in the age of supercomputing*" [1]. There, one can find how the development of microscopic reaction models, coupled with massive computing and the Backward-Forward Monte Carlo (BFMC) method can improve applied simulations which depend on nuclear data evaluations. In this brief paper, I will present the BFMC approach (and its combination with the Total Monte Carlo (TMC) method), the nuclear data correlations resulting from it, and finally Eric's visions for the future.

2 BFMC and TMC

The BFMC method was firstly developed by Eric and presented in Ref. [2]. It is an extension of the TMC method [3]: first vary all model parameters, and produce random cross sections. Then such cross sections (and all varied nuclear data) can be used in specific simulations, such as criticality calculations, leading to a number of random k_{eff} values. This is basically the TMC approach. Eric's addition is the quantification of the quality of each random cross sections by calculating a weight w based how far the calculated k_{eff} values are from the benchmark value. In his view, the weight w_i (for the random realization i) was calculated such as

$$w_i = \exp^{-\left(\frac{\chi_i^2}{\chi_{\mathrm{min}}^2}\right)^2} \qquad (1)$$

In this expression, χ_i^2 is the traditional chi-square distance between the calculated $k_{\mathrm{eff,i}}$ and the $k_{\mathrm{eff,benchmark}}$. The value χ_{min}^2 is the best chi-square from the random population. This approach is not per say exactly Bayesian because of the normalization of the exponent and of the additional global square, but it is in fact extremely efficient for applied problems. This deviation from a pure Bayesian approach can be justified by the account of model defects, which are in fact numerous in nuclear data modeling. The outcome of such calculations are posterior distributions, integrating both differential and integral information. Applications can be found for the evaluation of ^{89}Y [4] and ^{239}Pu [2], for the general application to nuclear data evaluation [5].

To illustrate the advantage of the combination of the BFMC and TMC methods, one can read Ref. [6], where different Bayesian-based methods are compared and applied to the well-known criticality benchmark Godiva, as presented in Fig. 1. Although this example is about a criticality benchmark and its k_{eff}, different calculated parameters can be found in the following. Here, the prior distribution, being voluntary large, can be sensibly reduced to correspond to the benchmark value. This leads to different weights w_i for each i cross section, indicating which cross section (and model parameters) are preferable.

We will now continue to exploit these methods, but in the perspective of nuclear data evaluation, and the estimation of cross-correlations between different nuclear data quantities.

3 Correlations from BFMC and TMC

The original description can be found in papers written by Eric and myself in Refs. [7, 8]. The idea is to use a criticality benchmark (in the present case Jezebel) being sensitive to different nuclear data quantities. For the Jezebel benchmark, the nuclear data of interest are the nubar, fis-

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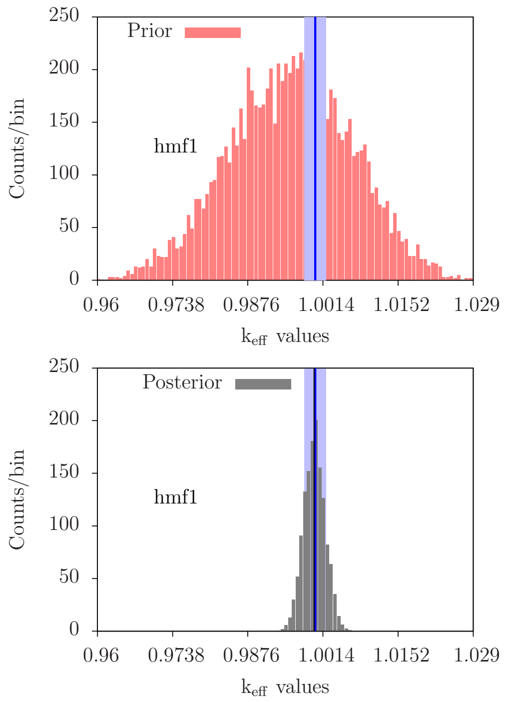

Figure 1. Prior (top) and posterior (bottom) k$_{\mathrm{eff}}$ for the Godiva benchmark, obtained from the BFMC and TMC methods. Figure taken from Ref. [6].

sion cross section and prompt fission neutron spectra from ^{239}Pu. As a prior, these three quantities are not correlated, as they are usually individually evaluated. By applying the BFMC and TMC methods, one can obtain posterior distributions as in Fig. 1, but also posterior correlation values between these three quantities. The main advantage is that one can obtain a reasonable calculated uncertainty, without artificially decreasing the uncertainties of these three nuclear data quantities. The obtained correlations are presented in Fig. 2. This approach was successful in com-

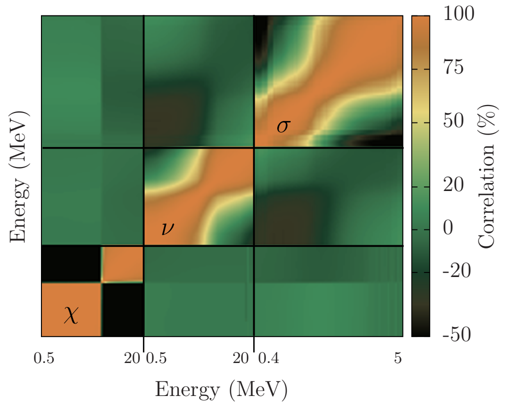

Figure 2. Posterior correlation matrix for ^{239}Pu ν, σ and χ. Note the cross-correlated non-zero values. Figure taken from Ref. [8].

bining differential and integral information, while helping the nuclear data evaluators to keep reasonable uncertainties. It was then decided to apply the same calculation method to more isotopes, more cases and virtually build bridges between different communities: criticality benchmarks for ^{235}U and ^{238}U [9], reactor application for U and Pu correlations [10], damage cross section for Si-based material [11], fission yield evaluation [12] and evaluation method [13].

4 Eric's visions for the future

Finally, although his work dramatically stopped, Eric helped us to expand his visions to the advantage of the whole community. First, the way of performing systematic calculations, representing a snapshot of the moment's knowledge in reaction theory, has proven to be a large success for the nuclear data evaluators and nuclear data users. Already in 2015, Eric supported the idea that the JEFF library could benefit from the massive calculations performed in the framework of the TENDL project. It is now a well-accepted idea that the JEFF library integrate in a very extended way the TENDL method and sub-libraries. His advice was then the use of "*soft power*", rather than imposing solutions, which has led to successful extension of JEFF outside its traditional reactor applications.

Then Eric's view on varying reaction models and their parameters, already discussed in 2017, was systematically applied in 2023 with the production of the TENDL-astro library. Such library follows Eric's recommendation to not only vary model parameters, but also models themselves.

At last, Eric was one of the first to recognize that (all) existing libraries were adjusted to integral data. This statement is not yet accepted by the whole nuclear data evaluation community, but it is nevertheless a fact which needs to be acknowledged.

5 Conclusion

It is now time to make one confession. Although I am a co-author of Ref. [1], I did not explicitly contribute to this paper. Eric was kind enough to include me, thanks to a number of discussions that we had on this subject. But by doing so, Eric also demonstrated his ability to connect people and think for the future. He saw that "*connecting the dots*" did not only meant to combine codes together, but also to bring people from different horizons and expertise to work together. This is exactly what has led to the success of the projects such as TENDL, TENDL-astro, BFMC, large-scale calculations based on microscopic approaches, and also to the rising quality and completness of many nuclear data libraries, such as JEFF. We need more scientists and colleagues like Eric.

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