NUCLEAR SCIENCE AND ENGINEERING: **172**, 287–299 (2012)

Random Adjustment of the H in H_2O Neutron Thermal Scattering Data

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Received January 11, 2012
Accepted March 26, 2012

Abstract—*The thermal scattering data for H in H_2O are adjusted to better fit a series of criticality safety benchmarks using the Petten adjustment method for optimizing nuclear data. This method is based on the "Total Monte Carlo" approach developed for nuclear data uncertainty propagation to a large-scale system, together with a selection based on a global distance to specific criticality benchmarks. This paper demonstrates the possibility to improve the agreement with integral benchmarks by modifying the thermal scattering data. It is an additional step toward defining a globally adjusted nuclear data library with the Petten adjustment method, including thermal scattering data and nuclear data at higher energy.*

I. INTRODUCTION

Thermal scattering nuclear data are one of the major inputs for model simulations of thermal systems, such as the current fleet of thermal reactors, or storage of nuclear spent fuel. As presented in many publications,[1,2] the binding of a scattering nucleus in a moderator affects the neutron cross section and the energy and angular distributions of secondary neutrons. This field of nuclear data evaluation is rather separated from the one of slightly higher neutron energy, mainly because of different models involved in the evaluation work. But, as with many other areas of neutron physics, the understanding, the calculations, and ultimately the evaluations of thermal scattering data are based on models. Therefore, if some models are used together with their parameters, the so-called Petten adjustment method can be applied.

The Petten adjustment method simply consists of randomizing model parameters for nuclear data in order to calculate random differential data (such as cross section, particle emission, etc.). The second step is to benchmark these random data with a defined set of "trusted" systems (such as shielding or criticality benchmarks). The last step of the method consists of selecting the random differential nuclear data having the best agreement with the benchmarks. As explained in Secs. III and IV, the Petten adjustment method was successfully applied to other nuclear data but not yet to thermal scattering data and cross sections for light elements (below mass $A = 19$).

In this paper, we will demonstrate that the agreement of thermal scattering data with integral benchmarks from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) list[3] can be improved using the Petten adjustment method, as was also presented in two different papers for other types of nuclear data: in Ref. 4 for the adjustment of the neutron-induced reactions of ^{239}Pu and in Ref. 5 for the adjustment of the neutron-induced reactions of ^{63}Cu and ^{65}Cu.

This work is part of a more general effort to generate the "best" modern nuclear data library. It is believed by the authors of these papers that new and different evaluation methods can be used to produce a nuclear data library with unprecedented characteristics and quality: quality on the style of production, the format, and its performance. The method of choice to achieve such an ambitious goal is the Petten adjustment method, being the result of reproducibility, quality assurance, and

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a bit of creativity. Previous publications by the present authors have demonstrated the advantages of the Petten adjustment method compared to "incremental approaches," usually exploited to improve one version of a nuclear data library to the next one. However, before succeeding in this enterprise, a few open questions must be answered. Can the Petten adjustment method be applied to low-neutron-energy nuclear data (such as thermal scattering), and to light element nuclear data? Which adjustment sequence should be pursued to avoid unwanted compensation and to effectively reach the "best" library?

This paper answers part of the first question by studying the impact of random H in H_2O thermal scattering data. As one of the most important thermal scattering data, H in H_2O was partially reevaluated in 2004 (Refs. 1 and 6), and this new evaluation is now included in the U.S. ENDF/B-VII.0 library[7] and the European JEFF-3.1.1 library.[8] The Japanese JENDL-4.0 library[9] includes an older evaluation from 1994. The latest work from 2004 (Ref. 1) includes a review of the available experimental data, updating of models and model parameters for the generation of $S(\alpha,\beta)$, and extended benchmarking for different kinds of systems.[6] Since 2004, no additional work has been performed on the thermal scattering data of H in H_2O.

Based on this extensive and high-quality work, we are proposing an adjustment of some of the model parameters to improve the global agreement with some criticality safety benchmarks. In this work, we are not presenting final "new" parameters, but rather, we are demonstrating that an adjustment method can be used for H in H_2O thermal scattering data.

II. MODEL FOR THERMAL NEUTRON SCATTERING

The complete description of the current knowledge on the theory of thermal neutron scattering can be found in the literature (see, for instance, Refs. 1 and 2). We will not repeat in the following what is better explained elsewhere, and we invite the reader to refer to other publications for an extensive description of thermal scattering theory. In this section, a minimum explanation of thermal scattering is given so that the adjustment procedure (given in Sec. III) can be understood.

In the case of H in H_2O, incoherent inelastic scattering is the major component, and coherent and incoherent elastic scattering can be neglected. Inelastic scattering is described by the scattering law $S(\alpha,\beta)$ at different temperatures. In this case, the double-differential scattering cross section for thermal neutrons is given by

$$\frac{\partial^2\sigma(E\rightarrow E',\mu)}{\partial E'\partial\mu} = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}S(\alpha,\beta) \ , \tag{1}$$

where

E, E' = incident and outgoing neutron energies in the laboratory system

μ = cosine of the scattering angle in the laboratory system

σ_b = characteristic bound scattering cross section for the material (water in this case)

kT = thermal energy (eV)

and $S(\alpha,\beta)$ = asymmetric form of the scattering law, which depends on two variables, i.e., the momentum transfer α and the energy transfer β:

$$\alpha = \frac{E + E' - 2\sqrt{EE'}\mu}{AkT} \tag{2}$$

and

$$\beta = \frac{E' - E}{kT} \ , \tag{3}$$

where A is the ratio of the scattered mass over the neutron mass. In the case of the incoherent and Gaussian approximations, the scattering law can be written as a function of $\rho(\beta)$, the frequency spectrum of excitations in the system. The asymmetric scattering law is the Fourier transform of the intermediate scattering function:

$$S(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\beta\hat{t}}e^{-\gamma(\hat{t})}\,d\hat{t} \ , \tag{4}$$

where $\hat{t}$ is the time measured in units of $\hbar/(kT)$ seconds. The function $\gamma(\hat{t})$ is given by

$$\gamma(\hat{t}) = \alpha\int_{-\infty}^{+\infty} P(\beta)(1 - e^{-i\beta\hat{t}})e^{-\beta/2}\,d\beta \tag{5}$$

and

$$P(\beta) = \frac{\rho(\beta)}{2\beta\sinh(\beta/2)} \ . \tag{6}$$

The frequency spectrum can be decomposed into a sum of spectra such as

$$\rho(\beta) = \sum_{i=1}^{K}\rho_i(\beta) \ , \tag{7}$$

where $\rho_i(\beta)$ are given by

$\rho_i(\beta) = \omega_i\delta(\beta_i)$ for the discrete oscillators ,

$\rho_i(\beta) = \rho_s(\beta)$ for the solid-type spectrum ,

and

$\rho_i(\beta) = \rho_t(\beta)$ for the translational spectrum.

As presented in Sec. III, some of these model parameters will be randomly selected to produce random inelastic thermal cross sections to be used in MCNP simulations.[10]

III. THE PETTEN ADJUSTMENT METHOD

The Petten adjustment method for nuclear data adjustment has been presented in Refs. 4 and 5. It is based on the principle that a calculated quantity (k_{eff}, neutron flux, cross section, or any other value obtained from a simulation) is not an absolute value but, rather, can be represented by a probability distribution with a central value (the k_{eff}) and a standard deviation ($\pm\Delta k_{eff}$). For cross sections, which is a term often used instead of nuclear data, their uncertainties reflect a restricted knowledge due to limited experimental conditions or limited theoretical understanding. One should then use not one cross-section value (at a given energy, for a given reaction) but should use a large number of them, all obtained following a probability distribution defined by its central value and standard deviation. As often happens in nuclear simulations, a Gaussian or uniform distribution is used. Each of these possible cross sections can be used for a system simulation and induces different calculated results, such as different k_{eff}. If one compares the calculated k_{eff} with the experimental value, it is possible to select the cross section that produces a calculated k_{eff} equal to the experimental one. The next step is then to consider this *special* cross section as the new central value.

This is the underlying method that is applied in this work. The generalization of this method to a large number of nuclear data (cross sections, resonance parameters, neutron emission, etc.) and of systems (a few tens of criticality benchmarks) is called "nuclear data adjustment" in the following. It has been recently shown that nuclear data (cross sections, emission spectra, etc.) can be adjusted using a Monte Carlo method to obtain better agreement with differential and integral data. In Refs. 4 and 11, a method of nuclear data evaluation and adjustment was first presented and applied to ^{239}Pu. Based on the TALYS reaction code,[12] hundreds of ^{239}Pu calculations (named "files," due to the format being ENDF-6 formatted files) were produced by varying all possible model parameters. All these files, different in content but alike in format were then benchmarked with a selection of k_{eff} benchmarks from the ICSBEP collection.[3] The result of this work was a randomly adjusted ^{239}Pu evaluation, performing better that any other random ^{239}Pu files obtained during this exercise. A second application of this method, presented in Ref. 5, concerns the ^{63}Cu and ^{65}Cu isotopes. In this work, the performance of the random files was tested against not only criticality integral benchmarks but also fusion benchmarks and differential data. It was shown that the best performing random ^{63}Cu and ^{65}Cu files also outperformed the copper evaluations from the ENDF/B-VII.0 library[7] and the JEFF-3.1.1 library.[8] The random adjustment method or Petten adjustment method as presented in Ref. 5 proved to be effective for two isotopes and produced evaluations performing better than the ones coming from classical approaches.

IV. APPLICATION TO THERMAL SCATTERING DATA

In the specific case of the thermal scattering data for H in H_2O, the procedure varies from the previous applications of the Petten adjustment method, but the philosophy stays the same. In order to generate thermal scattering data that can be used in a simulation, the following steps were taken:

1. Create input parameters for the LEAPR module[13] of NJOY (Ref. 14).

2. Run LEAPR to generate thermal scattering data in ENDF format "MF 7, MT 4" [incoherent inelastic data in terms of $S(\alpha,\beta)$ tables for different temperatures].

3. Use the ENDF file with the THERMR module of NJOY to generate pointwise thermal scattering cross sections.

4. Use the ENDF file and the output of THERMR with the ACER module of NJOY to generate thermal scattering data for the MCNP code in the ACE format.

5. Finally, repeat n times the previous steps with random input parameters for LEAPR.

The central (or nominal) values for all model parameters to be used in LEAPR are the values used for the JEFF-3.1.1 evaluation. Based on these values and uniform distributions, some parameters can be randomly modified. In the present work, seven different parameters were changed:

1. the translational weight ω_t (25%)
2. the oscillator weights ω_j (25%)
3. the free atom cross section for the scatterer σ_1 (10%)
4. the free atom cross section for the scatter σ_2 (15%)
5. the frequency spectrum $\rho(\beta)$ (30%)
6. the α value
7. the β values

$$\left.\begin{array}{l}\text{6. the } \alpha \text{ value}\\ \text{7. the } \beta \text{ values}\end{array}\right\} (25\%).$$

Each of these parameters has a different influence on the inelastic cross section, and because of high nonlinearity in Eqs. (1) through (7), their combined effect is not equal to the linear sum of their independent effects. The uncertainties of the above parameters were chosen in an ad hoc way. There is virtually no information on how to choose the uncertainties of these parameters in the open literature. The main constraint in the selection of these uncorrelated uncertainties was to reproduce the spread of the experimental inelastic cross section (as shown in Fig. 1). But, because of the high nonlinearity of the model, a different set of uncertainties could be selected, providing a similar cross-section spread. If permitted, we would vigorously advise the nuclear data community to reinvest in the knowledge of this part of the physics, abandoned over the past decades with a considerable and costly loss of expertise. The resulting random inelastic cross sections for H in H_2O are presented in Fig. 1, together with the experimental data and the calculated uncertainties. It can be seen that the rather large uncertainties in the model parameters have a limited effect on the inelastic cross section.

By generating random files, the correlation matrix for the inelastic cross section can also be extracted, as presented in Fig. 2. This correlation matrix reflects the types of models and parameters (and their uncertainties) used in this work. If a different set of parameters or different parameter uncertainties are used, a different correlation matrix and uncertainties for the inelastic scattering could be obtained. It can be noticed that the correlations presented in Fig. 2 are strong (always above 0.70), which is common for energy-energy correlation matrices obtained from random model parameters only. This denotes the rigidity of the model, compared to the relative low correlations obtained from the experimental data. One of the advantages of the current approach is clearly demonstrated: It is relatively easy to obtain uncertainties and correlations to construct a covariance matrix. Covariance matrices are used for uncertainty propagation methods based on perturbation theories. In the current ENDF-6 format, there is no definition for a thermal scattering covariance matrix (to be called “MF-37”), but if the need from the nuclear data user community is strong enough, the current method and results presented in Figs. 1 and 2 could be used. For a given cut at a specific energy, the obtained random inelastic cross sections presented in Fig. 1 are uniformly distributed as the probability function for random parameters is uniform.

At the end of a loop *i* for LEAPR-THERMR-ACER, an ACE file is obtained, which can be used by MCNP

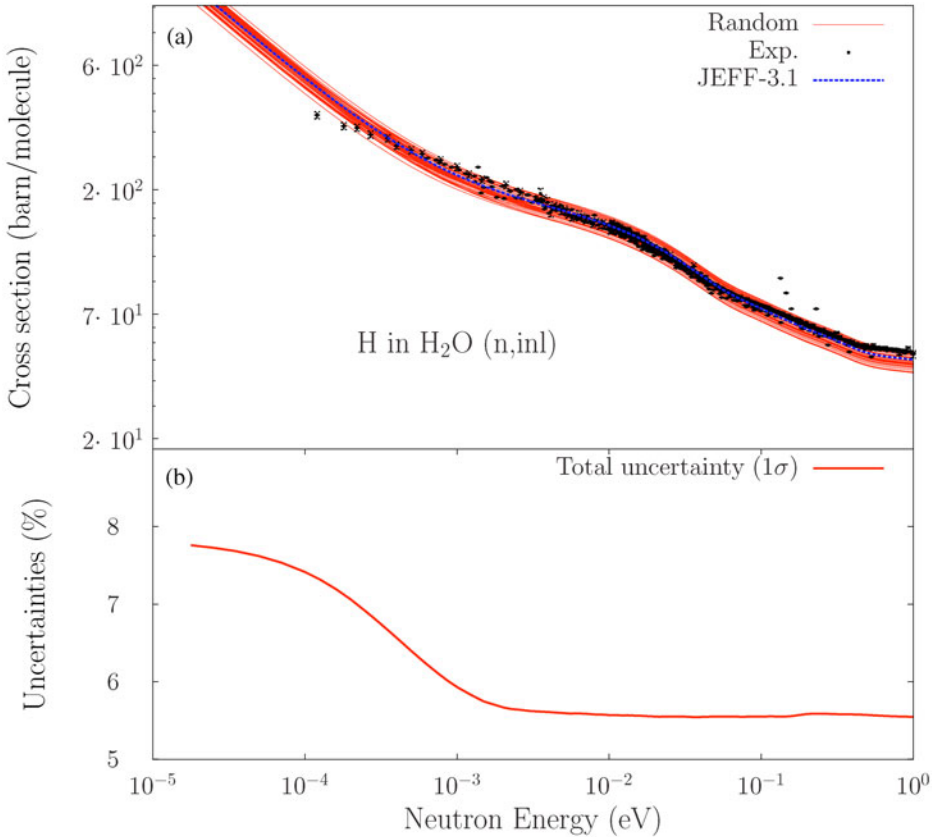

Fig. 1. (a) Incoherent random inelastic scattering cross section of H in H_2O compared to experimental data and the inelastic cross section from the JEFF-3.1 library. (b) Uncertainties in the inelastic cross section calculated from 1330 random inelastic cross sections.

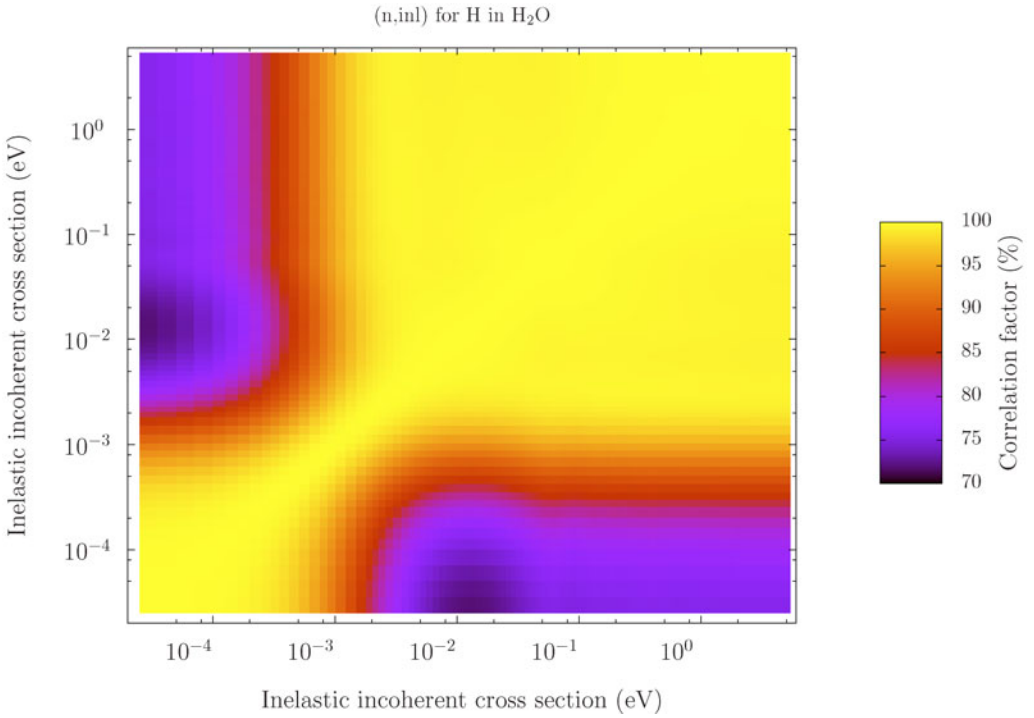

Fig. 2. Energy-energy correlation matrix for the incoherent inelastic scattering of H in H_2O. Note that the correlation values are always larger than 0.7.

TABLE I

List of Thermal Benchmarks Selected for the Random Search*

Name	Cases	Name	Cases	Name	Cases	Name	Cases
pst12	22	pst1	6	lst4	7	lmt1	1
lct7	10	lct6	18	ict3	2	hst32	1
hst42	8						

*Each criticality benchmark name consists of three letters. The first letter defines the degree of enrichment ("h" for high, "i" for intermediate, and "l" for low-enriched ^{235}U; "p" is used for a plutonium benchmark). The second letter defines the physical form ("m" for metal, "s" for solution, and "c" for compound). The last letter defines the neutron spectrum ("f" for fast, "t" for thermal, and "i" for intermediate).

with a criticality benchmark to calculate $k_{eff,i}$. After n loops, probability density functions for k_{eff} of each benchmark are obtained. A number of 75 thermal criticality safety benchmarks from the ICSBEP collection[3] are selected to evaluate the impact of random H in H_2O thermal scattering data. The list is given in Table I.

Finally, as a large number of benchmarks are considered, it is easier to compare the performances of different libraries with a unique number such as F, defined as

$$F = 10^{\sqrt{(1/N)\sum(\log(E_i)-\log(C_i))^2}} , \quad (8)$$

where

C_i = calculated value for the i benchmark

E_i = benchmark value

N = number of benchmarks.

The distance F can be calculated for the three libraries ENDF/B-VII.0, JEFF-3.1.1, and JENDL-4.0 and is equal to 1.0112, 1.0113, and 1.0114, respectively. As given by Eq. (8), a small F corresponds to better agreement with the experimental data compared to a larger F.

The minimization of F can then be performed, benchmarking all random nuclear data files and selecting the ones with the best performance. Even if in principle our current approach for H in H_2O adjustments can be used for all thermal scattering data at once (requiring a large number of MCNP runs), only the H in H_2O data at 293 K are varied, and the other thermal scattering data and nuclear data are kept constant and equal to the JEFF-3.1.1 evaluations.

As in any Monte Carlo calculation, the number of random runs needs to be high enough to ensure convergence of the distributions for the calculated k_{eff}. The averaged updated standard deviations Δk_{eff} as a function of the number of runs (second moment of the k_{eff} distributions) for some selected benchmarks are presented in Fig. 3.

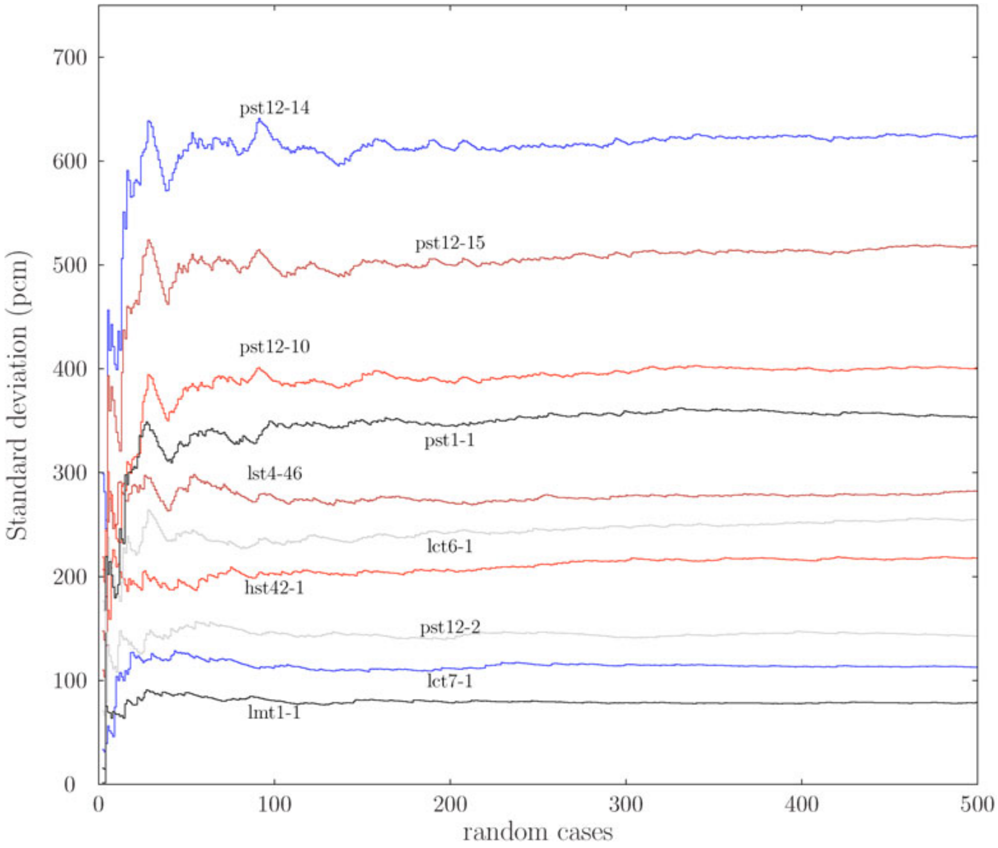

Fig. 3. Standard deviations for some benchmarks as a function of the number of random thermal scattering files.

It appears that the averaged Δk_{eff} are relatively stable after a few hundreds of runs, but a total of 1330 random thermal scattering data sets was used. The benchmarks presented in Fig. 3 are representative of the complete set, although the majority of the Δk_{eff} are <200 pcm. It is interesting to notice that the benchmarks with the higher sensitivity to the H in H_2O thermal scattering data are the plutonium benchmarks (denominated "pst") and not the uranium benchmarks. This is certainly related to the fact that ^{239}Pu has a strong resonance close to 0.4 eV, whereas ^{235}U and ^{238}U do not have strong narrow resonances in the thermal region, where the thermal scattered data are important. The complete list of benchmark results is presented in Table II for the averaged k_{eff} and standard deviation Δk_{eff}.

Examples of such k_{eff} distributions are presented in Fig. 4. As shown, the probability distributions for k_{eff} are significantly changing from the benchmarks with low sensitivities to thermal scattering data to the ones with high sensitivities. Single or double Normal distributions are indicated to guide the eye. The deviation from a Normal distribution for some of the benchmarks can be related to the results presented in Ref. 15, where deviations were also found in the case of high k_{eff} uncertainties. In Ref. 15, the non-Normal distributions were obtained from non-Normal cross-section distributions. Here again, the present distributions are related to the uniform probability distributions used for the model parameters, as shown in Fig. 5. Two kinds of parameter distributions are presented in Fig. 5: a uniform distribution (as in Fig. 4) and a Normal distribution for the model parameters ω_t, ω_j, σ_1, σ_2, $\rho(\beta)$, α, and β. In the case of the pst12-14 benchmark, which has a high sensitivity to the scattering data, the shapes of the k_{eff} distributions are different, depending on the type of distributions for the model parameters. This indicates that not only are the mean and the standard deviation of a probability distribution important, but also its shape is important.

V. RESULTS

V.A. Improved Thermal Scattering H in H_2O

Following this present evaluation method, a large number of ACE files are produced. As this paper demonstrates the feasibility of the method, the number of random files is kept to a relatively small number (fewer than 2000). Furthermore, as seen below, we believe we have sampled within the complete phase-space of the

TABLE II

Average $\overline{k_{eff}}$ and $\Delta\overline{k_{eff}}$ After 1330 Random Runs for the 75 Benchmarks Considered in Table I

Benchmark	$\overline{k_{eff}}$	$\Delta\overline{k_{eff}}$ (pcm)	Benchmark	$\overline{k_{eff}}$	$\Delta\overline{k_{eff}}$ (pcm)	Benchmark	$\overline{k_{eff}}$	$\Delta\overline{k_{eff}}$ (pcm)
hst42-1	0.99635	215	hst42-2	0.99616	210	hst42-3	0.99990	140
hst42-4	1.00120	110	hst42-5	0.99893	100	hst42-6	0.99928	110
hst42-7	1.00001	100	hst42-8	1.00063	90	ict3-132	1.00343	120
ict3-133	1.00820	115	lmt1	0.99812	80	hst32-1	0.99867	130
lct6-1	0.99944	140	lct6-2	1.00010	150	lct6-3	1.00006	160
lct6-4	0.99958	130	lct6-5	0.99959	145	lct6-6	1.00013	150
lct6-7	0.99998	170	lct6-8	1.00008	170	lct6-9	0.99970	125
lct6-10	0.99970	140	lct6-11	0.99995	150	lct6-12	0.99971	155
lct6-13	0.99956	155	lct6-14	0.99941	110	lct6-15	0.99941	115
lct6-16	0.99948	125	lct6-17	0.99945	135	lct6-18	0.99945	140
lst4-1	1.00037	280	lst4-29	1.00148	260	lst4-33	0.99935	250
lst4-34	1.00161	225	lst4-46	1.00146	215	lst4-51	1.00057	205
lst4-54	1.00067	190	lct7-1	0.99705	120	lct7-2	0.99881	145
lct7-3	0.99740	90	lct7-4	0.99706	130	lct7-5	0.99684	145
lct7-6	0.99885	155	lct7-7	0.99841	95	lct7-8	0.99792	120
lct7-9	0.99845	155	lct7-10	0.99851	100	pst1-1	1.00275	350
pst1-2	1.00464	350	pst1-3	1.00675	355	pst1-4	1.00106	340
pst1-5	1.00502	340	pst1-6	1.00628	300	pst12-2	1.00620	250
pst12-3	1.00736	250	pst12-4	1.00749	180	pst12-5	1.00936	140
pst12-6	1.00810	545	pst12-7	1.00693	540	pst12-8	1.00611	505
pst12-9	1.01132	430	pst12-10	1.00554	400	pst12-11	1.00790	340
pst12-12	1.00813	310	pst12-13	1.00966	140	pst12-14	1.00341	620
pst12-15	1.00968	520	pst12-16	1.00428	460	pst12-17	1.00745	380
pst12-18	1.00738	355	pst12-19	1.00865	290	pst12-20	1.00873	280
pst12-21	1.00891	200	pst12-22	1.00971	150	pst12-23	1.00956	150

possibilities allowed by the current modeling of the thermal scattering data. A higher number of random runs will not lead to a smaller distance (F).

Figure 6 presents the results of the benchmarks of the random files in terms of F as defined in Eq. (8). All single random files are represented by a unique F value, and to compare with existing evaluations, results from other libraries are plotted as lines.

In Fig. 6, the results for 1330 random H in H_2O libraries are presented. It is rather unconventional to visualize a library for which an isotope is represented by a set of files (corresponding to probability distributions for different types of thermal scattering data), and Fig. 6 is a collapsed way of looking at n random files applied to 75 benchmarks. As expected from a simple random approach, a number of files perform quite poorly compared to other libraries, reflecting the amount of knowledge, experience, and adjustment already included in traditional evaluations. But, an important set outperforms any of the three presented libraries ENDF/B-VII.0, JEFF-3.1.1, and JENDL-4.0. There is nevertheless a limitation in the results obtained with this approach. As shown in Fig. 6, random thermal scattering data do not permit the F value to be <1.006 to 1.007. This limitation can have at least three origins:

1. limitation of the thermal scattering model
2. limitation of the impact of thermal scattering data, as compared with other nuclear data
3. combined performance of the thermal scattering data with important nuclear data such as ^{235}U and ^{238}U.

The first limitation comes from the theoretical knowledge of the thermal scattering process. It can certainly be improved, and/or more freedom could be added to the model. This would lower the best F obtained, but because of the second limitation, random thermal scattering data cannot by itself solve all the differences between the calculated and the measured k_{eff}.

Another important parameter for the thermal scattering data is the incident energy grid used by the NJOY processing code.[16] NJOY transfers the $S(\alpha,\beta)$ to secondary energy distributions on an incident energy grid. The H in H_2O thermal scattering data can also vary by a large amount depending on the number of energies on this grid. In this work, the incident energy grid is not modified (or randomized) as it is not an input parameter of the LEAPR module of NJOY, but a separated study could be realized to assess the importance of some of the assumed quantities in the NJOY code.

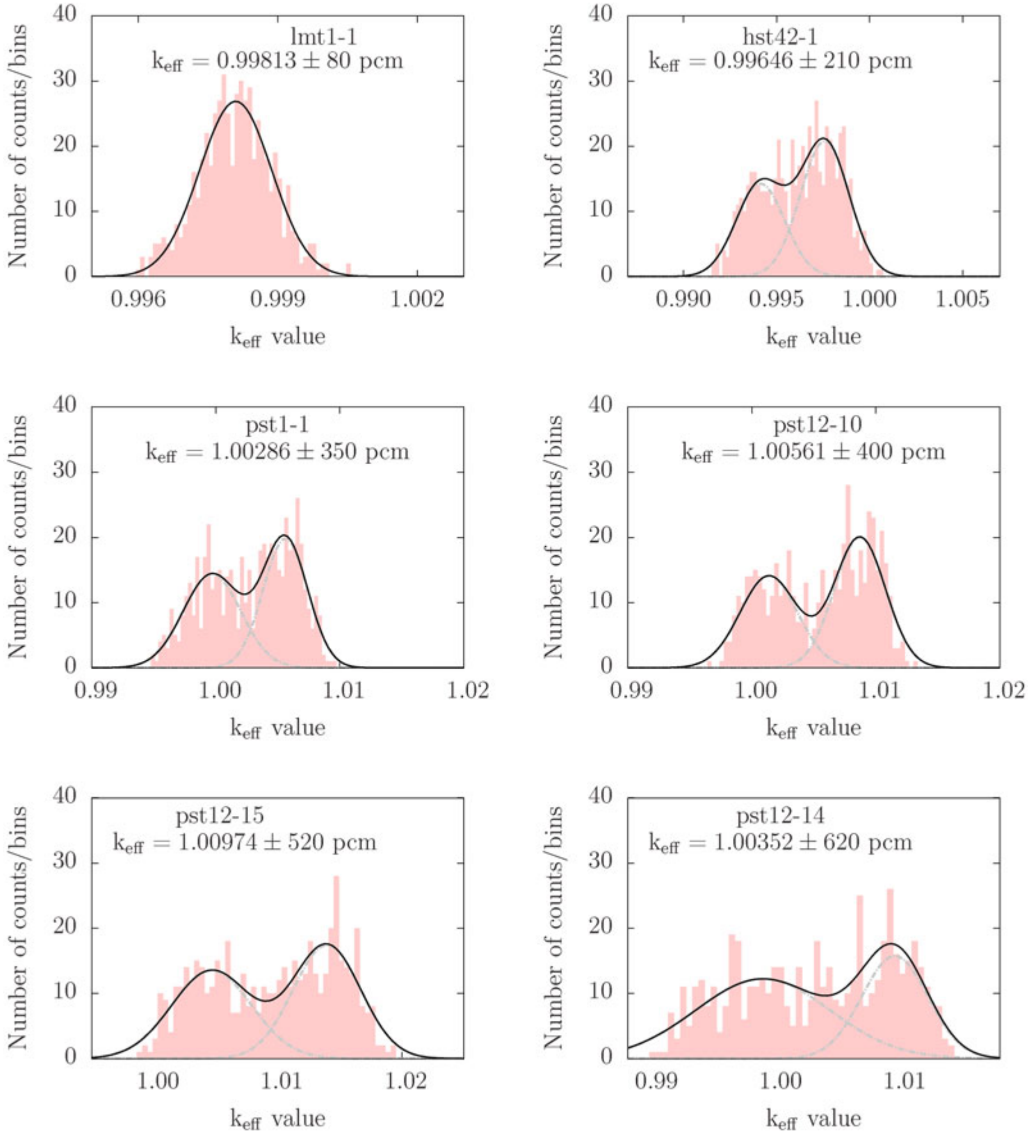

Fig. 4. Calculated k_{eff} values for six benchmarks. Note that the total standard deviation is increasing from the top left figure to the right bottom figure. The fits by one or two Gaussians are not used to extract the standard deviations but are presented to emphasize potential shifts from a Normal distribution.

Finally, the last limitation is related to the possible correlation between the H in H_2O thermal scattering data and the major actinides, regarding the benchmark performances. It can be expected that when a library such as JEFF is tested and adjusted, some deficiencies of the major actinides are compensated by specific thermal scattering data (or vice versa). It is then more difficult to find a "better" thermal scattering file, without also adjusting the major actinides.

A different way of representing the same results is shown in Fig. 7, where the F values in Fig. 6 are projected onto the y-axis and counted in histograms. In this representation, each F value (for each random H in H_2O thermal scattering data file) is represented by a step of height 1 in the histograms. The traditional JEFF-3.1.1 library has a single step for the F value and is presented with an arrow. This distribution is not symmetric and has a large number of counts toward low F values.

This kind of representation (Figs. 6 and 7) has already been used in Refs. 4 and 5, where nuclear data are modified, such as cross sections, angular distributions, or nubar. The distributions as presented in Fig. 7 were then different, following a lognormal distribution. In the present case, the projection of F (Fig. 7) is not similar to previously obtained results. This is not related to the definition of the "distance," where a simple χ^2 formula is used in Refs. 4 and 5. The type of distribution seems to be related to the type of nuclear data that is randomly

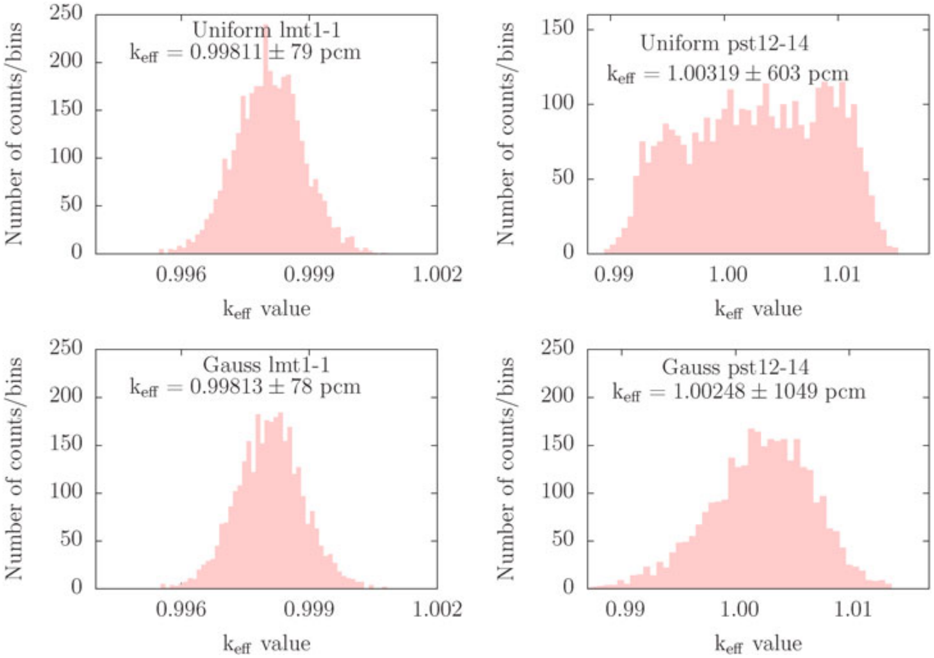

Fig. 5. Calculated k_{eff} values for two benchmarks: pst12-14 and lmt1-1 for two different distributions of the random model parameters: uniform (top plots) and Normal (bottom plots). The non-Normal distributions in Fig. 4 can be attributed to the uniform distributions for the model parameters.

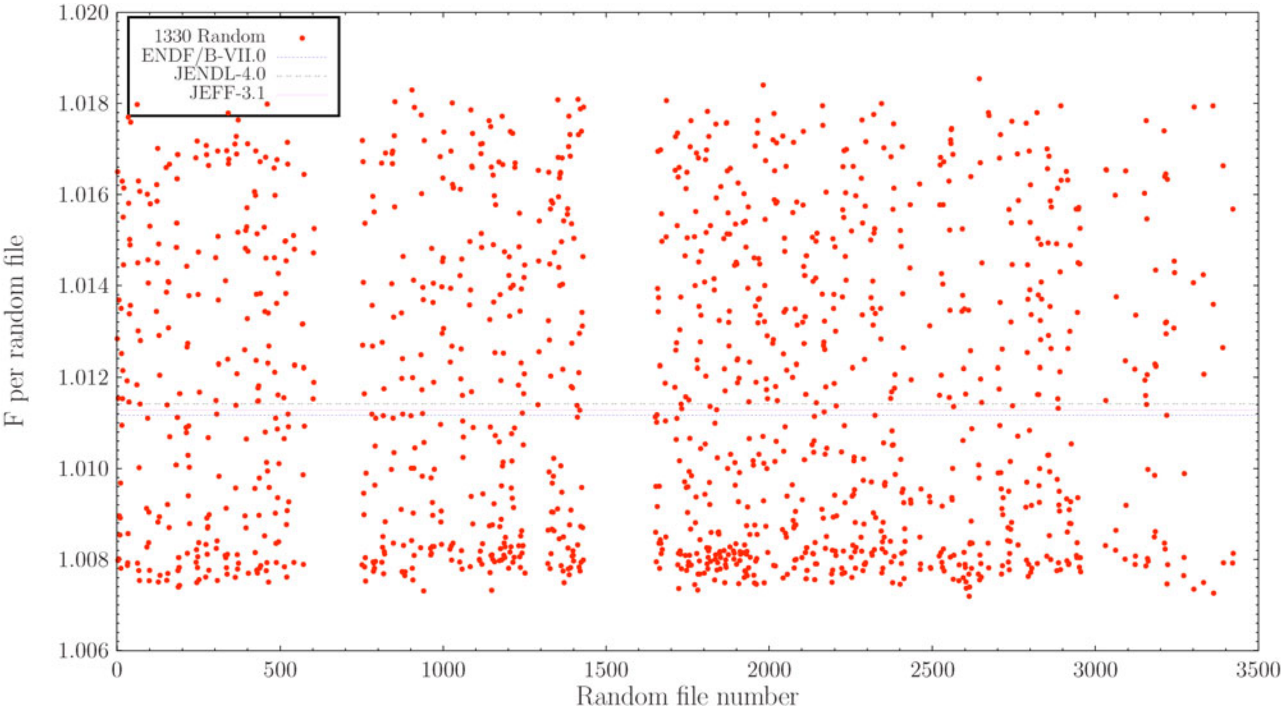

Fig. 6. The F distance values for random H in H_2O files (dots), compared to F for existing libraries (lines). F is defined in Eq. (8): The smallest F corresponds to the best agreement between the experimental data and the calculation. The lines represent the F values from the three libraries ENDF/B-VII.0, JEFF-3.1, and JENDL-4.0.

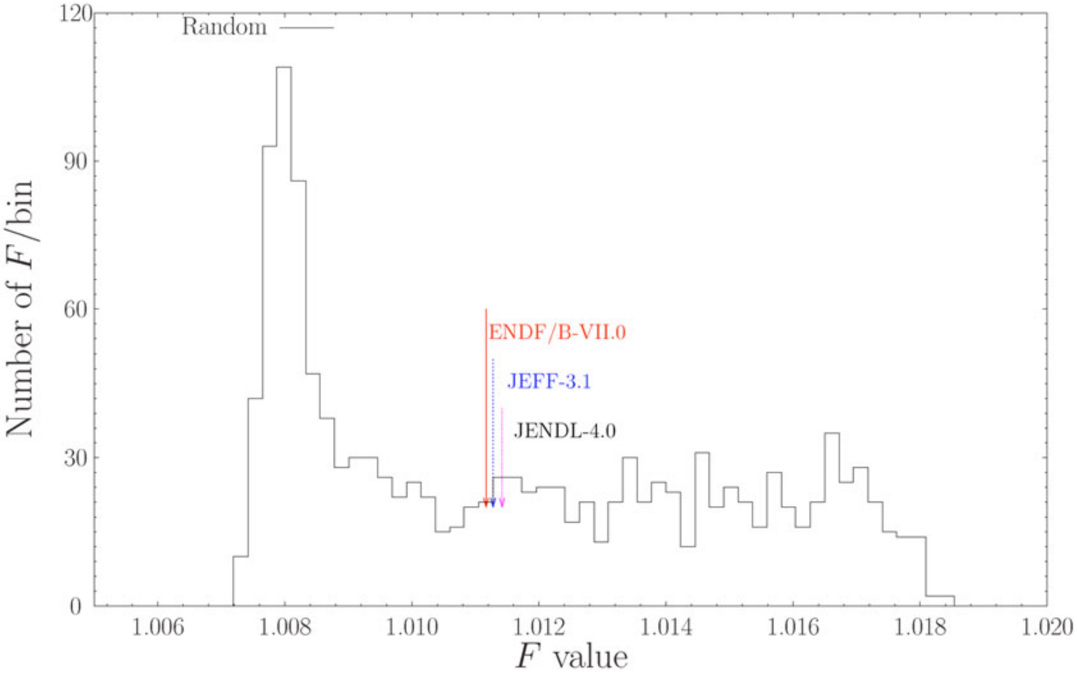

Fig. 7. The F values for each random H in H_2O files per bin, compared to the F values for JEFF-3.1.1, ENDF/B-VII.0, and JENDL-4.0. This figure is the projection on the y-axis of Fig. 6.

varied. More study would be necessary to understand the origin of the shape of the distribution, which defines the limit of the Petten adjustment method. If it could be shown that this type of distribution has a nonzero probability at $F = 1$, then it would be possible, by sampling enough, to find the perfect agreement between experiments and calculations.

Finally, based on the smallest obtained distance F, the best H in H_2O thermal scattering data can be selected for the given set of 75 benchmarks. In the present case, the smallest F is obtained for run 2613 with $F = 1.007192$, which is significantly smaller than the ones for ENDF/B-VII.0 or JEFF-3.1.1. Run 2613 is in fact equivalent to many other random runs that gave slightly larger F values. Considering a statistical uncertainty of 50 to 100 pcm for each benchmark, all F values within 0.0005 are equivalent. Figure 8 presents the calculated-to-experiment (C/E) values for the 75 considered benchmarks, obtained from run 2613. Values from the JEFF-3.1.1, JENDL-4.0, and ENDF/B-VII.0 libraries are also presented.

From Fig. 8, one can see that the benchmarks with the most improved C/E values are the plutonium benchmarks (pst1 and pst12). The C/E values are strongly decreased by as much as 1000 pcm and are now within the experimental uncertainties. For the low-enriched uranium benchmarks (lct and lst), the new C/E values are globally lower than those from other libraries. This would tend to increase the F distance but is compensated by the gain in the plutonium benchmarks. There seems to be an incompatible trend between the uranium and the plutonium benchmarks, where the C/E values for the uranium benchmarks are too low and the C/E values for the plutonium benchmarks are within the experimental uncertainties. But, again, the present study does not have the goal to produce absolute better thermal scattering data for H in H_2O but rather to demonstrate the possibility of using the Petten adjustment method to globally improve C/E results.

To conclude this section, we should put forward a few words about the drawbacks of the method. As in many applications of Monte Carlo methods, the main drawback is the multiplication of the calculations and, therefore, of the entire calculation time. It is partly compensated by the availability of computer clusters, easiness of the parallelization, and low-cost CPUs compared to human cost. The generalization of the methods to additional benchmarks and isotopes is not a difficulty as such and can almost be directly translated into the calculation time issue. The personal thinking of the authors is that the limitation due to the calculation time can easily be surpassed, but the acceptance factor corresponds to the actual struggle. The real challenge of such method is to be accepted by the scientific community as a reliable, capable, and competitive method, at a similar level as the past incremental improvements. Without acute optimism, we believe that the technical limitations are already fading away, but the real confinement of the method lies in human acceptance.

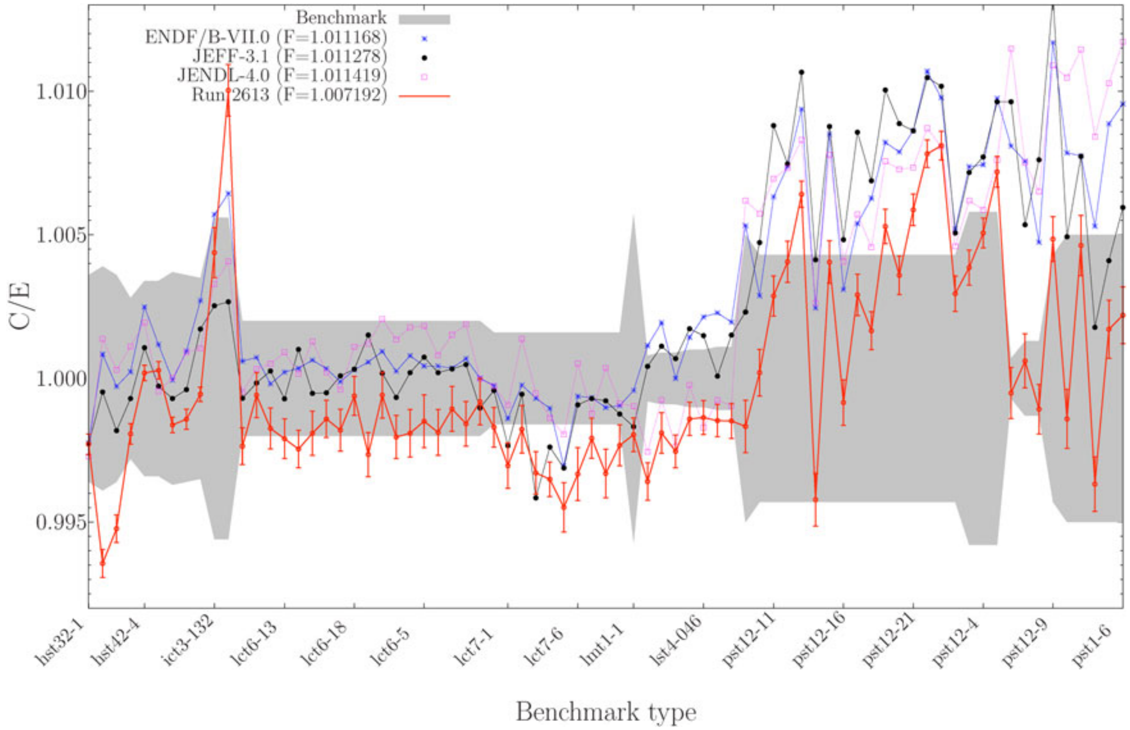

Fig. 8. Benchmark results for the best H in H_2O random file (run 2613), compared to the benchmark results with the JEFF-3.1, JENDL-4.0, and ENDF/B-VII.0 libraries. The uncertainty bars are the MCNP statistical uncertainties.

V.B. Benchmark Correlations

One the outcomes of the method is the large number of random k_{eff} values for each considered benchmark. The majority of these k_{eff} values are not better than the ones from JEFF-3.1.1 or JENDL-4.0, but additional information can be extracted from them. In a similar way as presented in Ref. 5 for the inelastic cross section of ^{63}Cu, correlations between the 75 benchmarks can be obtained based on the variations of the H in H_2O thermal scattering data.

The correlation between two k_{eff} benchmarks ρ_{xy} can be expressed as

$$\rho_{xy} = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{(n-1)s_x s_y} \quad , \tag{9}$$

where

x_i = random k_{eff} of the benchmark x

$\bar{x}$ = average k_{eff} of the benchmark x

y_i = random k_{eff} of the benchmark y

$\bar{y}$ = average k_{eff} of the benchmark y

s_x, s_y = standard deviations.

Correlation ρ_{xy} can be calculated for each of the 75 benchmarks, and $75 \times 75 = 5625$ correlation values can be obtained. They are plotted in Fig. 9, in a simplified ρ_{xy} scale showing large correlations (positive or negative) or weak correlations. As seen, most of the benchmarks are correlated (in fact, with positive correlation values). A few benchmarks are independent of others, such as the ict3 and lmt1 benchmarks, showing that their C/E values could be adjusted without affecting the values of the others. Also note that the plutonium and the uranium benchmarks are strongly correlated, which will make it difficult to obtain good C/E values for both types of systems by only changing the H in H_2O thermal scattering data.

VI. CONCLUSION

Using the Petten adjustment method, it is demonstrated that the H in H_2O thermal scattering data can be adjusted to obtain better C/E values for 75 thermal criticality benchmarks. Random $S(\alpha,\beta)$ were produced by randomly changing model parameters for the double-differential scattering cross section, and about 1330 random thermal scattering data for MCNP were obtained (as ACE files). Each thermal scattering data file was then benchmarked, and a large number of random H in H_2O

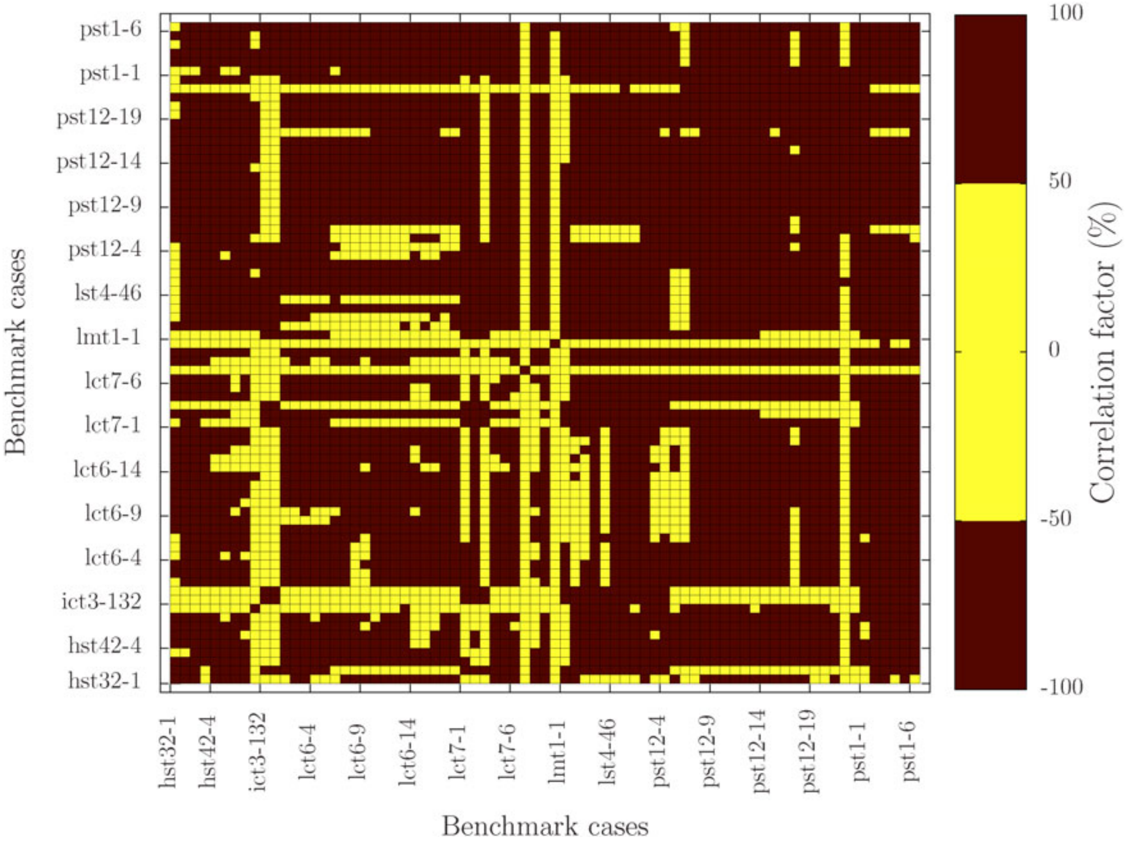

Fig. 9. Correlation between the different k_{eff} benchmarks from the random variations of the thermal scattering data of H in H_2O. Rounded values are presented to simplify the matrix.

thermal scattering data could provide better global C/E values. It is then proved that the Petten adjustment method can be applied to different types of nuclear data, from thermal scattering data to nuclear data up to 20 MeV, from structural material up to actinides. Two questions remain open. First, can the Petten adjustment method be applied to nuclear data for light elements (from hydrogen to oxygen)? Second, to which element should the method be first applied to achieve the best adjusted nuclear data library? Our future efforts will be directed to answering these two questions with the final goal being to produce one of the best (adjusted) nuclear data libraries.

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