Methodology for an efficient statistical cross sections sampling in the unresolved resonance range

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Abstract

Cross sections are crucial nuclear data that describe the probability for a particular nuclear reaction to occur between an incident particle and a target nuclide. In the context of neutron transport, accurate cross section calculations are notably crucial in that they provide the input for reactor physics and criticality safety calculations. Cross sections are computed from a large variety of models that sometimes involve experimental data, in particular to describe in detail the resonant shape of the cross sections at low energy. In this paper, the statistical contributions of compound nucleus resonances to the cross sections are investigated. This is particularly useful when artificial sets of statistical resonances must be sampled, eg. in the framework of the ladder method used to compute probability tables in the unresolved resonance range, where resonances are experimentally indistinguishable. The ladder method is a Monte Carlo based technique in which sets of resonances (called ladders) are sampled around reference energies in the unresolved resonance range from average resonance parameters. In this paper, a methodology is proposed to estimate the statistical weight of the resonances for cross sections calculations in the unresolved resonance range. This provides practical insights to determine the minimal number of resonances to be sampled in the unresolved resonance range, and the needed number of Monte Carlo histories. The methods of the present article can be extended to any physical problem based on a statistical sampling of nuclear resonances. In particular, the conclusions can be directly applied to nuclear data processing codes, to some evaluation techniques that require resonances sampling, and to Monte Carlo transport codes that handle the unresolved resonance range on-the-fly.

Keywords:
nuclear data, cross sections sampling, unresolved resonance range, processing, ladder method, elementary spingroups

1. Context and definition of the problem

Neutron-nucleus interactions are well characterized on the basis of cross sections, which are functions of the neutron energy that model the probability for particular reactions to occur. Cross sections constitute crucial input data for reactor physics and criticality safety calculations. At low energies below the continuum, resonances form sharp peaks in the cross section shape, which is intimately related to the reaction mechanisms of the compound nucleus model. Resonances arise from the coupling between the energy of the incident neutron and the discrete levels of the compound nucleus, at energies that constitute the so-called resolved and unresolved resonance ranges. In these domains, cross sections can be described using the R-Matrix theory, a semi-empirical mathematical framework developed in the late 40s by Wigner and Eisenbud [1], and further explored by Lane and Thomas [2]. R-Matrix theory relates cross sections to quantities called resonance parameters, evaluated from time-of-flight experimental data, and compiled in nuclear data libraries. Resonance parameters are mainly defined as resonance energies and resonance reaction widths, for several spingroups that do not interfere.

As the energy increases, the experimental resolution decreases, until it becomes impossible to distinguish the resonances. This defines the unresolved resonance range. In this case, the characterization of individual resonances is not possible, but average values of the resonance parameters can usually be determined. Statistical approaches are then privileged to model the fluctuations of the resonances. This is the central aspect of the well-known *ladder method* introduced by Levitt [3] to compute cross sections as probability tables in the unresolved resonance range: statistically acceptable sets of resonances are sampled in the vicinity of each reference energy at which average parameters are known. These resonance sets are called ladders, and serve to compute partial cross section values at the reference energy in question. Drawing several resonance ladders leads to a Monte Carlo procedure which results in a sampling of the possible cross section values. In the original approach of Levitt, probability tables are then derived from the sampling. This method is implemented in existing nuclear data processing codes, for instance in the PURR module of NJOY (LANL) [4], or in the module PURM of AMPX (ORNL) [5]. Let us mention that the baseline of the present work was the development of a module of the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) nuclear data processing code GAIA-2 [6], meant to handle nuclear data in the unresolved resonance range in a similar way. The present work does not deal with

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probability tables, however, and mainly focuses on the details of an efficient statistical resonance sampling. In particular, our goal is to estimate the number of resonances to draw and the required number of Monte Carlo iterations to ensure an accurate cross sections sampling.

In practice, evaluated resonance parameters are provided in the ENDF format [7], which introduces several restrictions, taken into account in our investigation. Notably, average resonance widths are only provided for elastic scattering, radiative capture, fission, and for a competitive reaction. Let us note that an average *reduced* neutron width is rather provided for the elastic scattering. Moreover, once resolved resonances have been sampled, cross sections are reconstructed using the Single-Level Breit-Wigner (SLBW) formalism of the R-Matrix theory, and $\psi-\chi$ Doppler broadening usually serves to take into account the effect of temperature. The SLBW formulas used to compute the cross sections at an arbitrary energy E are [7]:

$$\sigma_\gamma(E) = \frac{\pi}{k^2}\sum_J g_J \sum_l \sum_r \frac{\Gamma_{\gamma r}\Gamma_{nr}}{\Gamma_r^2}\psi_r \tag{1}$$

$$\sigma_f(E) = \frac{\pi}{k^2}\sum_J g_J \sum_l \sum_r \frac{\Gamma_{fr}\Gamma_{nr}}{\Gamma_r^2}\psi_r \tag{2}$$

$$\begin{aligned}\sigma_{el}(E) =& \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2(\phi_l) + \frac{4\pi}{k^2}\sum_J g_J \sum_l \sum_r \frac{\Gamma_{nr}}{\Gamma_r} \\ &\times\left[\left(\cos(2\phi_l) - 1 + \frac{\Gamma_{nr}}{\Gamma_r}\right)\psi_r - \sin(2\phi_l)\chi_r\right],\end{aligned} \tag{3}$$

where the sum is performed over all resonances r of a same spingroup (l, J) ; the subscript r applies here to the resonance parameters (energy, and widths Γ_n, Γ_γ, Γ_f, Γ) specific to the sampled resonance r. In the equations above, g_J is the statistical spin factor, k is the wave number, ϕ_l the hard-sphere phase shift, whose expressions can be found in reference [7]. ψ_r and χ_r are the Voigt profiles which depend on the temperature T and make use of the complex Faddeeva function, defined as $w(z) = e^{-z^2}\mathrm{erfc}(-iz) = e^{-z^2}\left(1 + \frac{2i}{\sqrt{\pi}}\int_0^z e^{t^2}dt\right)$, so that:

$$\psi_r(x,\zeta) = \frac{\sqrt{\pi}}{2\zeta}\mathrm{Re}\left[w\left(\frac{x}{2\zeta}, \frac{1}{2\zeta}\right)\right] \tag{4}$$

$$\chi_r(x,\zeta) = \frac{\sqrt{\pi}}{2\zeta}\mathrm{Im}\left[w\left(\frac{x}{2\zeta}, \frac{1}{2\zeta}\right)\right] \tag{5}$$

$$\text{using} \quad x = \frac{2(E'_r - E)}{\Gamma_r} \quad \text{and} \quad \zeta = \frac{\Delta}{\Gamma_r} \tag{6}$$

where $\Delta = 2\sqrt{\frac{|E|Mk_BT}{m}}$ is the Doppler width, and E'_r is the resonance energy, slightly shifted for l-values greater than 0 (cf. [7]). When T = 0 K, the expressions of ψ_r and χ_r are much simpler:

$$\psi_r(x,\zeta) = \frac{x}{1+x^2} \quad \text{and} \quad \chi_r(x,\zeta) = \frac{1}{1+x^2} \tag{7}$$

It is clear from these expressions that even if all resonances contribute to the cross sections calculated at an energy E, the more distant resonances have smaller weights because of the $(E'_r - E)^2 + \Gamma_r^2/4$ term in the denominator of the formulas. Moreover, elastic scattering plays a particular role compared to capture and fission, as the reaction entrance channel is necessary an elastic channel in the R-Matrix theory. The elastic scattering expression is correspondingly more complex, and shows an interference term.

Let us take an example to illustrate this. For this purpose, a ladder of 200 resonances has been randomly sampled for a single spingroup of ^{235}U at 2.25 keV, and the contribution of each resonance to the cross section values computed at this energy has been computed. These contributions for indexed resonances above and below 2.25 keV have been plotted in Figure 1 for the three reactions.

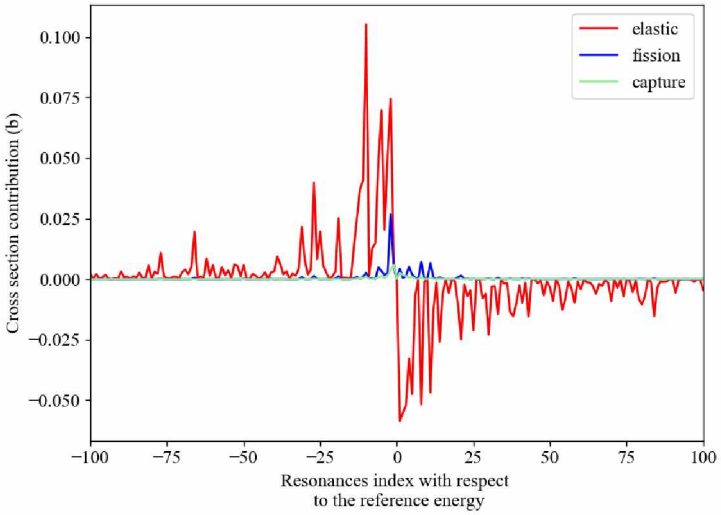

Figure 1: Contributions of resonances around a reference energy E = 2.25 keV to the cross sections calculated at this energy, for a random ladder of the spingroup (l = 0, J = 3) of ^{235}U.

The statistical decrease of the resonance contributions for each reaction is clearly apparent in Figure 1. The interference effect for the elastic scattering is also explicit: resonances above the energy of calculation bring negative contributions, as opposed to resonances below. Resonance contributions are thus likely to compensate each other for elastic scattering, resulting in a more complex situation.

This example provides an insight of the questions that we would like to address in our work: what is the statistical contribution of the resonances to the cross sections in the unresolved resonance range, or more pragmatically, how many resonances should be at least considered to ensure an accurate calculation of the cross sections at a given energy ? For the practical case of the ladder method, this indicates the number of resonances to sample. Before establishing a methodology to answer this question, it is of interest to describe in detail the sampling techniques used in the framework of the ladder method.

2. One by one resonance sampling strategies

The resonance sampling makes use of the statistical distribution laws of the resonance parameters. Usually, it is as-

sumed that the resonance *spacing* follows the Wigner surmise $W(x) = \frac{\pi}{2} x e^{-\frac{\pi}{4}x^2}$, and that reaction widths follow χ^2 distributions with certain degrees of freedom, provided in the evaluation. In fact, both these theoretical distributions are derived from a more rigorous mathematical framework used to model the nuclear energy levels statistics, which is the random matrix theory. For instance, the Wigner surmise corresponds to the law of the spacing between eigenvalues of a random matrix from the so-called Gaussian Orthogonal Ensemble (GOE) of size 2×2 only [8]. The use of the random matrix theory to replace the Wigner surmise for the resonance spacing is not dealt with presently in the processing codes. For now let us adhere to the usual practice, which is a one by one sampling of resonances. As such, correlations are not taken into account between resonances when one relies on the Wigner surmise and χ^2 distributions.

2.1. Choice of a starting point

One by one ladder sampling can be implemented in two ways, which correspond to the two possible choices of the first resonance to sample. A possible approach, implemented in the NJOY code, consists in setting up the energy limits of the resonance ladder E_1 and E_2, before filling it with successive resonances starting from the leftmost energy [4]. In order not to select E_1 as the first resonance energy for all ladders, a random shift can be introduced. For instance, the first resonance for each spin sequence can be legitimately placed at $E_{r,1} = E_1 + \xi\overline{D}$ ($\overline{D}$ being the average spacing between resonances for the considered spingroup, and ξ being sampled from an uniform distribution $\mathcal{U}[0, 1[$). Then, resonances are sampled one by one, until E_2 is reached. E_1 and E_2 must be chosen carefully so that enough resonances are sampled within the ladders, which is usually performed using *ad hoc* practices.

The second approach aims at sampling the resonances around the reference energy directly. This method has been initially implemented in a code called URR [9], and then in the module PURM of the AMPX code system [5]. First, a central spacing D_0 between the resonances surrounding the reference energy must be obtained. As previously, this central spacing must be randomly shifted for each ladder, in order to avoid a perfect symmetry between the first resonances. For example, the first resonances for each spin sequence can be placed at $E_{r,1} = E_{ref} + \xi D_0$ and $E_{r,-1} = E_{ref} + (1 - \xi)D_0$ ($\xi \sim \mathcal{U}[0, 1[$). Then, resonances can be drawn successively above and below the reference energy from these two resonances. Compared to the NJOY approach, the problem is shifted from the definition of energy limits $[E_1, E_2]$ to a possible condition on the sufficient number of resonances needed to compute cross sections, which looks more flexible. In order to avoid asymmetry effects, the same number of resonances must be sampled on each side. In practice, resonances are thus sampled as *pairs* around the reference energy.

Both sampling methods are illustrated in Figure 2.

2.2. About the central spacing

Both approaches are in fact exactly equivalent if enough resonances are sampled. To be more precise, special attention

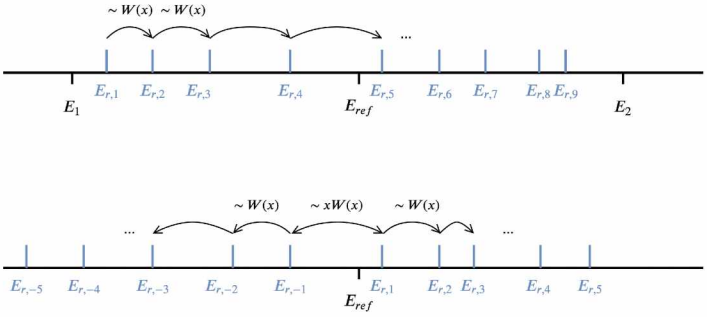

Figure 2: Successive samplings of resonances energies. The NJOY-like method determining $[E_1, E_2]$ is displayed on the upper figure. The bottom figure shows the AMPX-like method, where pairs of resonances are sampled around the reference energy.

should be paid to the central spacing, defined as the spacing that surrounds the reference energy. Indeed, in the NJOY approach, it[1] does not follow the Wigner surmise but a slightly modified distribution. In fact, the present situation is an application case of the so-called bus waiting time paradox [10]. It can be proved that the asymptotic distribution followed by the central spacing is[2] $W^*(x) = xW(x) = \frac{\pi}{2} x^2 e^{-\frac{\pi}{4}x^2}$. To our knowledge, this subtlety has not been stressed in literature. It has some strong consequences. For instance, one may remark that the statistical average value of central spacing is thus $\frac{4}{\pi}\overline{D}$ which is larger than the mean spacing between resonances.

It must be underlined that the W^* distribution constitutes an asymptotic result, valid in case of an infinite ladder. For the AMPX method, the central spacing can be directly chosen to follow W^*. For the NJOY approach, on the other hand, the lower energy limit of the ladder E_1 has to be chosen far enough from the reference energy so that the central spacing approximately follows W^*. In the general case, the choice of E_1 depends on the distribution law of the spacing. Here, a numerical simulation has been performed using the Wigner surmise. For several numbers of resonances N, E_1 has been chosen at energy[3] $E_{ref} - N\overline{D}$, and many ladders have been randomly sampled. The resulting histogram of the obtained central spacings is displayed in Figure 3, along with the theoretical W and W^* distributions.

It appears that after a very few resonances only (4 on average), the central spacing distribution gets close to the asymptotic result W^*. In practice, this criterion is always met. As a consequence, both sampling strategies behave equivalently. In the rest of this article, the calculations are made with the GAIA-2 code following the AMPX method for the resonance sampling, that is the paired sampling.

The remaining questions concern the number of resonances to be sampled and the number of Monte Carlo iterations to perform in order to ensure correct cross section sampling.

[1] The interest here is about the spacing distribution over all the Monte Carlo trials.

[2] This is true here because the Wigner surmise has a mean equal to one.

[3] Choosing $\overline{D} = 1$ is the most straightforward choice and does not change the issue.

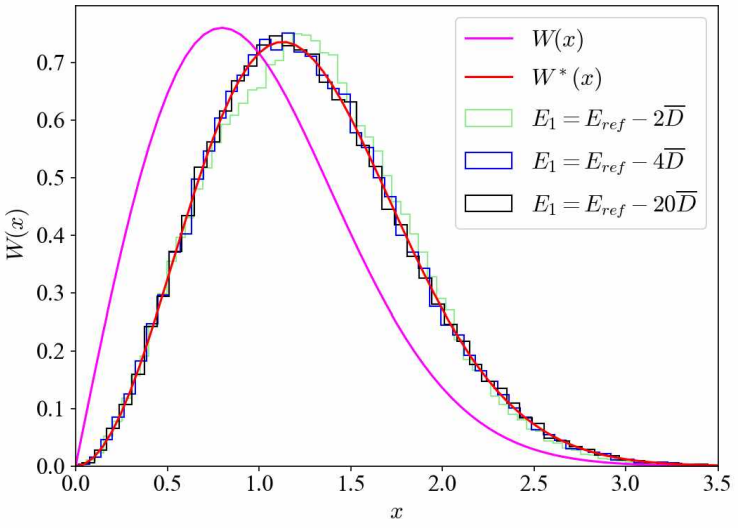

Figure 3: Convergence of the central spacing distribution to $W^*(x) = \frac{\pi}{2}x^2e^{-\frac{\pi}{4}x^2}$ for several choice of the left limit of the ladders.

3. A methodology to estimate the required numbers of resonances and Monte Carlo iterations to perform in the ladder method

As mentioned in Section 1, all resonances contribute to cross sections calculated at the reference energy E_{ref}, but distant resonances tend to contribute less[4]. In order to ensure the quality of the cross section sampling, it is extremely valuable to make sure enough resonances are sampled in the ladders, so that no significant contribution is missed. Let us stress that this latter statement has to be envisaged from a statistical point of view, that is, the n^{th} resonance contribution should only be considered averaged over many ladders. In other words, the outputs which have to be looked upon are the cross section samplings, which approach probability distributions. This suggests another issue, which is the impact of the amount of Monte Carlo iterations on the cross section samplings. In fact, both questions can be treated with very similar tools, as shown in the following.

The question of the statistical contribution of the resonances to the cross sections obviously depends on the resonance parameters. That implies that the inputs have to be carefully considered. In this paper, an ensemble of input parameters is introduced, called *elementary spingroups*.

3.1. Elementary spingroups

In practice, cross section samplings are performed around reference energies E_{ref} at which resonance parameters have been tabulated[5] for a given nuclide. A crucial point to underline is the conservation of total angular momentum J during a compound nucleus reaction. In addition, the conservation of the orbital angular momentum l is usually assumed in the evaluations as well. As a consequence, cross sections for a particular nuclide at a given energy are the sum of several contributions from spingroups that do not interfere, as actually displayed in Equations (1) to (3). Each subcalculation thus relies on 17 *scalar* parameters, that can be classified as follows:

1. Five nucleus-only related quantities: the target mass and spin, the competitive threshold, and two values for the scattering channel radius[6]. These quantities intervene in the calculation of the channel wave number, hard-sphere phase shift, and penetrabilities ;
2. One reference energy E_{ref}: the resonance parameters are defined at the reference energy, which is also the retained energy for the cross section calculations in this work[7]. Penetrabilities, wave number and neutron width are energy-dependent ;
3. Ten spingroup related quantities: the quantum numbers l and J, the resonance average spacing $\overline{D}$, four average widths (reduced neutron $\overline{\Gamma_n^0}$, capture $\overline{\Gamma_g}$, fission $\overline{\Gamma_f}$ and competitive $\overline{\Gamma_x}$), and their associated degrees of freedom (ν_n, ν_g, ν_f, ν_x). As many channels are open for capture, the degree of freedom for this reaction is huge. The ENDF format even imposes[8] the Dresner approximation, $\nu_\gamma \to \infty$, so that the degree of freedom for capture can be discarded as a relevant input parameter for our needs.
4. One temperature T, which is the only input parameter whose value is fixed by the user rather than found in libraries. This quantity plays no role in the resonance sampling, but intervenes at the cross section reconstruction step, when Doppler-broadening is taken into account.

From these considerations, it is possible to decompose a whole nuclear data library in the unresolved resonance range into a collection of sets of 16 scalar parameters[9], called now *elementary spingroups*, which serves as a basis of input cases to estimate the statistical weight of resonances. For instance, the nuclear data library JEFF-3.2 [11] can be turned from 307 nuclides for which an unresolved resonance range is defined into 41 486 elementary spingroups. JEFF-3.2 has been chosen because it includes many nuclides with an unresolved range, and is a good candidate to explore the unresolved resonance parameters phase space. The major interest of using elementary spingroups in place of nuclides is the ability to relate the resonance parameters to the outcome of the resonance sampling, and to provide physical interpretations. This will be discussed in our work, where the converted JEFF-3.2 library is used as a representative collection of the diversity of the nuclides, and of the computational effort in the unresolved resonance range when a whole library is processed.

[4] As mentioned, the resonance contributions are quite different for the considered reactions, and in particular for elastic scattering, which presents an interference phenomenon.

[5] Even if additional energies can be considered relying on parameter interpolations.

[6] The fact two radii can be provided is a trick of the ENDF format in order to give to the evaluators more "knobs". The evaluated files indicate the appropriate use of the radii using dedicated flags.

[7] One must note that this constitutes a choice of the present study, which seemed to be the most conservative. In particular, this is not the approach adopted by NJOY in the PURR module, where cross sections are reconstructed over a whole random energy grid, and directly stored in a probability table.

[8] Using the convention $\nu_\gamma = 0$ in the evaluated files.

[9] Excluding the temperature.

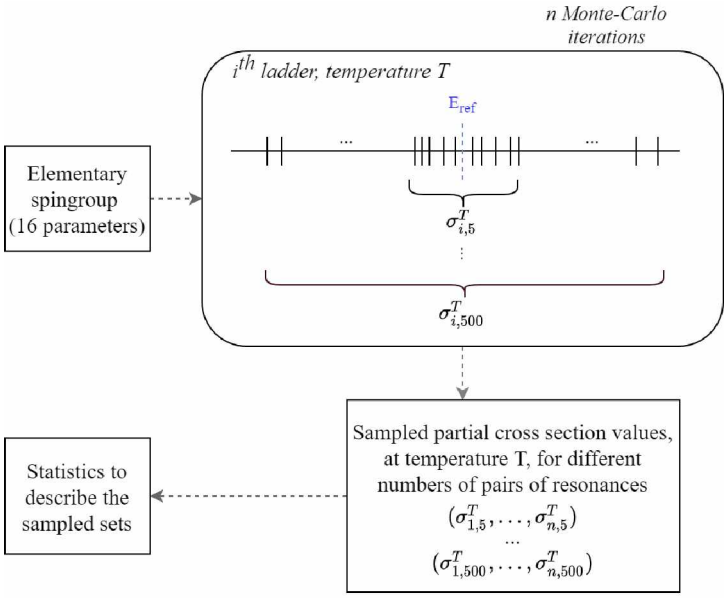

Figure 4: Computations methodology to estimate the required number of resonances to sample in the ladders.

3.2. Methodology for the number of resonances in the ladders

Once elementary spingroups have been identified as the relevant input quantity, a methodology to estimate the required number of resonances to sample for each of them can be established. As said before, considering a single ladder is meaningless. Here, the objective is to look at the outcome of the Monte Carlo procedure, that is, to the obtained cross section samplings that approach the underlying probability distributions of the partial cross section values at the reference energy. When it comes to describe and compare several samplings, statistics are required. Here, the four first moments of the samplings have been considered (mean, variance, skewness, and kurtosis), as well as several percentile statistics (1st quartile, 3rd quartile, and 95th percentile), and the two-sample Kolmogorov-Smirnov distance, that measures the absolute difference between empirical distribution functions associated to two samplings.

The principle is thus to estimate the impact of using ladders of different sizes (ie. composed of an increasing number of resonances) on the resulting cross sections calculated at the reference energy for each elementary spingroup, on the basis of the aforementioned statistics. Instead of sampling several ladders of different sizes directly, the following methodology is adopted for each elementary spingroup: first, a very large ladder is drawn using the paired sampling method. For the purposes of this study, 500 pairs of resonances have been sampled in the ladders. Then, cross sections have been computed considering increasing numbers of pairs of resonances, starting from the central ones. More precisely, cross sections values for elastic scattering, capture, and fission reactions have been computed at the reference energy, considering only the 5 first pairs of resonances around the reference energy, then 10, 15, and so on until 50, then 60, 70, and so on until the whole ladder (500 pairs) was taken into account. As a consequence, differences between cross sections obtained for ladders of different sizes were only due to the additional resonances considered, and no longer depended on the fluctuations of the first common resonances. At the end of the Monte Carlo sampling, several cross sections sets have been obtained considering increasing numbers of pairs of resonances. Then, the several statistics that describe the cross sections samplings have been computed, and compared to the 500-pairs result, considered as an "asymptotic" result[10]. It must be pointed out here that nothing ensures *a priori* this amount to be large enough to ensure asymptotic calculations. Nonetheless, results seem to indicate this is quite a good approximation. In order to take into account the effect of the temperature, the cross sections calculations have been performed at T = 0 K and T = 293.6 K using the same resonance ladders. The method is depicted in Figure 4.

3.3. Methodology for the number of Monte Carlo iterations

A very similar method has been adopted to estimate the impact of using additional Monte Carlo iterations on the resulting cross section samplings. Actually, the more iterations the better, but it is very relevant to provide an estimation of the convergence speed of the cross sections samplings towards the underlying probability distributions, in order to provide an estimation of a sufficient number of iterations. For each particular elementary spingroup, samplings composed of increasing numbers of Monte Carlo iterations have been compared. There, ladders have been chosen wide enough in order to get rid of the bias due to the finite number of sampled resonances, and 500 pairs have been considered. Contrary to the previous case, different random seeds have been considered in each case to take into account the randomness of the samplings, as a statistical uncertainty is estimated. The retained method is summarized in Figure 5.

In this work, we have chosen to compare samplings of size 10 000 and 20 000, and then to address the next order of magnitude, with 100 000 and 200 000 Monte Carlo iterations.

4. Statistical weight of resonances

4.1. Convergence for the several statistics

Calculations have been performed using a slightly modified version of the GAIA-2 code developed at IRSN, which enabled to implement the proposed methodologies. The statistical contribution of resonances has been investigated first. The convergence of the cross sections samplings statistics according to the number of pairs of resonances considered in the ladders is illustrated using *convergence plots* as in Figures 6 to 8 that correspond to the elastic, capture, and fission reaction respectively, at T = 0 K. Each subplot corresponds to a statistical quantity of interest, and each line represents the behavior of a single elementary spingroup[11]. The percentage difference to the asymptotic 500-pairs result is there displayed as a function of the size of the

[10] That means, as if an infinite number of resonances were sampled.

[11] This makes 41 486 lines for each elastic or capture plot, and only 5311 ones for fission as not all nuclides of JEFF-3.2 are fissionable.

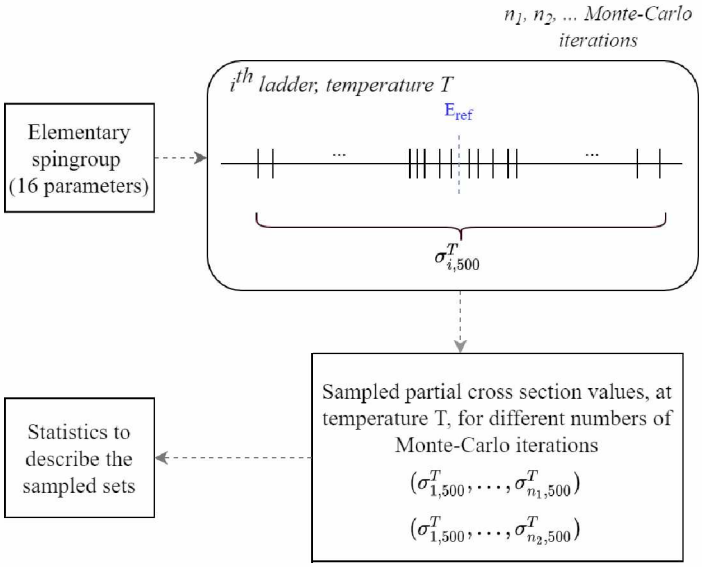

Figure 5: Computations methodology to estimate the number of Monte Carlo iterations to be run in the ladder method.

ladders, expressed in pairs of resonances. The cross sections samplings have been performed using 100 000 Monte Carlo iterations. The bottom-right subplot in both figures displays the outcomes for the Kolmogorov-Smirnov distance ; the absolute difference between the empirical distribution is computed between the 500-pairs sampling and the samplings obtained from fewer resonances. This quantity scales over [0, 1], but the outcome has been multiplied by 100 to be displayed on the same scale than the other statistics. For all statistics, the red line corresponds to the less converged case, that is the elementary spingroup for which the 490-pairs outcome differs the most from the 500-pairs result. The corresponding nuclide, energy, and quantum numbers l and J have been indicated on the figures. The next 50 less converged cases are also drawn in orange.

These graphs call several comments. First of all, it appears clearly that more resonances have to be sampled to obtain statistically accurate elastic scattering cross sections than for capture or fission, due to the interference effect depicted in Figure 1. This effect is explicit considering the mean statistics for instance. For the capture and fission, the mean always converges to the 500-pairs result from below, because each resonance brings a positive contribution. This is not necessarily the case for elastic scattering, hence the fact that some elementary spingroups seem to converge from above. The same considerations apply to the quantile-like statistics. For the variance, the convergence is from below for all reactions, which indicates that the variance is always larger for the 500-pairs samplings. This is probably because computations make use of nested ladders, so that the dispersion of cross sections is more important for larger ladders. For skewness and kurtosis, that respectively measure the probability distribution asymmetry and the weight of the tails compared to the central part, the situation differs between capture or fission, and elastic scattering. For capture and fission, the convergence is very fast and from above, which implies that the weight of the right tail of the distribution is reduced when more resonances are considered in the ladders. As a consequence, cross sections samplings obtained from larger ladders are more regular, which means that their values are closer to the mean (when corrected from dispersion, which is measured from the variance). There is thus a stabilization effect for large ladders. For elastic scattering, the situation is slightly more complex; skewness and kurtosis seem to be harder to converge than the mean and variance[12]. For some hundreds of cases, adding a dozen of resonances seem to be enough to impact the convergence. Finally, the Kolmogorov-Smirnov distance regularly converges from above, which comes from its definition.

These calculations, performed over all the data contained in JEFF-3.2, prove that elastic scattering is the more constraining reaction to take into account the long-range contributions of resonances. That being said, one may also remark that more resonances are often required for accurate fission cross section calculations than for capture, while SLBW Equations (1) to (2) are similar. This is notably explicit for the moment statistics. This can be simply explained, reminding that the degree of freedom for the capture width is set to zero, contrary to fission[13]. As a consequence, large fission widths are likely to be sampled, given further resonances a greater weight, hence the difference between fission and capture.

It must be stressed out however that, for almost all the elementary spingroups, the convergence is very fast. In order to highlight this statement, the percentages of "converged" cases after some arbitrary numbers of pairs of resonances (10, 50, 200, 490) have been summarized in Tables 1 to 3 for the several reactions. There, an elementary spingroup is said to be converged if, after a given number of pairs of resonances, the relative difference of the statistics of interest compared to the 500-pairs result is below a given threshold. For the purposes of this study, a threshold of 0.1% has been considered.

Level ϵ = 0.1%	**Mean**	**Var.**	**Skew.**	**Kurt.**
≤ 10 pairs	72.87 %	74.91 %	74.07 %	72.47 %
≤ 50 pairs	95.76 %	84.91 %	83.72 %	81.66 %
≤ 200 pairs	99.90 %	97.18 %	96.23 %	94.58 %
≤ 490 pairs	100.0 %	100.0 %	99.92 %	99.95 %
	Qt1	**Qt4**	**95 Pct.**	**K.S.**
≤ 10 pairs	0.11 %	0.32 %	26.76 %	0.0 %
≤ 50 pairs	3.85 %	10.67 %	57.13 %	0.0 %
≤ 200 pairs	32.49 %	76.90 %	88.26 %	5.30 %
≤ 490 pairs	98.68 %	100.0 %	100.0 %	100.0 %

Table 1: Proportion of cases for which the statistics values of the elastic cross section samplings converged for less resonances than indicated, for level of convergence ϵ = 0.1%. The convergence is measured from the percentage difference to the 500-pairs result.

[12] It is expected higher moments behave equivalently.
[13] It varies between 1 and 4 in JEFF-3.2.

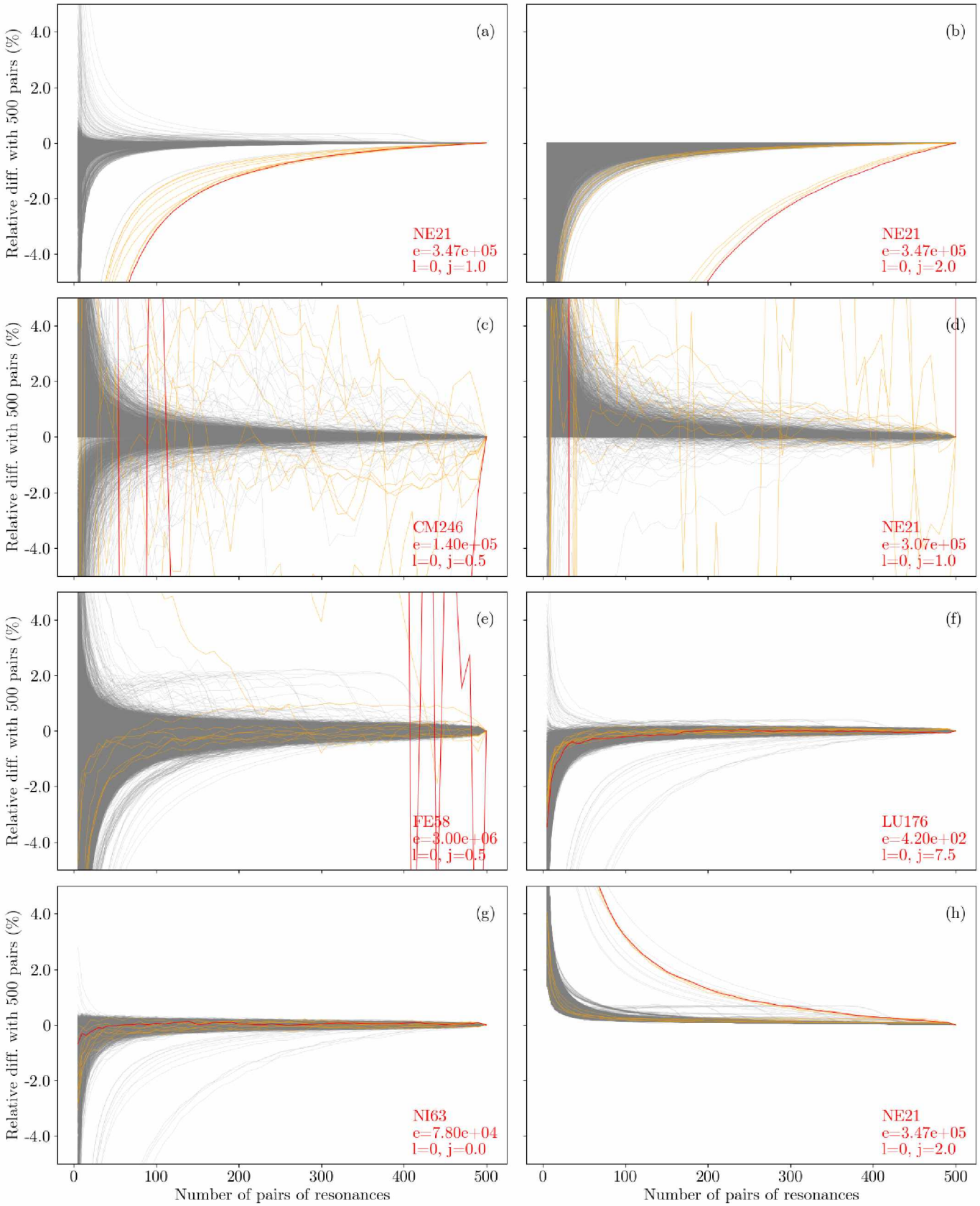

Figure 6: Convergence of various statistics of the sampled elastic cross sections toward the reference (500 pairs of resonances), at T = 0 K. (a) mean, (b) variance, (c) skewness, (d) kurtosis, (e) first quartile, (f) fourth quartile, (g) 95^{th} percentile, (h) Kolmogorov-Smirnov distance

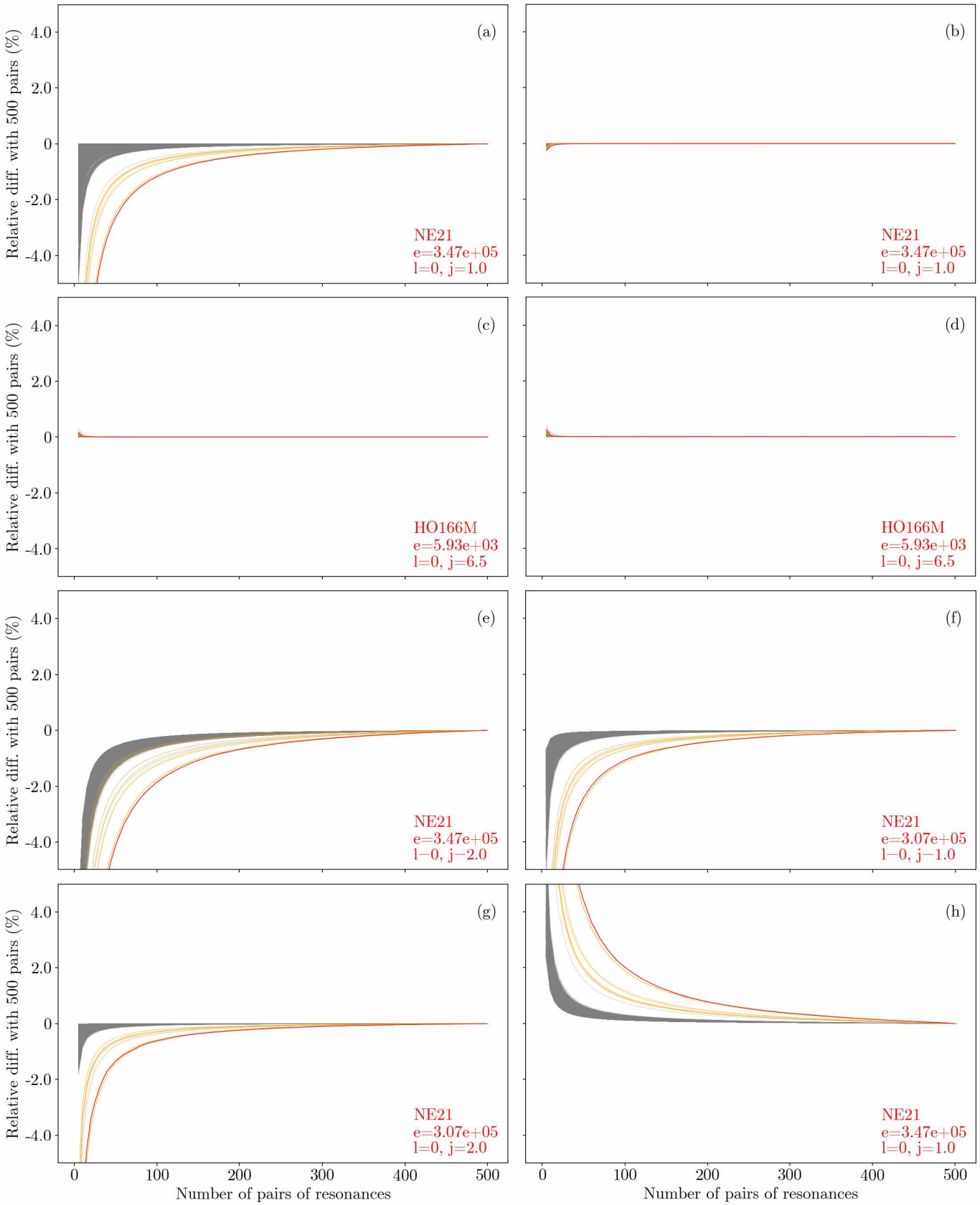

Figure 7: Convergence of various statistics of the sampled capture cross sections toward the reference (500 pairs of resonances), at T = 0 K. (a) mean, (b) variance, (c) skewness, (d) kurtosis, (e) first quartile, (f) fourth quartile, (g) 95^{th} percentile, (h) Kolmogorov-Smirnov distance

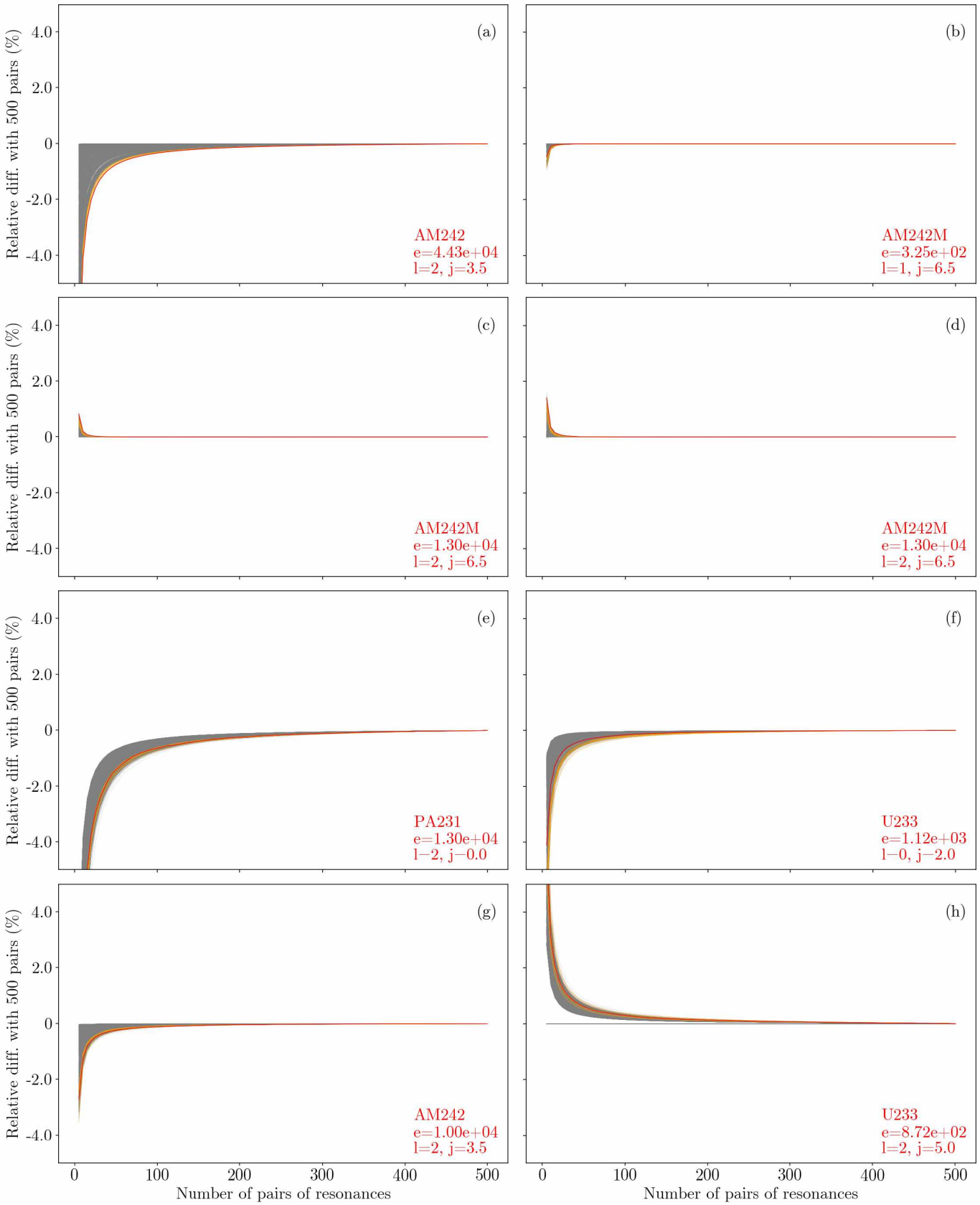

Figure 8: Convergence of various statistics of the sampled fission cross sections toward the reference (500 pairs of resonances), at T = 0 K. (a) mean, (b) variance, (c) skewness, (d) kurtosis, (e) first quartile, (f) fourth quartile, (g) 95^{th} percentile, (h) Kolmogorov-Smirnov distance

Level $\epsilon = 0.1\%$	**Mean**	**Var.**	**Skew.**	**Kurt.**
≤ 10 pairs	68.05 %	99.99 %	99.99 %	99.98 %
≤ 50 pairs	96.13 %	100.0 %	100.0 %	100.0 %
≤ 200 pairs	99.97 %	100.0 %	100.0 %	100.0 %
≤ 490 pairs	100.0 %	100.0 %	100.0 %	100.0 %
	Qt1	**Qt4**	**95 Pct.**	**K.S.**
≤ 10 pairs	0.0 %	97.44 %	99.97 %	0.0 %
≤ 50 pairs	98.88 %	99.97 %	99.99 %	99.97 %
≤ 200 pairs	100.0 %	100.0 %	100.0 %	100.0 %
≤ 490 pairs	100.0 %	100.0 %	100.0 %	100.0 %

Table 2: Proportion of cases for which the statistics values of the capture cross section samplings converged for less resonances than indicated, for level of convergence $\epsilon = 0.1\%$. The convergence is measured from the percentage difference to the 500-pairs result.

Level $\epsilon = 0.1\%$	**Mean**	**Var.**	**Skew.**	**Kurt.**
≤ 10 pairs	28.69 %	95.57 %	95.19 %	91.41 %
≤ 50 pairs	70.92 %	100.0 %	100.0 %	100.0 %
≤ 200 pairs	99.03 %	100.0 %	100.0 %	100.0 %
≤ 490 pairs	100.0 %	100.0 %	100.0 %	100.0 %
	Qt1	**Qt4**	**95 Pct.**	**K.S.**
≤ 10 pairs	0.0 %	77.70 %	93.466 %	0.0 %
≤ 50 pairs	32.31 %	100.0 %	100.0 %	100.0 %
≤ 200 pairs	100.0 %	100.0 %	100.0 %	100.0 %
≤ 490 pairs	100.0 %	100.0 %	100.0 %	100.0 %

Table 3: Proportion of cases for which the statistics values of the fission cross section samplings converged for less resonances than indicated, for level of convergence $\epsilon = 0.1\%$. The convergence is measured from the percentage difference to the 500-pairs result.

As an example, after only 50 pairs of resonances, around 95.76% of the elementary spingroups of JEFF-3.2 reach an elastic mean value closer than 0.1% to the 500-pairs outcome. That means that, taking a random test case, accurate results are likely to be obtained with a few resonances only. It must be stressed that the hard-to-converge cases are not related to the usual differentiation between "heavy" or "light" nuclides: the lightest ^{21}Ne, the medium ^{55}Mn, and the heavy ^{242}Am require many resonances, whereas the second-lightest ^{22}Na converges quickly. A better criterion to discriminate between the cases that require many resonances and the others is thus of high interest, and is addressed in the following.

4.2. Role of the resonance parameters

The most interesting question is about the impact of the resonance parameters on the required number of resonances in the ladders. In other words, why some elementary spingroups seem to converge faster than others ? As a first step, a criterion is required to state whether enough resonances have been sampled. As previously, the most straightforward way is to consider a threshold for the relative difference between the 500-pairs outcomes and the statistics values considering fewer resonances. The threshold value is arbitrary, and depends on the precision of the convergence required. Thus, for each statistics and reaction, the minimal number of resonances for which the threshold is reached can be deduced for each elementary spingroup. It is then possible to look for a relation between the 16 scalar parameters of each elementary spingroup that could provide an insight about the number of required resonances.

After several attempts, a very interesting quantity turned out to be the strength-like ratio $\overline{\Gamma}/\overline{D}$ of the total average width associated to the elementary spingroup, and the average spacing. The competition between the $\overline{\Gamma}$ and $\overline{D}$ plays a major role in the Single-Level Breit-Wigner formulas, where it notably appears in the cross sections denominator. The average total width $\overline{\Gamma}$ is evaluated here at the reference energy of the elementary spingroup[14]:

$$\overline{\Gamma} = \overline{\Gamma_n}(E_{ref}) + \overline{\Gamma_\gamma} + \overline{\Gamma_f} + \overline{\Gamma_x} \tag{8}$$

It must be stressed out that a proper definition of this quantity is thus possible in the framework of the elementary spingroups calculations. In order to fix the ideas, for most elementary spingroups of JEFF-3.2 the ratio $\overline{\Gamma}/\overline{D}$ is below 1, which is typical of the unresolved resonance range. The median value is around 10^{-2}, while the maximal found ratio equals 4.552, and is obtained for the upper limit of the unresolved resonance range of the first spingroup of the light nuclide ^{21}Ne, namely $E_{ref} = 0.347221$ MeV, $l = 0$, $J = 1$.

The required numbers of pairs of resonances estimated for each elementary spingroup to reach a relevant level of convergence compared to the asymptotic case have been plotted against the corresponding $\overline{\Gamma}/\overline{D}$ values in Figure 9 for T = 0 K. The threshold level has been set to 0.1% of the reference 500-pairs outcome.

From Figure 9 a positive relation between the number of resonances to be sampled in the ladders and the $\overline{\Gamma}/\overline{D}$ value emerges. Physically, that means the bigger the resonances spacing is compared to the total width, the less resonances are required. This result is not surprising, considering the previous discussions about the influence of the distant resonances, and the competition between the spacing and the total width in Equations (1) to (3). The present calculations clarify this competition.

For capture and fission, the number of required resonances as a function of $\overline{\Gamma}/\overline{D}$ seems to follow an exponential-like growth for all statistics once $\overline{\Gamma}/\overline{D}$ exceeds a particular value. This remains of course a crude statement. In particular, identifying a precise threshold value of $\overline{\Gamma}/\overline{D}$ so that more resonances are required depends on the convergence precision required (here 0.1%). For elastic scattering, the situation is even more complicated, because the cross sections have a more complex shape. A

[14] To be more precise, the neutron width is evaluated at the reference energy from the reduced neutron width.

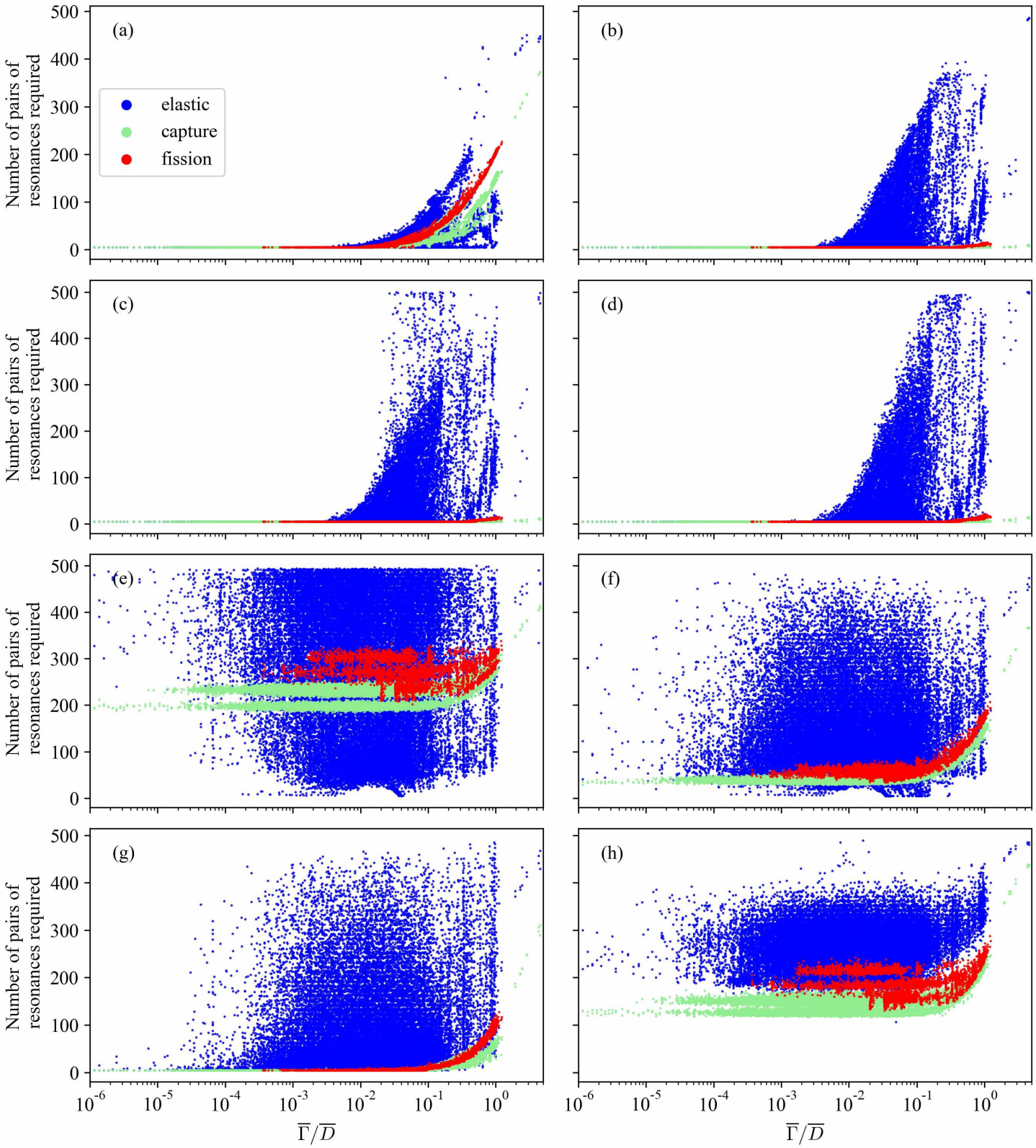

Figure 9: Required number of resonances to reach close to 0.1% of the 500-pairs values for each spingroup, plotted against their $\overline{\Gamma}/\overline{D}$ value, at T = 0 K. Each figure corresponds to a statistics of interest: (a) mean, (b) variance, (c) skewness, (d) kurtosis, (e) first quartile, (f) fourth quartile, (g) 95^{th} percentile, (h) Kolmogorov-Smirnov distance

positive correlation appears for most statistics, even if some elementary spingroups with high $\overline{\Gamma}/\overline{D}$ ratio are converged after a few resonances only. Nonetheless, some very relevant practical conclusions can be drawn.

Approximately half of the cases encountered in JEFF-3.2 have a $\overline{\Gamma}/\overline{D}$ ratio below 10^{-2}. For very important statistics such as the first moments, elementary spingroups with smaller $\overline{\Gamma}/\overline{D}$ than 10^{-2} are converged up to 0.1% compared to the 500-pairs result after a dozen of resonances only. This means that special attention should be paid on the contrary to the elementary spingroups with greater ratios. This statement will be made more precise further. Let us focus on the second important aspect of this work, which is the estimation of a sufficient number of Monte Carlo iterations.

5. Number of Monte Carlo iterations

The methodology proposed in Section 3.2 for the number of Monte Carlo iterations has been implemented using a slightly modified GAIA-2 version once again. For each elementary spingroup, cross section samplings obtained with several numbers of Monte Carlo iterations have been compared using the previous moment and quantile statistics. There, large ladders of 500 pairs of resonances have been used at each iteration. The relative differences between samplings composed of 10 000 and 20 000 iterations have been computed, as well as between 100 000 and 200 000 iterations. These relative differences are displayed in Figure 10 for T = 0 K, on the left and right columns respectively. On these graphs, the x-axis displays the indexed 41 486 elementary spingroups of JEFF-3.2, so that each elementary spingroup is represented by a point. Elementary spingroups have been sorted in ascending $\overline{\Gamma}/\overline{D}$ values, which appeared as a relevant quantity according to the previous analysis. The x-axis has not been chosen as the $\overline{\Gamma}/\overline{D}$ quantity directly, although such a choice would have been possible. However, it turned out that choosing an x-axis where all points are arbitrarily fixed and equally distant was just more efficient to exhibit the calculations sensibility to fluctuations. To be more precise, setting the $\overline{\Gamma}/\overline{D}$ as the x-axis would have resulted in many points in the middle of the graphs, making it less readable. As a consequence, sorted-indexed x-axis were preferred for the present analysis.

Two main conclusions can be drawn from Figure 10. First of all, it is clear that the relative difference between 100 000 and 200 000 iterations is smaller for all statistics than between 10 000 and 20 000 iterations. This is a strong insight of the validity of the ladder method. When the number of iterations is doubled, the statistics are more stable at the next order of magnitude. This also suggests that performing only 10 000 Monte Carlo trials is not sufficient in numerous cases, as a 100% difference is regularly reached for moments-related statistics of the elastic scattering.

The second important conclusion is related to the influence of the resonance parameters. There, an apparent correlation emerges between low $\overline{\Gamma}/\overline{D}$ values and high percentage differences, especially for the mean. This means elementary spingroups with large average spacings compared to the average total width are likely to require more Monte Carlo iterations for the calculations to be accurate.

This behavior is actually related to the apparent size of the sampled ladders at the reference energy. As seen previously, low $\overline{\Gamma}/\overline{D}$ lead to only a few resonances contributing to the cross sections at E_{ref}. However, this also means that their randomness is less susceptible to be compensated by other resonances from the ladder. In other words, when $\overline{\Gamma}/\overline{D}$ is huge, many resonances from the 500-pairs ladders effectively contribute to the cross sections, so that, from the point of view of random number generation, more generated numbers are taken into account. As a consequence, the Monte Carlo technique that underpins the ladder method is more efficient and less ladders are required.

From these considerations, a trade-off seems to emerge. Large $\overline{\Gamma}/\overline{D}$ values suggest that large ladders must be sampled. On the other hand, small $\overline{\Gamma}/\overline{D}$ imply more Monte Carlo iterations. This has some serious implications for the computational effort required to produce accurate cross sections. It is relevant to consider the temperature effect before concluding.

6. Effect of the temperature

The same calculations to statistically estimate the necessary numbers of resonances and Monte Carlo iterations have also been performed at room temperature, at T = 293.6 K. There, the same sampled ladders have been used, but the cross sections have been calculated taking into account a $\psi - \chi$ Doppler broadening. Let us focus on the changes induced by taking into account the temperature.

6.1. Number of resonances

The obtained convergence plots are very similar to those of the T = 0 K case, except for a very important detail: overall, more resonances are required to obtain the same level of convergence to the 500-pairs result. This is notably true for the variance, which has been plotted in Figure 11 for elastic scattering, Figure 12 for the capture, and Figure 13 for the fission reaction[15]. The same applies for the mean, skewness and kurtosis especially, even if the effect is less marked. This phenomenon is simply explained, reminding that the Doppler effect broadens the cross sections around the resonances. As a consequence, farther resonances are likely to have a more significant contribution than at T = 0 K.

There again, the $\overline{\Gamma}/\overline{D}$ ratio looks like a relevant quantity. More resonances are needed for elementary spingroups with high ratios. Figure 14 displays for all statistics the relation between the number of pairs of resonances required and the $\overline{\Gamma}/\overline{D}$ ratio of all elementary spingroups of JEFF-3.2. The figure looks slightly more complex than Figure 9, but the correlation between the two quantities is again apparent.

6.2. Number of Monte Carlo iterations

As in the T = 0 K case, the relative differences between 10 000 and 20 000 Monte Carlo iterations have been computed

[15]Other statistics have not been plotted here to make this document lighter.

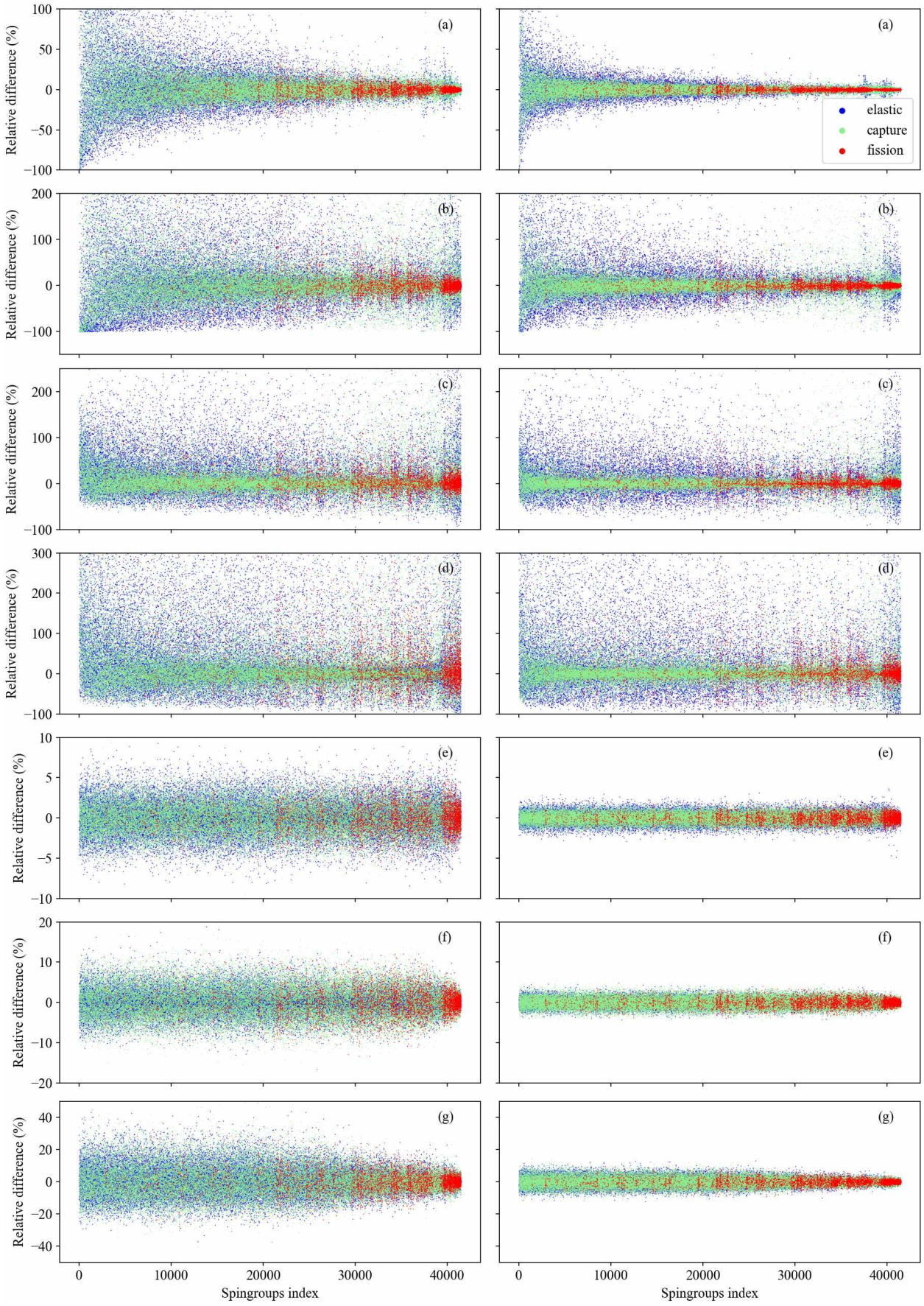

Figure 10: Percentage of difference for several statistics ((a) mean, (b) variance, (c) skewness, (d) kurtosis, (e) first quartile, (f) fourth quartile, (g) 95^{th} percentile) of the cross section sets corresponding to the elementary spingroups of JEFF-3.2 sorted in ascending $\overline{\Gamma}/\overline{D}$, at T = 0 K. On the left, the comparison is between 10 000 and 20 000 iterations, on the right for between 100 000 and 200 000 iterations.

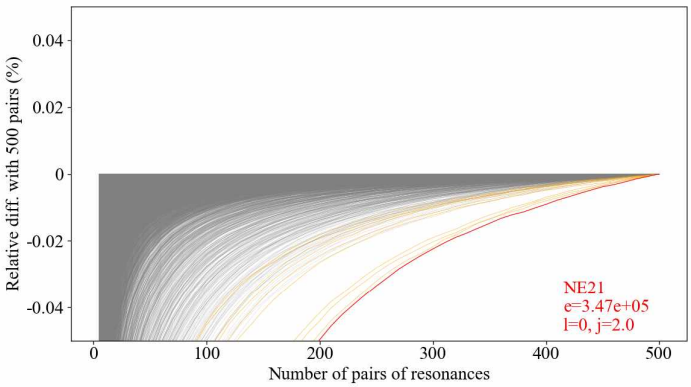

Figure 11: Convergence of the variance of the elastic cross sections samplings for all elementary spingroups of JEFF-3.2 toward the reference (500 pairs of resonances), at T = 293.6 K

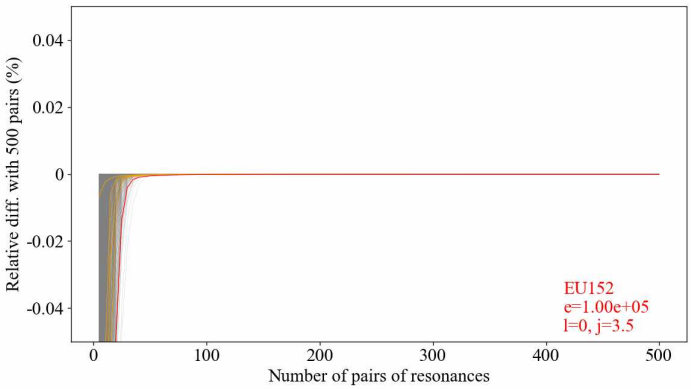

Figure 12: Convergence of the variance of the capture cross sections samplings for all elementary spingroups of JEFF-3.2 toward the reference (500 pairs of resonances), at T = 293.6 K

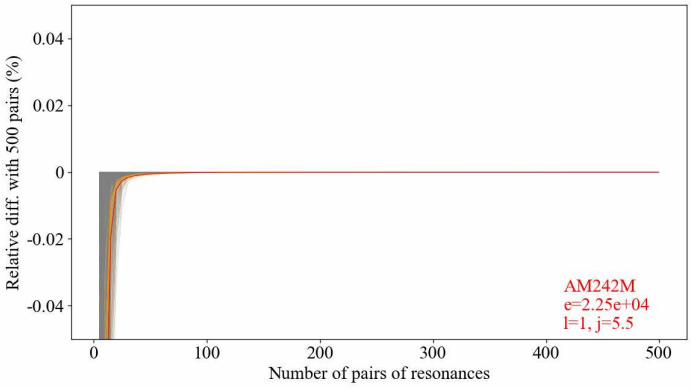

Figure 13: Convergence of the variance of the fission cross sections samplings for all elementary spingroups of JEFF-3.2 toward the reference (500 pairs of resonances), at T = 293.6 K

for moments and quantiles statistics, as well as between 100 000 and 200 000 iterations. Results are displayed in Figure 15, where indexed elementary spingroups sorted with respect to increasing $\overline{\Gamma}/\overline{D}$ have been distributed on the x-axis. For the sake of comparison, the y-axis has been scaled like in Figure 10.

Compared to the T = 0 K results, the same trends can be observed. The differences when 10 000 iterations are used are quite larger than at the next order of magnitude. Moreover, larger differences are reached for smaller $\overline{\Gamma}/\overline{D}$ ratios. Nonetheless, a significant change compared to the T = 0 K case can be spotted. When temperature increases, the percentage difference between the several numbers of iterations tends to decrease. This is true for all statistics, reactions, and elementary spingroups. The reason is related to the flattening effect of the Doppler-broadening, which implies that, for a same ladder, more resonances contribute to the cross sections. As a consequence, the Monte Carlo fluctuations for all statistics are less relevant than at T = 0 K. This has a strong effect, as the number of elementary spingroups for which a 100% difference can be identified for the moments statistics becomes marginal.

7. Conclusions

This work aimed at characterizing some aspects of the technique used to handle cross sections calculations in the unresolved resonance range, namely the ladder method. This method is based on a Monte Carlo sampling of resonance ladders around reference energies in the unresolved resonance range. The main objective was to estimate the statistical weight of the resonances in order to answer crucial questions related to the number of resonances required to fill the ladders, and the number of ladders to sample. A very conservative implementation of the ladder method has been retained. In particular, cross sections were computed using the usual SLBW formalism, at the reference energy only.

First of all, it has been shown that the two classical methods used to sample resonances, implemented in the NJOY and AMPX codes respectively, are equivalent if at least a dozen of resonances are sampled in the ladders. However, special care must be taken concerning the central spacing. The choice has been made to sample resonances as pairs around the reference energies, as it makes the subsequent investigations simpler.

The starting point of the present work has been to observe that cross section computations in the unresolved resonance range can be subdivided into sub-calculations that make use of 16 scalar input parameters (plus the temperature). These sets of data have been called *elementary spingroups*. The content of the whole JEFF-3.2 library in the unresolved resonance range has been decomposed into a collection of 41 486 elementary spingroups. Processing JEFF-3.2 in the unresolved range is thus exactly equivalent to processing these elementary spingroups. This decomposition is the keystone of this work. Once performed, the cross section samplings have been studied on the basis on several statistics, for all elementary spingroups rather than nuclides.

Actually, relying on elementary spingroups enables to relate the required numbers of resonances and Monte Carlo iter-

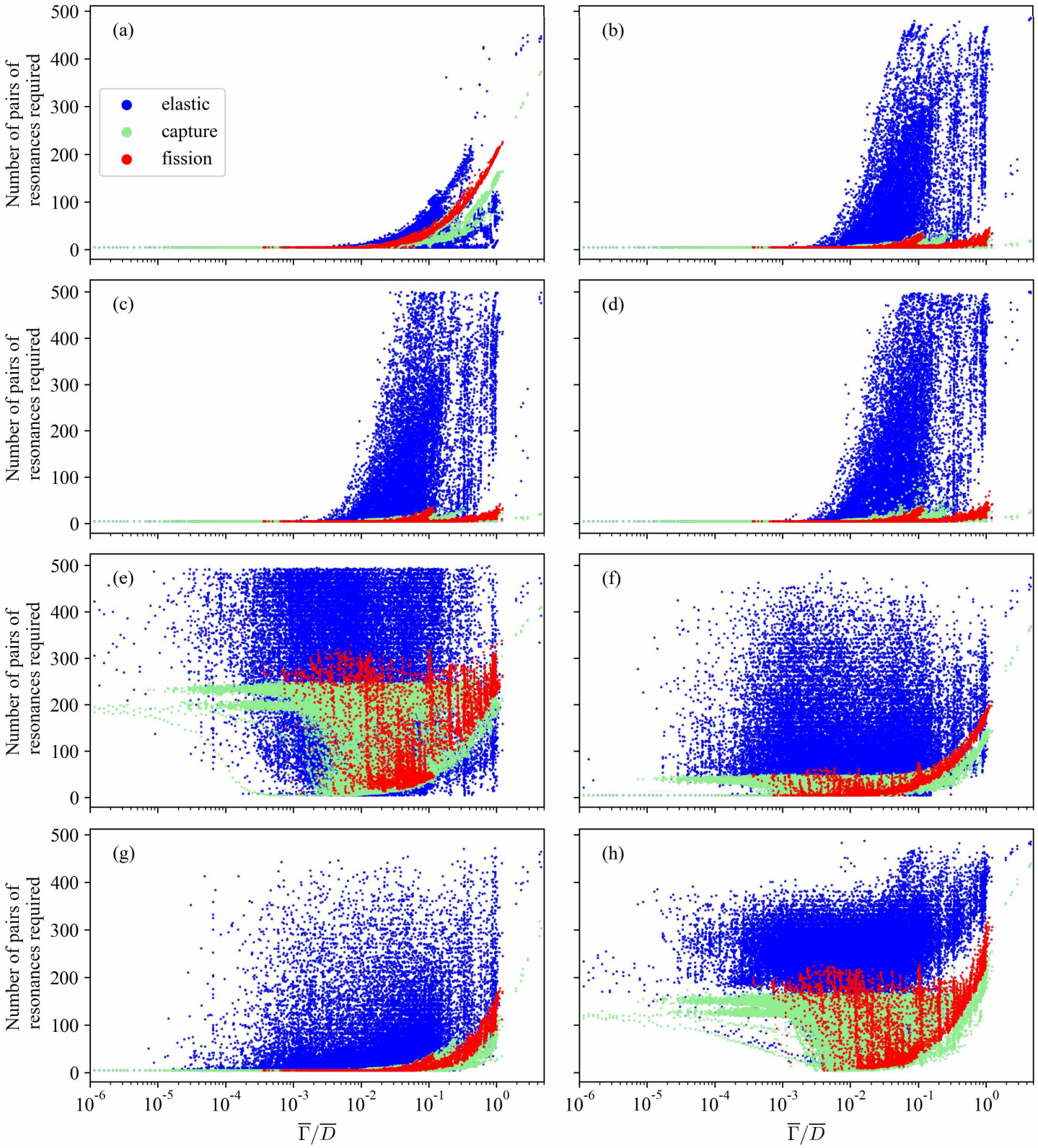

Figure 14: Required number of resonances to reach close to 0.1% of the 500-pairs values for each spingroup, plotted against their $\overline{\Gamma}/\overline{D}$ value, at T = 293.6 K. Each figure corresponds to a statistics of interest: (a) mean, (b) variance, (c) skewness, (d) kurtosis, (e) first quartile, (f) fourth quartile, (g) 95^{th} percentile, (h) Kolmogorov-Smirnov distance

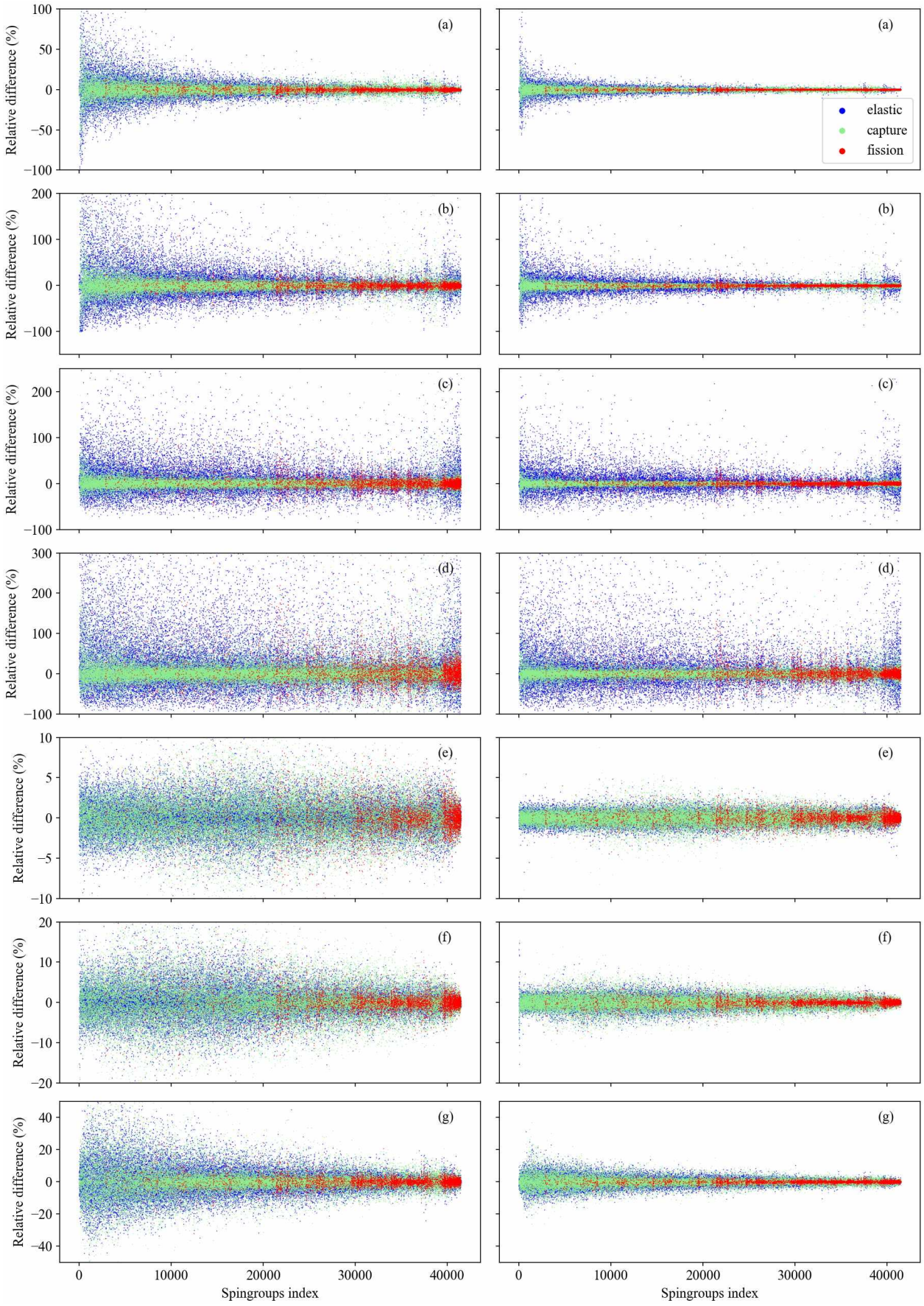

Figure 15: Percentage of difference for several statistics ((a) mean, (b) variance, (c) skewness, (d) kurtosis, (e) first quartile, (f) fourth quartile, (g) 95^{th} percentile) of the cross section sets corresponding to the elementary spingroups of JEFF-3.2 sorted in ascending $\overline{\Gamma}/\overline{D}$, at T = 293.6 K. On the left, the comparison is between 10 000 and 20 000 iterations, on the right for between 100 000 and 200 000 iterations

ations to the resonance parameters themselves. In particular, we have found that the ratio $\overline{\Gamma}/\overline{D}$ of the elementary spingroup total average width to the average spacing is a relevant quantity. It has been shown that cases with small $\overline{\Gamma}/\overline{D}$ ratios require only a few resonances but many Monte Carlo iterations, whereas more resonances and less iterations are required for elementary spingroups with higher $\overline{\Gamma}/\overline{D}$ values. This trade-off has a simple explanation, since distant resonances contribute less to the cross sections. When $\overline{\Gamma}/\overline{D}$ is small the average spacing tends to be large compared to the total average width, hence less resonances are needed. However, as less resonances actually contribute in a single ladder, their statistical fluctuations have a larger impact.

Investigating the effect of temperature reinforces the previous statement. Calculations at room temperature rather than at T = 0 K show that, for all elementary spingroups, more resonances in the ladders contribute to the cross section. However, the statistical Monte Carlo fluctuations are significantly reduced when the temperature effect is taken into account. This can be understood by observing that the Doppler effect broadens and flattens the resonances. As a consequence, distant resonances are more likely to contribute than at T = 0 K.

Finally, this work confirmed that obtaining relevant elastic cross sections requires to sample more resonances than for capture or fission, because of the interference effect, which means that elastic scattering will be preponderant in determining the appropriate ladder sizes. Moreover, it has been shown that fission calculations may require more resonances than capture, because the fission width degree of freedom is not set to zero. This enables sampling large distant resonances, having a significant contribution to the fission cross section.

This work has some very practical applications. It provides an estimation of the number of resonances to be sampled during the ladder sampling for every nuclide in the nuclear libraries, as well as an estimation of the required number of Monte Carlo iterations. This is very useful for processing codes which implements the ladder method in the unresolved resonance range to compute probability tables. Usually, both the number of resonances and the number of ladders are supposed to be chosen by the user for each nuclide. This work shows that this choice can be non-trivial. Providing a quantitative estimation for both these variables requires to establish a criterion for the convergence of the probability distribution of the sampled cross sections, which is very delicate. This is however mandatory for practical applications, and we believe that the role of this work is also to provide some useful advice. We thus suggest to work at the spingroup scale, and compare the $\overline{\Gamma}/\overline{D}$ value to 10^{-2}. Below this value, choosing 100 pairs of resonances around the reference energy provides quite accurate results. Above, the number of resonances has to be increased. Furthermore, 100 000 Monte Carlo iterations looks like a minimal number to perform, which should probably be increased if the $\overline{\Gamma}/\overline{D}$ ratio is small.

This work also has some strong implications for Monte Carlo codes that handles the unresolved resonance range on the fly, such as in reference [12]. There, the question of the number of resonances to be sampled is crucial, because too many resonances would slow down the Monte Carlo calculations. Our work shows that, for several cases, the number of resonances cannot be chosen too small. This is thus a real stake for the Monte Carlo codes.

Future work will concern the introduction of some more complex features. Among them, one of the most promising is the introduction of correlations between resonances, relying on the random matrix theory. Another appealing idea would be to investigate the influence of reconstructing a whole continuous-energy cross section in the vicinity of the reference energy, instead of performing cross section calculations at the reference energy only.

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