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From average parameters to statistical resolved resonances

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ABSTRACT

This paper presents a novel approach using average parameters from statistical models in the continuum to produce statistical resolved resonances in the resonance range. Based on unresolved resonance parameters and the random ladder method, average parameters such as the scattering radius, level spacing, reduced neutron width and the radiative width are used to create resolved resonances from thermal energy up to the first excited level. Using the TALYS reaction code and the CALENDF processing code, the method is tested on ≃2400 isotopes and will be used to produce resolved resonance ranges in the TENDL libraries for reactions missing experimental resolved and unresolved parameters. Additionally, the R-matrix code AVEFIT is used to approximate the resonance structure effects above the first excited level of selected isotopes.

1. Introduction

Two types of neutron reaction theories are usually employed for the modeling of low-energy neutron reaction mechanisms (below a few tens of MeV). The first one is the R-matrix theory, exact or with approximation, depending on the mass and charge of the target nucleus (Hale, 1981; Larson, 2006; Moxon et al., 2010). It is based on special few-body techniques and can be applied to a limited set of nuclei in a limited energy range. The second one is based on direct models or statistical models (many-body) resulting from the averaging over many resonances, e.g. Hauser–Feshbach or preequilibrium models, as implemented in Young et al. (1996), Herman et al. (2007), Raynal (1994), and Koning et al. (2007).

In practice, a mixture of these approaches is used to reproduce observables (such as cross sections) and to extract their characteristics. The R-matrix approximations are used at low neutron energy and the statistical models are applied for higher incident neutron energy as soon as competitive channels are opened (with the exception of light isotopes, where the R-matrix theory can be applied over a broader range of energy). As a consequence, there is often a separation between the phenomenological parameters used in the many-body theories and their counter-parts in the lower energy range. This separation is reflected in the variations of the cross sections (smooth at high energy and resonant at low energy) and in the average parameters (such as average capture width, level spacing, strength functions) which are often not consistent between the two ranges. A "gray zone", where these two methods are partially connecting is called the "unresolved resonance range", defining a region where resolved resonances get so close together that they cannot be measured and given separately. Instead, average values for the resonance spacing and the various characteristic widths are given. These parameters can be obtained from both the lower and higher energy ranges. From the lower energy range, the average parameters such as strength functions, effective potential scattering radius, mean-level spacing and reduced neutron width can be derived from R-matrix analysis. From the higher energy range, the optical model, usually valid above the first excited level, can be extended to lower energy to provide similar parameters. These analysis are gathered in an "evaluation" (a recommendation of nuclear data) and the agreement between the average parameters from low and high energy ranges are part of the quality of such work.

There are individual efforts to harmonize the parameters coming from these two branches of the neutron reaction theories, such as in Bouland et al. (2011). A few examples can be found for ^{242}Pu (Rich et al., 2007), ^{103}Rh (Dupont et al., 2004), but these efforts are often marginal and only applied on a case-by-case basis. In the nuclear data community, the majority of libraries presents evaluations where the low and high energy range are indeed disconnected by means of evaluation procedures. The main reasons can be found in the historical background of such libraries, in the ways the measurements of the different energy ranges are performed and in their range of applications. One of the most perceptible

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consequence of this separation can be found in the covariances associated with these evaluations. Without exception, they present no correlation between the resonance and the fast neutron ranges. It can be advocated that state-of-the-art studies of the neutron reaction modeling (and therefore their evaluations) cannot ignore these types of deficiencies because it underlines the global consistency of the work.

In an attempt to have another view on the existing evaluation work, we are proposing the implementation of a more systematic approach, for a large number of nuclides, using a different attitude towards the usage of nuclear models. Our principal motivation is therefore to produce a set of resolved resonances, consistent with average parameters used at higher incident neutron energy, for a large amount of isotopes.

If successful, this method will be applied for a large number of isotopic evaluations included in the future TENDL nuclear data libraries (Koning and Rochman, 2008, 2010; Rochman and Koning, 2010, 2012). The TENDL libraries are based on a global approach for a large number of isotopes and on specific and detailed evaluations for the important isotopes. But in both cases, the same methodology is applied, with reproducibility as the main mantra. Whether a nuclear reaction calculation is based on default parameters or adjusted ones, any evaluation can be reproduce at any time. The same approach needs to be applied in the present case, which will guarantee global applicability. This method of work (based on reproducibility) has already produced unexpected outcomes such as random nuclear data evaluations for uncertainty propagations (Koning and Rochman, 2008; Rochman and Koning, in press) or an original procedure of nuclear data adjustment (Rochman and Koning, in press, 2011).

2. Method

As presented in the following, the majority of tools and input data are already available. The originality of this work is to combine together different pieces of information on a systematic basis. The theoretical advantage is to obtain parameter consistency. The applied advantage for nuclear simulations consists in having a unique type of basic outputs (resolved resonance parameters), which are in principle always treated the same way by different processing codes (contrary to the unresolved resonance range).

2.1. Precursory ideas

The idea to obtain approximate cross sections in the resonance range when no measurements exist is not new. The first and easiest solution was then to extend the optical model calculation to low energy or to use a $1/v$ function and calculate smooth cross sections from 0 to the MeV region. No structure can be obtained, but this approximation allows to obtain a correct thermal cross section if the parameters of the optical model and the level densities are adjusted. An example of such an approach is presented in Fig. 1 for the ^{90}Sr (n,γ) cross section.

A drawback of this method can be seen from Fig. 1: there is a clear separation between the "pseudo resonance range" and the fast neutron region. Additionally, it was also difficult to adjust the resonance integral I_γ if measured values existed (see C/E values in Fig. 1).

An elaborate approach was developed in 2001 for the EAF-2003 library (Forrest, 2007), where the Single Resonance Approximation (SRA) was presented. The physical idea was to represent the large thermal cross section (>10b) of some reactions by one strong s-wave resonance superimposed on a $1/v$ background. The advantage of this method is the possibility it gives to reproduce the resonance integral in a better way than the $1/v$ component alone. The single-level Breit–Wigner formula was used for a unique resonance, with a few additional approximations on the statistical weight factor (constant and equal to 0.5), the radiative width (equal to $1593/A^2$, with A the mass number of the target) and the thermal capture cross section (Kopecky et al., 1992): if no experimental information is available, as for radioactive targets, an attempt was made to develop systematics both for thermal and 30 keV data. The prediction of thermal cross sections is almost impossible, due to the fact that only a very limited number of resonances determine these values and thus no statistical assumption can be applied. However, in spite of the expected very large uncertainty in these predictions, they account at least for the global trend.

Starting from the expression for the average capture cross section in the statistical region, after several simplifications, the parameterized formula

$$\sigma_{\mathrm{th}}(n,\gamma) = C \times (a \times U)^x \tag{1}$$

can be used to fit the constants C and x to the measured data. U is the effective excitation energy, defined as $U = S_n -$ pairing energy, and a is the level density parameter. The application of this approach at 30 keV is generally justified, however, at thermal energy the influence of the resonance region on the cross section value is dominant and any dependence on $a \times U$ is masked by large Porter-Thomas fluctuations. Nevertheless, a least square fit was applied to the thermal cross section data. Values of $C = 1.5 \times 10^{-6}$ barns and $x = 3.5$ are found (Kopecky et al., 1992). An example is presented in Fig. 1. This method allows for a better adjustment of both the thermal capture cross section and the resonance integral, but the separation between the fast and resonance neutron region is still visible.

Starting in 2008 and up to 2011, a different version of the SRA was implemented in the TENDL libraries. Instead of using a single resonance, many hypothetical resonances were invoked, with a single negative resonance. In the case of non-fissioning nuclei, five parameters for each resonance need to be given: l, j, E, Γ_n, Γ_γ. The l value is assumed to be zero, and the spin of resonances j is the spin of the target nucleus plus 0.5. The three other parameters are changing with the resonance numbers i. The resonance energy E_i

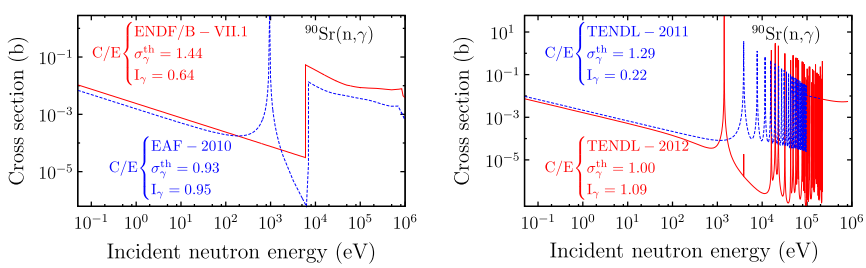

Fig. 1. Examples of different approaches for ^{90}Sr ($h_{1/2}$ = 28 years) in the low energy region. Left: basic optical model calculation for ENDF/B-VII.1 and Single Resonance Approximation (SRA) for EAF-2010. Right: multi-SRA for TENDL-2011 and the present methodology for TENDL-2012.

is equal to $E_i = D_0 \times i$, with D_0 the s-wave average level spacing, estimated from the level densities of Koning et al. (2008). For the neutron width Γ_n, according to the extreme compound, or black nucleus model (Feshback et al., 1947) the strength function is constant for all nuclei, and for s-wave neutrons is given by

$$\frac{\left\langle \Gamma_n^0 \right\rangle}{D_0} = \frac{2k_0}{\pi K} = 1 \times 10^{-4} \tag{2}$$

where $\left\langle \Gamma_n^0 \right\rangle$ is the average s-wave reduced neutron width, D_0 is the average s-wave level spacing, k_0 is the wave number for a 1 eV neutron while K is the wave number inside the nucleus. For a potential well depth of 42 MeV, the black nucleus value of the strength function is 1×10^{-4} (note that the strength function is a dimensionless quantity). It is then assumed that

$$\left\langle \Gamma_n^0 \right\rangle \simeq \Gamma_{nj}^{\ell=0} = \sqrt{\frac{1\text{eV}}{E_0}} \frac{\Gamma_{nj}}{V_{\ell=0}} \tag{3}$$

with the penetrability $V_\ell = 1$ for s-waves ($l = 0$). We can then extract the neutron widths for the ith resonance being:

$$\Gamma_{ni} = S_0 \times D_0 \times \sqrt{D_0 \times i} \tag{4}$$

with S_0 the strength function for s-wave resonances. The last parameter, the radiative width $\Gamma_{\gamma i}$ was evaluated in an iterative process with the following approximation (with the condition that $E_0 \gg \Gamma$):

$$\sigma_{\text{th}}(n,\gamma) = 4.1 \times 10^6 \left(\frac{A+1}{A}\right)^2 \sum_i^N \frac{g\Gamma_n^0 \Gamma_{\gamma i}}{E_{0i}^2} \tag{5}$$

with $\sigma_{\text{th}}(n,\gamma)$ the thermal capture cross section based on the systematics from Eq. (1). An example is presented in Fig. 1. As seen, the unique resonance from the SRA approach (EAF-2010) is replaced by a series of hypothetical resonances (20), and the connection with the fast neutron range is improved. Nevertheless, the resonance integral is not correct and there is still a difference between the resolved resonance parameters and the average parameters from the fast neutron range.

As presented, these three methods can be improved to satisfy basic requirements such as good C/E for integral data, use of consistent parameters through the complete evaluation, minimization of sudden changes between the resonance and fast neutron ranges. The technique presented in the following is developed to achieve these goals in a more satisfactory manner.

2.2. Modern development

The proposed method consists to expand the region of overlap (unresolved resonance range) and "*resolve*" it (or reconstruct it). Down to low energy, virtually to 0 eV in the case of isotopes without known resonances, and up to the first excited level in general.

Depending on the degree of knowledge for a given isotope, the above proposition can be implemented with different degrees of difficulty. It is then convenient to introduce a classification depending on the amount of knowledge for a given isotope. In the following, we will only consider isotopes with half-lifes longer than one second, including stable isotopes, representing ≈2400 cases (depending on how the isomers are counted).

1. At the first extreme, isotopes without any experimental reaction information (about 1600 isotopes). In this case, as no specific information can be used to adjust calculations, we fully rely on systematics, as defined in TALYS from Kopecky et al. (1992) or the underlying optical model potential and level density model (Kopecky and Nierop, 1995, 1992). The largest approximation is realized for these isotopes, meaning to expend the statistical models at low neutron energy, outside their scope of application. We will therefore obtain smooth cross sections in the complete energy range, together with average parameters. The next step is to use the *ladder* method (see next section), as described in CALENDF (Sublet et al., 2011) and AVEFIT (Moxon, 2012) to reconstruct statistical resonances. The evaluations for these isotopes are only included in the TENDL libraries.
2. In between the two extreme, isotopes with scarce experimental data, such as thermal cross sections, resonance integrals, average cross sections at high energy (about 400 isotopes). Such isotopes are for instance ^{40}K, ^{54}Mn, ^{60}Co, ^{90}Sr, ^{105}Rh, ^{106}Ru, ^{109}Cd, ^{111}Ag, ^{138,143}Ce or ^{204}Hg. The approach for these isotopes is very similar to the previous case, with two noticeable differences. First the model parameters are adjusted to reproduce the existing data (such as cross sections or existing resonances). In practice, if the thermal capture cross section is known, the average neutron width is adjusted. Secondly, if one of a few experimental resolved resonances are reported, the statistical models are not extended to 0 eV but to the highest energy of the known resonance (as for instance for ^{192}Os). All the isotopes are also included in the TENDL and EAF libraries (Sublet et al., 2011).
3. At the other end of the spectrum, isotopes with measured pointwise cross sections, resonances, integral measurements, and resolved resonance parameters (about 400 isotopes). These isotopes represent the most sensitive range for fission applications. Nuclear data cannot be modified without important consequences on benchmarks and other nuclear simulations. The above method can still be applied, but great care should be taken that the modifications do not deteriorate their performances. In this case, the TALYS model parameters are adjusted to the experimental data but the proposed method is only applied in energy ranges where resonances could not be resolved for experimental reasons (for instance the unresolved resonance range, but also energy ranges where it is known that resolved resonances are missing, as for ^{95}Mo, ^{170}Er, ^{100}Ru or ^{198}Hg). These isotopes are usually included in all major world libraries (the above mentioned plus (Chadwick, 2006; Koning et al., 2008; Shibata et al., 2011)).

2.3. Necessary quantities and parameters

Independently of the degree of experimental knowledge for a given isotope, the following method can be applied. In very simplistic description, the approach can be described as presented in Fig. 2.

As a starting point energy-dependent statistical parameters as well as specific cross sections are needed in the whole energy range. These parameters are for each orbital angular momentum l and spin of the resonance state j:

- the scattering radius r,
- the average level spacing D_0,
- the average reduced neutron width Γ_n^0,
- the average radiation width Γ_γ,
- and if relevant the average fission width Γ_f.

The necessary cross sections, consistent with the above parameters are the elastic, capture, inelastic and fission cross sections. These pointwise cross sections can be kept as is above an arbitrary energy limit, usually lower than the first inelastic level. Below this energy limit the average parameters can be converted into statistical resonance structures. This energy limit can be arbitrary chosen,

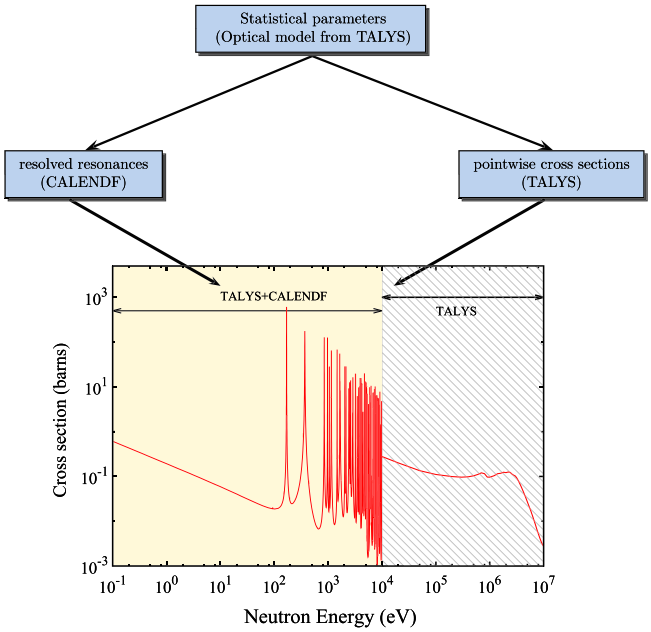

Fig. 2. Schematic approach to use in combination TALYS and CALENDF. At low energy (below 10^4 eV) the statistical parameters from the optical model and the level density model are use to generate statistical resonances. At higher energy, smooth cross sections coming from TALYS (or the optical model) are kept as is.

but in practice, it defines the number of resolved resonances and should therefore not be too high.

As an example, some needed quantities are presented in Fig. 3. These parameters are extracted from TALYS, using the global optical model (Koning and Delaroche, 2003) and the global and local level density models (Koning et al., 2008).

These models have been used and extensively tested within the TALYS code and with the TENDL libraries. The comparison with experimental data, when they exist, presents good agreements.

2.4. Converting average parameters to statistical resonances

The basic idea is to generate random ladders of resonances using the statistical properties of the unresolved resonance range (Brissenden and Durston, 1965; Sublet et al., 2011; Moxon, 2012). Ladders can be generated at an energy E by randomly selecting a starting resonance energy for one (l,j) sequence, and also randomly selecting a set of widths for that resonance using the appropriate average widths and χ^2 distribution functions. The next higher resonance energy can be selected by sampling from the Wigner distribution for resonance spacings, and a new set of widths for that resonance can be chosen. The process is continued until a long ladder of resonances for that (l,j) is obtained. The process for the other (l,j) sequences is then repeated, each such sequence being uncorrelated in positions from the others.

In the current implementation of CALENDF, for each (l,j) couple, a GOE random matrix (Gaussian Orthogonal Ensemble) (Ribon, 1986) is used to generate resonance energies. The random generation of resonance sequences and the impact of their fluctuations were first presented in Moldauer (1963, 1964). The CALENDF implementation allows to follow the Wigner law and to include correlations between two successive resonances. Following the average parameters obtained in the unresolved resonance range, CALENDF determines "segments", in which a few tens of s-wave resonances are included. Using stratified random numbers, the widths of the resonances are obtained.

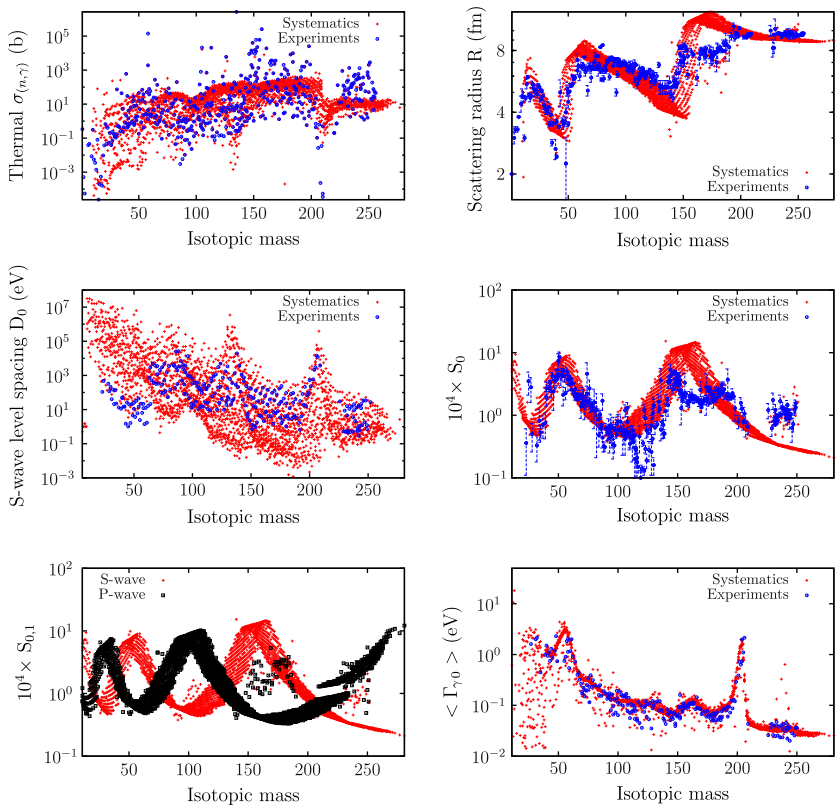

Fig. 3. Some parameters as a function of isotopic mass, needed to produce statistical resonances. From the top left to bottom right: thermal capture cross sections, scattering radius (at 10 keV), s-wave level spacing D_0, s- and p-waves neutron strength functions s_0 and s_1, and s-wave radiative widths.

3. Examples

This methodology is now applied to all isotopes included in the TENDL libraries, about ≈2400. In the following, examples for the most striking cases are presented.

3.1. Isotopes with unknown resolved resonances

These isotopes represent the vast majority of the cases, but are also considered the least important ones. As explained previously, the absence of experimental data gives a large freedom. The average parameters r, D, Γ_n^0, Γ_γ, and Γ_f are not adjusted and are taken directly from TALYS, based on the global optical model and the level density model from Koning and Delaroche (2003, 2008) and systematics from Kopecky and Nierop (1995, 1992). Fig. 4 presents examples of the resolved resonance range for twelve short-lived isotopes, from Cr to Cf. The resolved resonances are based on the TALYS unresolved resonance range extended to 0 eV, adjusted to systematics from Kopecky and Nierop (1995, 1992).

As no other evaluations exist for this kind of isotopes, it is not possible to compare the present resonance data with other source of information. But based on the described systematics used for average resonance parameters, the obtained cross sections are consistent with the expected values.

3.2. Isotopes with restricted average experimental data

As for the previous case, there are no available experimental resonance parameters. The difference lies in the known thermal capture (or fission) cross sections and in some cases in the known resonance integral values. These experimental values allow to adjust the resonance parameters. Only the capture thermal cross sections are used in the adjustment procedure. The resonance integral and the thermal fission cross sections are used as additional checks but are not used to modify resonance parameters. In the case of nonfissile isotopes, the neutron widths Γ_{ni} are multiplied by the $\sigma_{th}^{exp}/\sigma_{th}^{calc}$ ratio for each resonance. For fissile isotopes, the capture width $\Gamma_{\gamma i}$ are used instead of Γ_{ni}. Examples of such isotopes are presented in Fig. 5 and comparisons for the integral values are presented in Tables 1 and 2.

Fig. 5 presents a few advantages of the method: no unphysical cut-off between the resonance and the fast neutron ranges, no constant cross sections at low neutron energy and better agreement with integral data (as presented in Table 1). The capture and fission integrals are not used to adjust the different resonance widths and are therefore not expected to give a C/E equal to one. The comparisons between calculated and measured capture and fission integrals should nevertheless not be too different. In the case of fissile actinides, the adjustment method is not as efficient as for non-fissile isotopes. Although thermal values are not equal to measured ones, the differences are still acceptable. A better adjustment method would be to iteratively modify the capture and fission widths until the measured thermal values are obtained. This method presents the drawbacks to be slow and to diverge in some cases.

In the case of isotopes with no experimental resonance information, the present method can produce resonances close to the thermal energy. In this case, the thermal cross section, both in amplitude and shape, is affected, leading to possible high cross section values and Westcott factor very different from 1. To correct for the high amplitude, the renormalization of the neutron widths Γ_{ni} as presented earlier can adjust the thermal cross section and the capture integral. It should nevertheless be kept in mind that this approach is based on the generation of random resonances following a given statistical behavior. Their individual resonance parameters are random and if corresponding measurements would later come, strong differences in their values may occur. However, as presented in many cases in this paper, the obtained parameters and cross sections are often comparable to the SRA results, bringing a global confidence in the current approach.

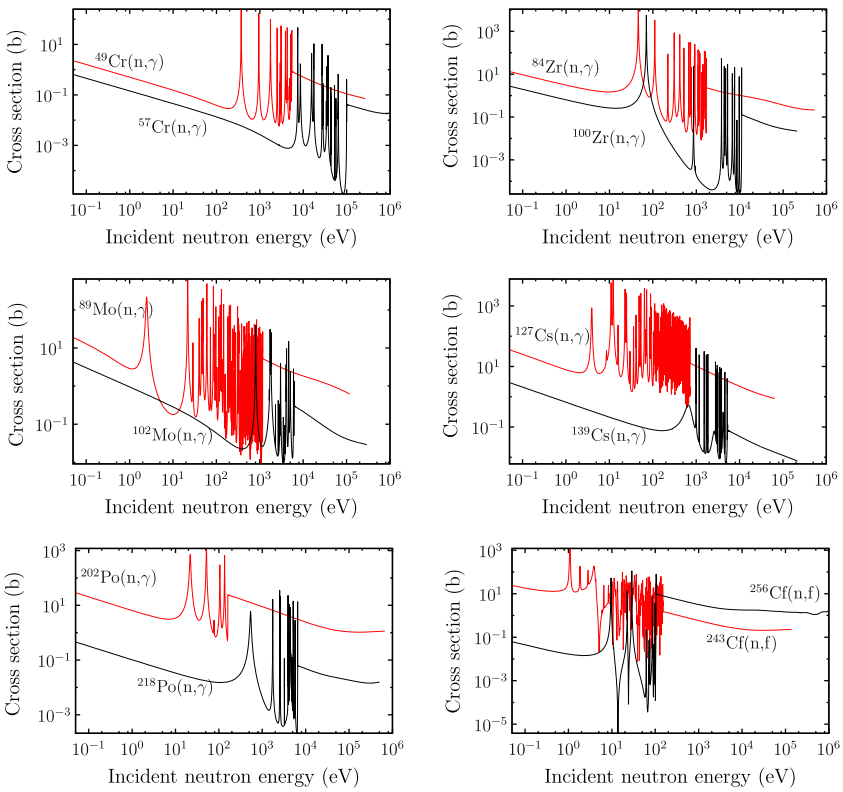

Fig. 4. Example of reconstructed resolved resonances based on the TALYS unresolved resonance range and CALENDF for 12 short-lived isotopes.

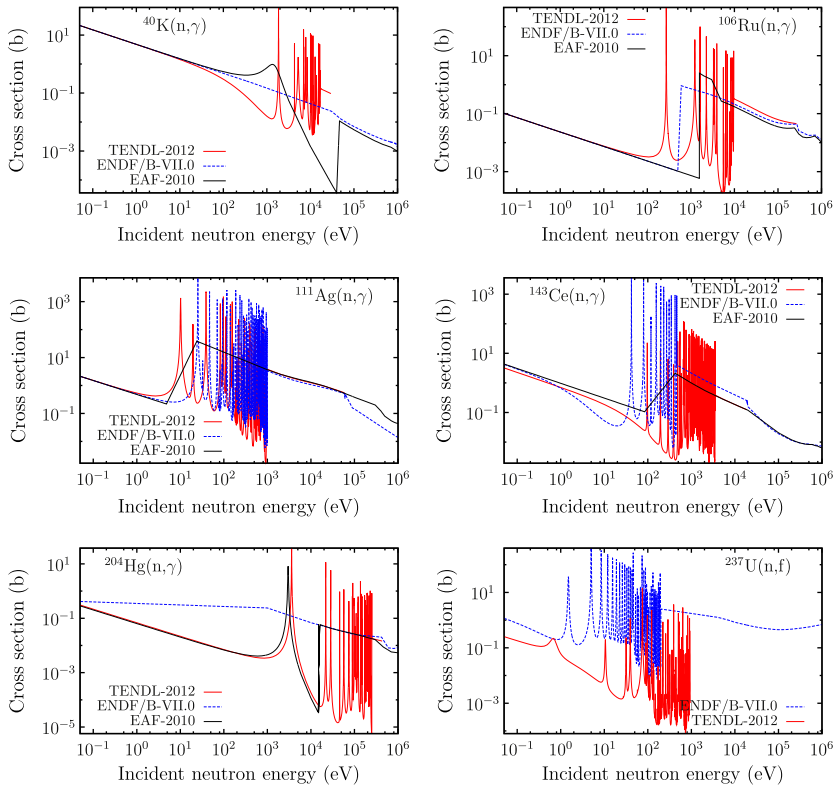

Fig. 5. Example of reconstructed resolved resonances based on the TALYS unresolved resonance range and CALENDF for 6 short-lived and low abundance isotopes, compared to other evaluations.

Table 1
Comparison of *C*/*E* for the thermal capture cross section σ_{th} (n,γ) and for the capture integral I_γ for a selection of isotopes.

Isotope	*C*/*E* σ_{th} (n,γ)			*C*/*E* I_γ			σ_{th} (n,el) (barns)	
	TENDL 2012	ENDF/B-VII.0	EAF 2010	TENDL 2012	ENDF/B-VII.0	EAF 2010	TENDL 2012	ENDF/B-VII.0
^{40}K	1.00	1.00	1.00	1.02	1.03	1.10	2.75	16.4
^{54}Mn	1.00	–	0.26	0.94	–	0.69	4.00	–
^{60}Co	1.00	–	1.00	0.95	–	0.76	1.37	–
^{105}Rh	0.99	0.75	0.52	0.84	1.00	0.19	65.7	8990
^{106}Ru	1.00	1.00	1.00	1.43	0.95	1.01	4.04	3.34
^{109}Cd	0.99	–	0.25	0.83	–	0.43	27.8	–
^{111}Ag	1.00	0.99	1.00	1.03	0.94	0.71	5.36	4.58
^{138}Ce	1.00	0.85	0.83	1.07	1.36	0.86	3.55	2.59
^{143}Ce	1.00	1.35	1.33	1.73	13.2	2.28	8.07	4.63
^{192}Os	1.00	–	0.64	1.46	-	1.48	0.67	–
^{204}Hg	1.00	1.00	0.93	0.92	3.14	0.67	7.52	29.4

Table 2
Comparison of *C*/*E* for the thermal capture and fission cross sections and for the capture and fission integrals for a selection of fissile isotopes.

Isotope	*C*/*E* σ_{th} (n,γ)		*C*/*E* σ_{th} (n,f)		*C*/*E* I_γ		*C*/*E* I_f	
	TENDL 2012	ENDF/B-VII.1	TENDL 2012	ENDF/B- VII.1	TENDL 2012	ENDF/B-VII.1	TENDL 2012	ENDF/B-VII.1
^{223}Ra	1.00	1.00	1.08	1.00	–	–	–	–
^{233}Th	0.99	0.97	0.99	1.00	0.22	0.34	–	–
^{239}U	1.00	1.01	1.00	1.02	–	–	–	–
^{238}Np	–	–	0.95	1.05	–	–	0.89	1.25
^{243}Pu	1.00	1.01	1.18	0.92	0.22	1.01	0.76	1.01
^{250}Bk	0.90	2.20	1.01	1.02	–	–	–	–

3.3. Stable isotopes

In the case of stable isotopes, resonance parameters are often known up to a given energy value. In some cases, gaps can be found where resonance parameters are partially known for a given energy range (the position of resonances might be known, but not their partial widths). As these isotopes are of importance for many types of applications, their resolved resonance range is not changed for measured resonances and is extended at higher energy by a limited number of statistical resonances. Depending on the

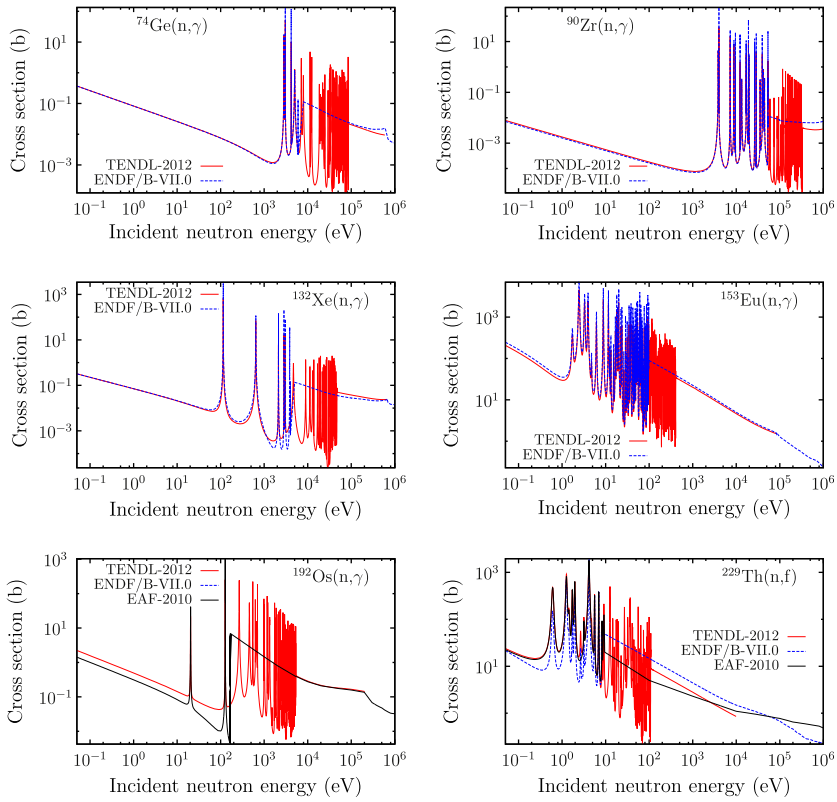

Fig. 6. Example of reconstructed resolved resonances based on the TALYS unresolved resonance range and CALENDF for six stable isotopes with high or relatively high abundance, compared to other evaluations.

average level spacing D_0, the above limit of the resolved resonance range is increased in order to keep a reasonable number of resonances. Above the resolved range, a shorter unresolved resonance range is used together with pointwise cross sections (as in all evaluations). Examples for isotopes with important modifications are presented in Fig. 6.

In these cases, the resolved resonance range is sensibly increased, with a limit of one or two hundred added resonances. But in the majority of cases, the modification of the resolved resonance range is minor or nonexistent.

4. Extension at higher neutron energy

The presented methodology can practically be applied up to the first inelastic level of a given nucleus. This limitation is related to the processing codes and the formalism used, which apply different rules for the resonance reconstruction and broadening depending on the number of open channels. The most dramatic effect is that the NJOY99 processing code by default stops to Doppler broadened resonances as soon as a competitive channel, given as a pointwise cross section in the evaluation, is opened (such as the (n,inl^{1st}) or the (n,α) reactions).

Accepting this limitation, any resonance effect above the first inelastic level should not be given as a suite of resonance parameters, but instead as pointwise (or groupwise) cross sections. It is well-known that resonance effects can appear at relatively high energy as for instance for ^{23}Na or ^{56}Fe. On the other hand, codes such as TALYS are using compound nucleus theories and cannot account for these effects. In order to represent the fluctuations still appearing above the first inelastic level, we are proposing to apply a R-matrix analysis with the AVEFIT code (Moxon, 2012). AVEFIT calculates the capture, fission and inelastic cross-sections from a randomly generated set of resonance parameters, using both the single level approximation and the full R-Matrix formalism. The program AVEFIT was developed from the earlier fitting program that used only the simple single level approximation to determine average nuclear parameters from data in the unresolved neutron energy region. The cross-section can now be calculated either by the single level approximation or a full R-matrix formalism. The calculation of the R-matrix formalism uses a similar subroutine to that used in the resonance fitting program REFIT (Moxon et al., 2010), the only modification being the ability to calculate the cross-section for up to five fission channels per spin and up to 60 inelastic levels. At each energy interval the program carries out several calculations to determine the average value of all the partial cross-sections and the spread due to the use of a finite number of resonances. The resonance parameters are selected randomly from the appropriate distribution using the (adjusted) average parameters, as previously presented.

In AVEFIT, resonance parameters are determined as follows.

- The spacing between the resonances are selected from a Wigner distribution. The spacing $D(j,E_n)$ for spin j at a neutron energy E_n uses a modified equation from Lang and Le Couteur (1954). The dependence of the level density $\rho_j(E_n)$ with spin is given by Lynn (1968). The level density observed at near zero neutron energy for spin $j = 0$ is determined from the observed values in the resolved region.
- For a given spin j and angular momentum l, the reduced elastic neutron widths Γ_n^0 are selected randomly from a Porter-Thomas distribution, using a mean value obtained from the strength function S_l and level spacing $D(j,E_r)$. If more than one elastic channel is open they are considered to be completely independent. The total elastic width $\Gamma_n(E_r)$ at the resonance energy E_r is written as the sum of the widths for all the open channels.

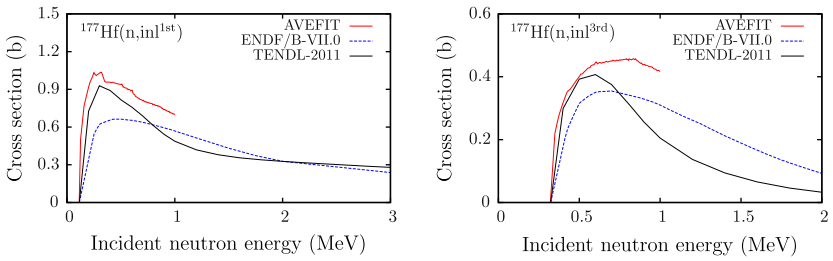

Fig. 7. Example for the inelastic cross sections to the first (left) and third (right) level for ^{177}Hf from the ENDF/B-VII.0 and TENDL-2011 libraries, compared with the AVEFIT calculations.

- The reduced inelastic widths, like the elastic widths, are selected randomly from a Porter-Thomas distribution. The inelastic widths are calculated from the reduced widths using a penetration factor that takes into account the energy and parity of the emitted neutron as well as the spin of the compound nuclear level. Again like the elastic scattering if more than one channel is open, they are assumed to be independent and summed in the same way as the elastic channels.
- The radiation width is assumed to be constant *i.e.* the width does not vary from resonance to resonance for a given spin j and momentum l, but its value does vary with incident neutron energy.
- The reduced fission widths for up to five channels in each spin can be selected from a Porter-Thomas distribution. The simple Hill–Wheeler fission barrier "penetration factor" $P_f(E_n)$ is used to calculate the neutron energy E_n dependence from the reduced width. The energy E_B and width ΔE_B of the barriers are input parameters of the program and can be different for each compound nuclear spin and channel if required.

Based on this description, cross sections in the fast energy range can be calculated. An example is given in Fig. 7 in the case of the inelastic cross sections on ^{177}Hf with average parameters $D(j,E_r)$ and inelastic levels from TALYS. Especially visible for the inelastic cross section to the first level, resonance structure in the grouped cross sections appear up to 1 MeV. In the case of the inelastic cross section to the third level, the resonance structure is less pronounced but still present.

A possible application, if pertinent for a large number of isotopes, is to use the relative cross sections from AVEFIT and to normalize them to the TALYS values. The new cross section, on average equal to the TALYS value, but with the AVEFIT structure can eventually be included in the TENDL library. For the time being, more efforts are needed before these results can systematically be included in TENDL.

5. Conclusion

A unique approach to create parameters for resolved statistical resonances for a large number of isotopes is presented. This method invokes global average parameters from the different systematics and from the TALYS reaction code. These parameters are then used by either the CALENDF code or by the R-matrix code AVEFIT. Statistical resonance parameters are then obtained from 0 up to the first excited level, reflecting the average resonance parameters coming from compound model calculations. Above the first inelastic level, grouped inelastic cross sections with local fluctuations are obtained. This method complements the measured resonance parameters, or provides a resolved resonance range when measurements are not existing. In between these two cases, statistical resonance parameters are adjusted to integral measurements when available. Successfully applied to all isotopes living longer than one second, this method will be used for the TENDL libraries starting in 2012.

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