Proposed changes to the ENDF-6 format

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0 Introduction

The ENDF-6 format [1] is still the world-wide used format in the nuclear data community. However, progress in the processing and calculational methods and computer performance increase the requirement for additional information which has traditionally been ignored. Therefore, we propose three minor changes to the existing ENDF-6 format, which will enable the users a better understanding of the nuclear data evaluations and consequently a more reliable and accurate interpretation and calculations.

1 Introducing a flag for lognormal distribution of inherently positive parameters

Inherently positive parameters with large relative uncertainties (typically $\gtrsim 30\%$) are often considered to be governed by the lognormal distribution. This assumption has the practical benefit of avoiding the possibility of sampling negative values in stochastic applications. Furthermore, it is typically assumed that the correlation coefficients for comparable multivariate normal and lognormal distributions are equivalent. However, this ideal situation is true only in the linear approximation which happens to be applicable only for small uncertainties. The paper [2] derives and discusses the proper transformation of correlation coefficients between both distributions for the most general case which is applicable for arbitrary uncertainties. It is seen that for lognormal distributions with large relative uncertainties strong anti-correlations (negative correlations) are mathematically forbidden. This is due to the asymmetry that is an inherent feature of these distributions.

In ENDF-6 format [1], the parameter distributions are usually presented in the form of mean values and corresponding covariances. As indicated above, the correlation coefficients between variable may differ significantly for either of the considered distributions. The decision whether to assume normal or lognormal distribution is not straightforward and depends on the evaluator. However, in order to prevent misinterpretations by the nuclear data users, the possibility of using a flag to define which distribution the covariance file in ENDF-6 format corresponds to would be strongly recommended.

Here, we suggest one of the many possible options of how to include the flag into the covariance files of the ENDF-6 format. To ensure backward compatibility we suggest that the default flag value "0" always corresponds to normal distribution for all parameters, and "1" corresponds to the lognormal distribution for inherently positive parameters and normal distribution for other parameters. Below, possible positions for the flag in individual covariance files are proposed:

File 30: Covariances of model parameters. In the part "Covariance Matrix (MT=2)", the flag could be introduced as the third parameter in the first row (after the parameters ZA and AWR).

File 31: Covariances of fission $\bar{\nu}$. For neutron induced fission, the formats are exactly the same as in File 33. For spontaneous fission, only one parameter is used; no flag is needed.

File 32: Covariances of resonance parameters. The flag could be introduced as the last parameter in the first row of the subsection for each energy range (after the parameters SPI, AP, IFG, LCOMP and NLS).

File 33: Covariances of neutron cross sections.

- "NC-type" subsubsections: covariances are taken from other files; no flag is needed.
- "NI-type" subsubsections: The flag could be introduced as the second parameter in the first row of the subsubsection (before the parameters LT, LB, NT and NP).

Since the reaction cross section is an inherently positive quantity, in new evaluations all covariances should be given in lognormal representation! (The reader is again reminded that for small relative uncertainties normal and lognormal representations are equivalent.)

File 34: Covariances for angular distributions. The only possible representation is in form of covariances of Legendre coefficients. From the covariance of the first coefficient (which is by definition $a_0 = 1$) correlation to the cross section can be derived. Since only the first Legendre coefficient is inherently positive, there is no need to introduce any flag.

File 35: Covariances for energy distributions. Unfortunately, there is no redundant position for a flag in subsections, corresponding to each covariance matrix. Therefore, only a general flag for all covariance matrices can be introduced, for example as the third parameter in the first row of each section (after the parameters ZA and AWR). Since any distribution is by definition an inherently positive quantity, in new evaluations with tabulated values all covariances should be given in lognormal representation!

File 40: Covariances for radionuclide production. The formats of the subsubsubsection for File 40 are exactly the same as the formats for the subsubsections for File 33; the flag could be introduced in the same way as in File 33. Since radionuclide production is an inherently positive quantity, in new evaluations all covariances should be given in lognormal representation!

The following specific changes in the ENDF-6 manual [1] are proposed:

- *Page 220, add after line 4:*

  LDST Recommended distribution for random sampling:
  LDST=0 normal distribtion for all parameters.
  LDST=1 lognormal distribtion for inherently positive parameters and normal distribution for other parameters.

- *Page 220, replace line 25 by:*

  `[MAT,30,1/ ZA, AWR, LDST, 0, 0, NP] HEAD`

- *Page 233, replace line 6 by:*

  `[MAT,32,151/ SPI, AP, 0, LCOMP, NLS, LDST] CONT.`

- *Page 233, add after line 11 (end of Section 32.2):*

  If LDST=0, use of the normal distribution is recommended for all parameters. If LDST=1, use of the lognormal distribution for inherently positive parameters and normal distribution for other parameters is recommended.

- *Page 262, add after line 3:*

  LDST Recommended distribution for random sampling:
  LDST=0 normal distribtion for all parameters.
  LDST=1 lognormal distribtion for inherently positive parameters and normal distribution for other parameters.

- *Page 262, replace line 16 by:*

  [MAT,33,MT/ 0.0, LDST, LT, LB, NT, NP/ $E_k, F_k E_l, F_l$]LIST

- *Page 285, add after line 3:*

  LDST Recommended distribution for random sampling:
  LDST=0 normal distribtion for all parameters.
  LDST=1 lognormal distribtion for inherently positive parameters and normal distribution for other parameters.

- *Page 285, replace line 21 by:*

  `[MAT,35,MT/ ZA, AWR, LDST, 0, NK, 0] HEAD`

2 MT=50

The ENDF manual administratively forbids the use of MT=50 for the cross sections and angular distributions of incident neutrons. By analogy with other reactions this would represent the compound-elastic scattering, which is by definition included in the elastic scattering MT=2, but with present restrictions cannot be retrieved from legal ENDF-6 files.

Elastic and inelastic cross sections and angular distributions in nuclear models are defined by the optical model parameters, which are usually fitted to available data at higher energies. At lower energies a mismatch between the calculated and measured values is sometimes observed. In some cases, the measured values also exhibit fluctuations in the cross sections and the average cosine of scattering (mu-bar), which cannot be fitted by model parameters that generally predict average behaviour.

The shape-elastic and the compound-elastic cross sections together make the scattering cross section, but compound-elastic angular distributions are symmetric in the CM coordinate system, while the shape-elastic angular distributions are anisotropic. By adjusting the relative contribution of each to the elastic cross section in nuclear model calculations, the mu-bar can be tuned to agree with measured values without adverse effects on the consistency of other quantities. The same kind of adjustment can be made to tune backward scattering (e.g. in the reflectors of critical assemblies), since the compound elastic cross section is the dominant contributor to the scattering at backward angles. Some experiments are highly sensitive to backward scattering [3], so the issue is not of purely academic interest. The alternative to the adjustment of angular distributions would be to modify the optical model parameters, which is very impractical and could lead to unphysical situations.

The proposal is to remove the administrative restriction on defining MT=50 for incident neutrons to define the compound-elastic cross section.

The impact of the change on the processing codes is negligible, since MT=50 does not appear in the summations for the inelastic and the total cross sections. Essentially, it is not required by the transport problems, but could be used for sensitivity studies and cross section adjustment schemes due to its influence on the mu-bar and backward scattering, while preserving the consistency with nuclear model calculations.

The following specific changes in the ENDF-6 manual [1] are proposed:

- *On Page 15 replace text*

  "...therefore, do not use MT=50 for incident neutrons, do not use MT=600 for incident protons, and so on."
  with the following:

  "...therefore, use MT=50 optionally to explicitly describe compound elastic scattering for neutrons, use MT=600 optionally to explicitly describe compound elastic scattering for protons, and so on." Note that these reactions are implicitly included in the elastic scattering cross section MT=2 and do not appear in the summations for MT=2 or MT=4.

- *In Table 14, replace the definition of MT=4 by:*

4	51-90	Total of neutron level cross sections (n,n') for incident neutrons
4	50-90	Total of neutron level cross sections (z,n') for other particles.

- *In appendix B.1. replace the Description of MT=4 by:*

  Production of one discrete-level neutron in the exit channel.
  Sum of MT=51-90 for neutrons; sum of MT=50-91 for other incident particles.

- *In appendix B.1. replace the text in Comment to MT=4:*

  "(MT=50 is undefined)."

  by the following:

'(MT=50 is optional and represents the compound-elastic cross section; it is implicitly included in the elastic MT=2)."

- *In appendix B.1. replace the text in Description of MT=50:*

  "Production of a neutron, leaving the residual nucleus in the ground state. For incident neutrons this is the compound-elastic cross section."

- *In appendix B.1. replace the Comment to MT=50 with the following:*

  "Compound-elastic cross section is optional for incident neutrons. It is implicitly included in MT=2."

3 Introducing a flag for fictitious statistically places resonances in the resolved resonance energy region

In some evaluations, resolved resonance extends to an energy above possible detection of all resonances with existing experimental methods, i.e. the upper part of the resolved resonance region is to a certain extend unresolved. If the contribution of missing resonances is small, they might be ignored. However, if this is not the case, some small resonances can be added for a better description of the interference effects. Since their exact position is usually not known, the statistical distribution of resonance parameters based on average values obtained from an energy region with good average resonance parameters values is used. In general, statistically placed resonances in the resolved resonance range can be a reasonable method to correct for missing resonances, however in future evaluations such artificial resonances should strictly be "flagged" in order to avoid possible confusion.

If all the widths of a resonance are below 10^{-10} eV, its contribution is truly negligible in any real evaluation. We believe that there are no real resonances below that value present in any application. On the other hand, resonance width cannot reach 10^{10} eV in nature. Therefore, a unique way to flag fictitious resonances would be to multiply all their assumed widths by a factor of 10^{-20}. This would ensure that they are ignored by default (which is also backward consistent), but a user still has the possibility to multiply them by 10^{-20} and use them. They can be detected simply by checking if all the widths are below 10^{-10} eV.

The following specific changes in the ENDF-6 manual [1] are proposed:

- *Page 59, replace lines 7-13 by:*

  GT Resonance total width, Γ, evaluated at the resonance energy ER.
  If GT $< 10^{-10}$, the resonance is placed statistically and the assumed width is $\Gamma = 10^{20}$ GT.

  GN Neutron width Γ_n evaluated at the resonance energy ER.
  If GN $< 10^{-10}$, the resonance is placed statistically and the assumed width is $\Gamma_n = 10^{20}$ GN.

  GG Radiation width, Γ_γ, a constant.
  If GG $< 10^{-10}$, the resonance is placed statistically and the assumed width is $\Gamma_\gamma = 10^{20}$ GG.

  GF Fission width Γ_f, a constant.
  If GF $< 10^{-10}$, the resonance is placed statistically and the assumed width is $\Gamma_f = 10^{20}$ GF.

  GX Competitive width, Γ_x, evaluated at the resonance energy ER.
  It is not given explicitly for LRF=1 or 2 but is to be obtained by subtraction, GX = GT - (GN + GG + GF), if LRX$\neq$0.
  If GX $< 10^{-10}$, the resonance is placed statistically and the assumed width is $\Gamma_x = 10^{20}$ GX.

- *Page 60, replace lines 9-10 by:*

  GFA First partial fission width, a constant.
  If GFA $< 10^{-10}$, the resonance is placed statistically and the assumed width is $\Gamma = 10^{20}$ GFA.

  GFB Second partial fission width, a constant.
  If GFB $< 10^{-10}$, the resonance is placed statistically and the assumed width is $\Gamma = 10^{20}$ GFB.

- *Page 65, replace line 17 by:*

GAM Channel width in eV or reduced-width amplitude in $eV^{1/2}$.
If $|GAM| < 10^{-10}$ and IFG=0, the resonance is placed statistically and the assumed width is $10^{20}|GAM|$. If $|GAM| < 10^{-5}$ and IFG=1, the resonance is placed statistically and the assumed reduced-width amplitude is 10^{10} GAM.

Conclusion

We believe the proposed changes to the ENDF-6 format would provide new options for some ENDF users in specific cases, thereby improving the accuracy of the nuclear data processing, while staying compatible with existing processing codes.

References

[1] Cross Section Evaluation Working Group, ENDF-6 Formats Manual, CSWEG Document ENDF-102, Report BNL-90365-2009 Rev. 2, SVN Commit: Revision 85, October 24, 2012.

[2] Gašper Žerovnik, Andrej Trkov, Donald L. Smith, Roberto Capote, "Transformation of correlation coefficients between normal and lognormal distribution and implications for nuclear applications," Nuclear Instruments and Methods in Physics Research A 727 (2013) 33-39.

[3] Daskalakis, A. M., Bahran, R. M., Blain, E. J., McDermott, B. J., Piela, S., Danon, Y., Barry, D. P., Leinweber, G., Bblock, R. C., Rapp, M. J., Capote, R., Trkov, Andrej. "Quasi-differential neutron scattering from ^{238}U from 0.5 to 20 MeV. Annals of Nuclear Energy, ISSN 0306-4549. [Print ed.], 2014, vol. 73, p.p. 455-464, doi: 10.1016/j.anucene.2014.07.023