Covariance Data in Unresolved Range

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Introduction

- The ENDF format in the URR has several limitations. Here we will focus on the covariance information.
- Some of these limitations are addressed in GNDS

Note: The following slides do not aim to present a definitive solution.

We would like briefly outline the limitations and foster a discussion that can lead to format proposals.

Current Unresolved Resonances ENDF format

File 2

E_1: Resonance parameters
E_2: Resonance parameters
…
E_N: Resonance parameters

Resonance parameters are always for SLBW.
(SAMMY converts from Fröhner parameters)

Drawbacks:
- No energy dependence
- Does not represent File 2
- Cannot be used as a prior for Bayesian evaluation

File 32

Average resonance parameters
Upper triangular of relative covariance data for average parameters.

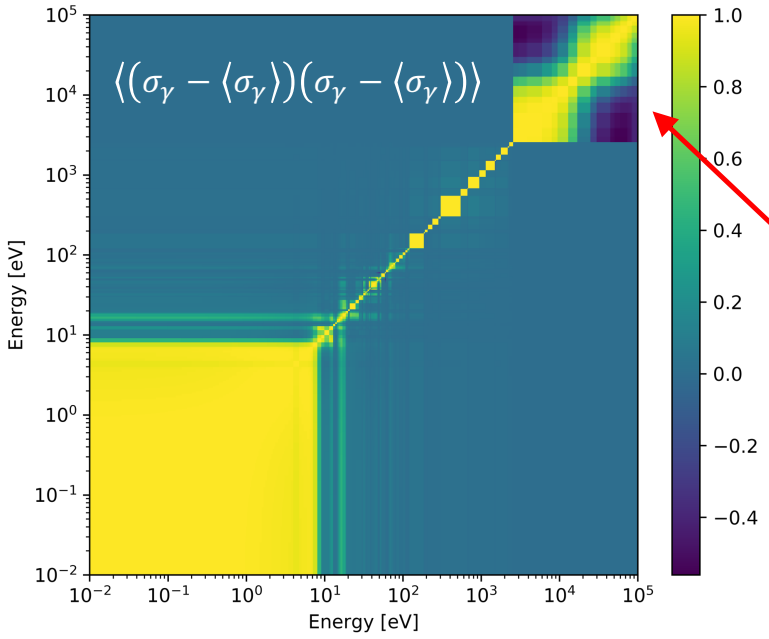
Thus, resonance covariance does not reflect resonance parameters

Note: SAMMY does Froehner algorithm. Conversion isn't loss less

Solution 1 (no format change necessary):

File 33

Covariance for each reaction with respect to cross section on suitable energy grid



This gives a covariance that can easily processed into a grouped covariance matrix suitable for transport codes

Drawbacks:

- Covariance matrix for resonance parameters is not available. Therefore, it can't be used as a prior for future evaluation.

Example: Ta-181 evaluation recently submitted to NNDC GitLab for review

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Solution 2 (no format change necessary):

File 32 allows *multiple energy ranges**

$[E_1, E_2]$: Covariance matrix for resonance parameters at E_1, same as existing format for average parameters
$[E_2, E_3]$: Covariance matrix for resonance parameters at E_2, same as existing format for average parameters
…
$[E_{n-1}, E_n]$: Covariance matrix for resonance parameters at E_{n-1}, same as existing format for average parameters

Drawbacks:

- How to set the energy ranges to capture all parameters
- Ignores all cross correlation between energies.
  Therefore, still unsuitable as a prior for future evaluation.

Note: A similar format will not work for File 2, as processing codes need to interpolate on URR resonance parameters at the desired energy.

*See Chapter 32.2 of ENDF manual

Solution 3 (format changes needed):

Change the format to allow the full covariance for all resonance parameters and all energies.

- Internally SAMMY can already write the full covariance matrix in LCOMP=2 (correlation, converted to integers by multiplying by 100). A similar format exists for the resolved range in ENDF manual - but for most evaluations doesn't give enough precision.
- Define a new format where the full covariance is given for all resonance parameters and all energies.
  - It would be preferrable to not repeat the resonance parameters in File 32 and just require that the covariance matrix is given for resonance parameter and energies as given in File 2. Since there are usually not a lot of URR parameters, this does not make the file unreasonable large.

Do we need a new format?

- In the URR File 2 there are two options:
  1. File 3 contains partial "background" cross sections, to be added to the average unresolved cross sections calculated from the parameters in File 2.
  2. File 3 contains the entire dilute cross section for the unresolved resonance region. File 2 is to be used solely for the calculation of the self-shielding factors

Transport codes use the covariance for the average (energy dependent) parameters. Thus, as stated before, covariances with respect to average cross section are sufficient.

Remaining problem: Reproducibility

It would be very useful to have the covariance with respect to all parameters in the URR, for use as a prior in future evaluation.

Since the transport and processing codes only need the covariance with respect to the cross section, could we:

- Let SAMMY write out File 33 covariance information in the URR (already implemented in the newest version). Other codes can also easily do that as they have the derivatives already calculated.
- Save the full covariance in GNDS format only (possible after some format updates). We propose to update SAMMY to read/write this covariance information. It can then be used as a prior.

Note: The RR parameters for U235 in Endf/B-VIII.0 are already stored in GNDS only, File 33 in ENDF format. Both available from NNDC.

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