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Subgroup 20: Covariance Matrix Evaluation and Process
in the Resolved/Unresolved Resonance Regions
Status Report 2004

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This report includes the activity of SG20 from April 2003 to April 2004.

Covariance Evaluations in the Resonance Range

- ORNL/LANL meeting at Oak Ridge (Jul. 15–18, 2003)

  Kawano visited Oak Ridge National Laboratory, and had a meeting on covariance evaluations for resonance parameters. The discussions included:

  - MF32, A new ENDF format for resonance parameter covariance — **compact format**.
    * Although the current ENDF-6 format can be used to store a covariance of resonance parameters, this format is practically inconvenient when the number of resonances is large. The compact format enables us to store the full covariance matrix within a reasonable file size. The format is really needed to store the huge covariance of ^{235}U resonance parameters evaluated with SAMMY.
    * This format is still pending as a part of ENDF-7 format, however it was mentioned at the 2003 CSEWG meeting that the covariance format can be separated from the main ENDF-7 format proposal.
  - Generation of covariance data for existing libraries.
    * Larson implemented "Retroactive Method" to estimate a covariance matrix of resonance parameters in SAMMY.
    * We recommend to use this capability for generation of resonance parameter covariance. SAMMY generates the covariance both in the original ENDF-6 format and in the new compact format.
    * The method can be found in the SAMMY distribution (test cases No.82 and 83).

- ORNL/LANL collaboration on Criticality Safety and Space Reactor

  - For the criticality safety and space reactor studies, we have evaluated resonance parameter covariances and the covariance for the higher energy part. The evaluated covariance files (ENDF-6 format) are complete, therefore the data are good examples to show our capability of covariance evaluation and processing.
  - For the criticality safety study
    * We have evaluated covariance data of ^{152,154,155,156,157,158,160}Gd.
    * The quantities included are resolved and unresolved resonance parameters, cross sections of total, elastic, inelastic, neutron capture, $(n, 2n)$, and $(n, 3n)$ reactions.
    * For the resonance parameters, SAMMY's retroactive method was used at ORNL.

    - For the cross sections above the resonance range, covariance data were evaluated with the KALMAN and SOK codes at LANL.
    - These two parts were combined at ORNL, and processed with ERRORJ.
  - For JIMO (Jupiter Icy Moons Orbiter) Space Reactor
    - Rhenium is used to terminate a chain reaction in the reactor, and Re covariance data are required to quantify the design margin.
    - Covariance matrices were given for ^{185}Re and ^{187}Re.
    - The same evaluation method as for Gd isotopes was adopted.
  - These data were stored in the ENDF-6 format, and processed with NJOY and ERRORJ codes. It was found that, in some cases, ERRORJ cannot process SAMMY's resonance covariance data. The problem was already noted by Shibata of JAERI in 2004. Chiba of JNC is fixing this problem.

- Development of SAMMY
  - An issue of major interest : "How believable or accurate are the covariance matrices being created for the resonance region."
  - Evaluated covariances should include all the known uncertainties in the experimental data and in the model calculation.
  - For example:
    - If the resolution-broadening function is known to have a certain form with certain parameter values, with uncertainties on those values, one might wish to use those parameter values (not allow them to vary) but also include the effect of the uncertainties.
    - Similarly for many other parameters (normalization, backgrounds, sample thickness, detector efficiencies, etc.).
  - SAMMY will have the ability to propagate uncertainties for virtually any parameters.
  - The final covariance matrix will then properly reflect all uncertainty information available to the evaluator.

The Retroactive Method to Estimate Covariance Matrices

In the SAMMY distribution, you can find two test cases — TR82 and TR83. Those contain an explanation on how to generate covariance matrices of existing resonance parameters.

The test case TR82 contains some typical experimental data of transmission, fission, and capture reactions. This test case calculates Y and W matrices defined as

$$Y = \sum_i G_i^t V_i^{-1} (D_i - \overline{T}_i), \quad (1)$$

$$W = \sum_i G_i^t V_i^{-1} G_i \quad (2)$$

where T and D are the calculated / experimental cross sections, G is the sensitivity matrix, and i stands for the index of experimental data set. These equations calculate the error propagation from experimental data to resonance parameters.

In the retroactive method, SAMMY's output covariance matrix, i.e., the covariance of output parameter values, is assumed to be associated with the initial parameter values.

If resonance parameter covariances in the compact format are needed, the TR83 directory contains an explanation on how to make them, and the ^{235}U resonance parameter covariance matrix is given there as a realistic example.

Data processing with NJOY, AMPX, PUFF-2

- ERRORJ (JNC)
  - The ERRORJ code that processes Reich-Moore covariance data can be used with NJOY, AMPX, and PUFF-2 data processing systems.
  - Chiba and Ishikawa of JNC maintain the code. The new version (ver.2.0) was released in May, 2003.
  - ERRORJ will be extended in order to read the compact covariance format generated by SAMMY.
  - ERRORJ still has some limitations; for example, it cannot calculate covariance data for a self-shielding factor.
  - The code has been distributed to Sumitomo Atomic Energy Industries, JAERI Nuclear Data Center, JAERI ADS Project, Toshiba, ORNL, ANL, LANL, NEA Dababank, and IPPE.
- NJOY (LANL)
  - Larson provided a subroutine that calculates derivatives of R-matrix theory (not numerical but analytical). This subroutine will be incorporated into NJOY to process resonance covariances. With this code, it may enable NJOY to calculate covariances of self-shielding factors.
- SAMMY (ORNL)
  - Although SAMMY is not a processing code, it also has a capability to generate group-averaged cross sections and their covariance. This would help us to check the generated group constant covariance.