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COVARIANCE MATRIX EVALUATION AND PROCESSING IN THE RESOLVED/ UNRESOLVED RESONANCE REGIONS

A report by the Working Party
on International Evaluation Co-operation
of the NEA Nuclear Science Committee

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FOREWORD

A Working Party on International Evaluation Co-operation was established under the sponsorship of the OECD/NEA Nuclear Science Committee (NSC) to promote the exchange of information on nuclear data evaluations, validation, and related topics. Its aim is also to provide a framework for co-operative activities between members of the major nuclear data evaluation projects. This includes the possible exchange of scientists in order to encourage co-operation. Requirements for experimental data resulting from this activity are compiled. The working party determines common criteria for evaluated nuclear data files with a view to assessing and improving the quality and completeness of evaluated data.

The parties to the project are: ENDF (United States), JEF/EFF (NEA Data Bank member countries) and JENDL (Japan). Co-operation with evaluation projects of non-OECD countries are organised through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

The following report was issued by Subgroup 20, whose task was to investigate methods for assessing the uncertainties associated with evaluated nuclear data in the resonance range. These uncertainty (covariance) data are essential for practical applications of evaluated nuclear data, for example for the adjustment of group constants and the estimation of design accuracies. The objectives of the subgroup were to:

- identify the needs of the user community;
- develop a methodology for the production of covariance matrices;
- produce a few examples of covariance matrices and review the formats used to store the data.

The opinions expressed in this report are those of the authors only and do not represent the position of any member country or international organisation. This report is published on the responsibility of the Secretary-General of the OECD.

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SUMMARY

This document serves as a summary of the work of Subgroup 20 (SG20) on covariance matrix evaluation and processing in the resolved/unresolved resonance regions, organised under the auspices of the Nuclear Energy Agency's Nuclear Science Committee Working Party on International Evaluation Co-operation (WPEC).

The work described in this report focuses on:

- summarising the issues related to covariance evaluation in the resonance region;
- discussing the retroactive method used in the SAMMY code [1];
- describing the compact format for storing huge covariance matrices in ENDF-6 files;
- recent developments and upgrades of processing codes to generate a multi-group covariance matrix from resonance parameter covariance data.

COVARIANCE MATRIX EVALUATION AND PROCESSING IN THE RESOLVED/UNRESOLVED RESONANCE REGIONS

1. Introduction

Requirements for covariance data for advanced technologies of nuclear energy applications are steadily growing. The evaluation of covariance data is, however, difficult and normally requires more effort than the cross-section evaluation itself. To provide the covariance data for nuclear data users is to give a qualitative assessment of the data library. Major customers of the covariance data are the reactor core calculations (estimation of uncertainty in the k_{eff}, criticality safety study, adjustment of nuclear data libraries [2,3]) and radiation shielding designs.

In WPEC/Subgroup 2 (SG2) [4], methods to evaluate the covariance of ^{56}Fe were investigated. After the completion of SG2, extensive progress was made by the JENDL group, and the JENDL-3.2 covariance file [5] for some important nuclides for fast-reactor applications was released. In practice this covariance file would be used for a few limited purposes. However, a long-standing problem remains, concerning the resonance region. For the JENDL-3.2 covariance file in the resonance region, a simple method was adopted to estimate the covariance matrices of the ^{235,238}U and ^{239}Pu resolved-resonance parameters [6]. The technique was not applicable to the ^{235}U resonance parameters in JENDL-3.3, because there are more than 3 000 resonances in one energy region.

As many nuclear data libraries – ENDF, JENDL and JEFF, for example – adopted the same ^{235}U resonance parameters obtained by Leal, Derrien, Larson and Wright [7], the issue to be resolved is of general interest among the nuclear data communities in the world.

Our main objective is to evaluate and report the resonance parameter covariance matrix in such a way that processing codes can make use of it. Both the method and some of the tools for the evaluation are described in this report. To demonstrate our achievements, we first apply our method to the gadolinium resonance parameters as a simple example, and then extend the technique into the actinide region.

2. Summary of issues discussed in the subgroup

2.1 Covariance for resonance parameters

An alternative to providing resonance parameter covariance matrices (RPCM) would be to evaluate uncertainties in multi-group-averaged cross-sections [8]. In this method, nuclear data users would find the covariance data in MF=33 of ENDF-6 files, not in MF=32. Although this may be practical for estimating the uncertainties in the resonance region for one energy group structure, the RPCM method is preferable for the following reasons:

- Use of the RPCM method makes it possible to calculate uncertainties for a self-shielding factor.

- The cross-section covariance matrix (CSCM) depends on the energy group structure used. It is easy to construct a covariance of grouped cross-sections in any kind of structure if the RPCM is available.

- Correlations between different reaction channels, such as fission and capture, can be generated using the RPCM.

Nevertheless, the CSCM method may be used for those cases where high-quality covariance data are not required. One example is resonance parameters for fission products with weak absorption, because few people use this kind of covariance data at present. For such cases, the simple solution is to estimate uncertainties in the averaged capture or total cross-sections in the resonance region, and give them in MF=33.

2.2 Data size problem

In the current ENDF-6 format, the RPCM is stored in MF=32, for which the number of elements is $N_\gamma N_p \times (N_\gamma N_p + 1)/2$, where N_γ is the number of resonances and N_p is the number of parameters per resonance. If there are 100 resonances with three parameters (E, Γ_n, Γ_γ), which might be a common case for many fission-product and structural materials, there are 45 150 elements (= 7 525 lines), and the file size is about 600 kB. It is still possible to store everything in a single file.

However, when the number of resonances is large, this format is not practical. In the case of ^{235}U, there are more than 3 000 resonances, and each resonance has five parameters. The covariance file for the resonance parameters may exceed one gigabyte.

The compact format proposed by Larson [9] permits storage of the full covariance matrix within a reasonable file size by dropping information that is not so important. This new format is essential to store the huge covariance of resonance parameters of actinides. The proposal was approved by the Cross-section Evaluation Working Group (CSEWG) in 2004, and now it is a part of the official ENDF-6 format.

2.3 The retroactive technique

For new resonance analyses, uncertainty information is obtained as a by-product of the fitting procedure used to determine the resonance parameters. Resonance analysis codes such as SAMMY [1] first generate the RPCM and then write it into an appropriate format, i.e. either the original ENDF-6 or the new compact format. The resonance parameter set and the RPCM data are then included in a single ENDF file.

However, it is not always possible or practical to perform completely new evaluations. Instead, RPCM must be found for resonance parameters in the existing nuclear data libraries. To generate these RPCM, it is necessary to collect information regarding how the resonance analysis was carried out in the past, and mimic the analysis procedure to obtain uncertainty information for the parameters.

The retroactive technique is essentially a simulation of previous resonance analyses. The reliability of the RPCM obtained with the retroactive method depends on the accuracy with which the information used for the resonance analysis can be reconstructed. This information includes experimental data, resolution functions of experiments and other systematic error sources in the data.

In the retroactive technique, experimental data are recreated from the given resonance parameters. Uncertainties in these simulated data are estimated from experimental conditions, etc., and should be realistic. The RPCM is then found by propagating all the errors from the simulated data to the resonance parameters, i.e. by using the R-matrix code to fit the simulated data by varying the resonance parameters. If the resulting fitted parameter values are very nearly the same as the original resonance parameter values, then the associated RPCM is expected to be a good approximation of the RPCM for the original resonance parameters.

2.4 Processing problem

The current release of the NJOY [10] nuclear data processing system can process neither the Reich-Moore [11] resonance parameter covariance matrix

nor the compact format. However, the ERRORJ code [12,13] can process both of them. This code can be used as a module of NJOY to generate the covariance matrix for multi-group cross-sections. We have encouraged the development of ERRORJ throughout the subgroup activity.

The ERRORJ code [12] was initially written by Kosako and Yamano of Sumitomo Atomic Energy Industries as a means of processing the JENDL-3.2 covariance file [5]; the code was then taken over by Chiba and Ishikawa [5] of Japan Nuclear Cycle Development Institute (JNC) [present affiliation, Japan Atomic Energy Agency (JAEA)]. They developed the code in order to make it usable with the other libraries, and implemented new features. The code has been distributed to many institutes, including JAEA, Toshiba, ORNL, ANL, LANL, NEA Databank, IAEA and IPPE.

Recently, ORNL established a new capability for processing covariance data. The PUFF code [14,15] can now process resonance parameter covariance matrices in both the original and the new compact format.

Although SAMMY is not a processing code, it also has the capability of generating the multi-group averaged cross-sections and the associated covariance matrix in the resonance region. SAMMY has therefore been used to check the multi-group cross-section covariances generated by ERRORJ and PUFF.

3. Procedure to evaluate resonance parameter covariances

3.1 Retroactive method

The retroactive method is a simulation of the resonance analysis. Instead of performing a full resonance analysis, it is simulated with reconstructed fictitious experimental data. Figure 1 shows a usual procedure of resonance analysis. Point-wise cross-sections are generated once from initial parameters taking into account the experimental resolution function, Doppler broadening, self-shielding effects and so forth, and the calculated cross-sections are compared with the experimental data. With a Bayesian update technique, a set of resonance parameters and the associated covariance matrix are obtained, which give a good fit to the experimental data within the accuracy of the data.

The retroactive method (Figure 2) starts with the existing resonance parameters. We assume that resonance parameters in the nuclear data libraries are the best estimates based on the experimental data available for the data analysis. Point-wise cross-section data (or transmission data) are reconstructed from the resonance parameters with the appropriate resolution function and the

target temperature. A typical resolution function can be found at several time-of-flight (TOF) facilities, such as ORELA (ORNL) and GELINA (IRMM).

The data generated are used as the simulated experimental data, and the parameter fitting to the data is performed. The uncertainties in the simulated data are also simulated, using typical statistical and systematic errors found in the literature. The parameter fitting gives χ^2 very close to zero, and there is essentially no change in the parameters, because the generated experimental and calculated cross-sections are identical.

Larson has implemented the retroactive covariance generation option into the SAMMY code, and we recommend that this capability be used for covariance evaluations. The JENDL-3.2 resonance covariance data [6] adopted a similar but simplified method. Table 1 shows a comparison of methods used in JENDL-3.2 and those used in SAMMY.

Table 1. **Comparison of JENDL-3.2/3.3 and SAMMY retroactive methods**

	JENDL	SAMMY retroactive
Data point	Averaged over several resonances	Reconstructed (simulated) from original resonance parameters
Resolution	N/A	Taken from typical experiments
Uncertainties	Inferred from real experiments, but rounded into a single value – 5% for example	Estimated from real experiments, can be rounded into a single value
Correction	N/A	Doppler and resolution broadening, multiple scattering, normalisation, and background, etc.
Sensitivity	Sensitivity to the σ	At each data point

3.1.1 Example 1, simple case

The covariance matrix of resonance parameters obtained in this manner reproduces the accuracy of the simulated data, so the generated data uncertainties should be realistic. As a simple example, we ignore all the data broadening and distortion effects, and just calculate cross-sections with the given resonance parameters. Figure 3 shows the change in the capture cross-sections of ^{156}Gd when the capture width Γ_γ of the 33 eV resonance was increased by 50%. This

results in a 30% increase in the calculated capture cross-section at 10 eV, and a relative sensitivity of 30/50 = 0.6. If we assume that the uncertainty in the capture cross-section at 10 eV is 5%, Γ_γ should have an uncertainty of 5/0.6 = 8.3%.

We generate the "simulated experimental data" using the ^{156}Gd resonance parameters in ENDF/B-VI, which were evaluated using the Multi-level Breit-Wigner formula. First, we consider the capture data only. Important quantities are the number of data points included (relevant to the TOF data energy interval) and the energy resolution. Here we consider simple Gaussian broadening due to the experimental energy resolution. In the measurement of the ^{99}Tc capture cross-section [16] at the KURRI TOF facility, there are about 100 energy points in the TOF data. Sources of uncertainty in the neutron capture measurement are statistical errors (3-10%), normalisation errors (6%) and other corrections (about 2%). We assumed that the simulated neutron capture data are of a similar quality as the KURRI ^{99}Tc data, so 10 uncertainties in the capture cross-sections with 50% correlation that comes from normalisation are given to the simulated data. The correlation coefficients tend to be large because of the uncertainties in the data normalisation. The energy resolution (FWHM) of 1% was also taken from the real experiment.

It should be emphasised that the data uncertainties are not copied from the KURRI experiments. Rather, the uncertainty information is estimated by referring to a typical experimental set-up, assuming that accuracies of measurements at each experimental facility are not very different.

The KALMAN code [17] was used to estimate the RPCM. The CSCM was reconstructed from the RPCM and the sensitivity matrices; calculated uncertainties in the capture cross-section are shown in Figure 4. The average uncertainty in the capture cross-sections in the energy range 0-1 keV is 5.4%. The total cross-section has larger uncertainties, because transmission data were not included in this evaluation.

The neutron transmission data for gadolinium isotopes were analysed by Mughabghab and Chrien [18]. Since no experimental transmission data are available in EXFOR, we simulated the data and included realistic estimates of experimental conditions. The simulated data are based on the following assumptions: transmission data energy interval of $\delta E \sim 0.01 E_n$ (obtained from the literature), energy resolution of 1% and 10% total uncertainties with 50% correlation. We did not include the data in the off-resonance region, because they are not informative. The calculated uncertainties in the total cross-sections are shown in Figure 5. The average uncertainty is 2%. Since capture data were not used in this calculation, the uncertainties in the capture cross-section became unrealistic.

The combined result, which includes simulated total and capture data, is shown in Figure 6. The average uncertainty in the total cross-section is 1.7%, and in capture is 3.2%.

3.1.2 Example 2, using the SAMMY retroactive option

Experimental data in the resonance region, as discussed before, often reveal a strong correlation due to the data normalisation. If the data are strongly correlated, statistical errors are not so important because they disappear when many data points are included, and only systematic (normalisation) error remains. In this situation the retroactive analysis of the resonance covariance with SAMMY becomes fairly efficient.

The normalisation error is nn important quantity in the SAMMY retroactive method. We again employ the gadolinium isotope as an example. It is assumed that the capture normalisation error is 5% and the total normalisation error is 3%. Those values were chosen so as: (1) to reproduce the evaluated uncertainties in the thermal cross-sections reported by Mughabghab [19]; and (2) to be reasonably consistent with realistic situations of measurements.

Figure 7 shows generated neutron capture cross-sections for ^{155}Gd with SAMMY. The data were made for 12 370 energy points in the energy range 0-183.3 eV, which covers the entire resolved-resonance region. The total cross-section data were also generated on the same energy grid. The statistical uncertainty in the capture reaction was assumed to be 20%, and in the total was 2%. Those values do not have a large impact on the final result. Note that those uncertainties are just statistical, and they are not correlated.

SAMMY generates the RPCM by fitting the resonance parameters to the simulated experimental data. The resonance parameters do not change during the fitting process, because the calculated and experimental cross-sections are the same. The RPCM is then written into the ENDF-6 format (standard ENDF-6 or compact format); this RPCM is shown in the standard format in Figure 8.

3.2 Compact format

The compact covariance matrix format proposed by Larson drastically reduces the file size of resonance parameter covariance. The format was approved by CSEWG, and the ENDF-6 data format manual (Revision 2005) [9] explains this format in detail. In this format, the covariance of resonance parameters is decomposed into the correlation matrix and uncertainties. The correlation

coefficients, which range from -1.0 to 1.0, are scaled by a factor of 100, and expressed by signed integer numbers, from -99 to 99.

The following procedure to compact the correlation coefficients is defined in the ENDF-6 manual [9]:

1. Drop (set to zero) all values of correlation between -0.02 and +0.02.
2. Multiply the remaining coefficients by 100.
3. Map all positive values grater than K and less than or equal to $K + 1$ to the integer K.
4. Map all negative values less than $-K$ and greater than or equal to $-K - 1$ to the integer K.

As an example, the resonance parameter covariance for ^{157}Gd in the compact format is shown in Figure 9.

The compact covariance matrix format has a great advantage in storing the resonance parameter covariances of actinides. For many of the major actinides such as ^{233,235}U, only the compact format can hold the complete covariance data in the nuclear data library. Leal, *et al*. [20] performed the R-matrix resonance analysis of ^{233}U, and the full covariance matrix of 769 resonance parameters were obtained with SAMMY. When the data are stored using ENDF-6 format, the file size becomes 94 MB; with the compact format, the size is a mere 2 MB.

3.3 Processing

The ERRORR module of NJOY [10] is able to process the RPCM if it is given by the Multi-level Breit Wigner (MLBW) formula. A long-standing problem regarding the processing code, however, involves processing the covariances of the ENDF LRF=3 format (the so-called Reich-Moore format) [11].

The problem was resolved by the JENDL project. The ERRORJ code [12], an improved version of ERRORR, was developed to process the JENDL-3.2 covariance file [5]. The code was later extensively improved by Chiba and Ishikawa [13], and Chiba reported on the current status of the ERRORJ code at the workshop of “Perspectives on Nuclear Data for the Next Decade” [21].

To generate the covariance matrix of multi-group cross-sections, the processing code calculates error propagation from the resonance parameter covariance to the cross-section, for which it requires the sensitivity coefficients $\partial\sigma_i/\partial p_j$, where σ_i is the i-th group cross-section, and p_j is the resonance

parameter. ERRORJ calculates the sensitivity coefficients numerically. These numerical derivatives have been tested through comparison with SAMMY's analytic calculations of $\partial\sigma_i/\partial p_j$.

Recently Wiarda made improvements in the PUFF code [15] at ORNL. PUFF now has the capability to process a LRF=3 resonance parameter covariance matrix, using the same analytical derivatives as SAMMY.

3.4 Unresolved resonance region

Issues to be discussed regarding the unresolved resonance region mainly concern the format, comprising two parts: (1) uncertainty on the nuclear radius, and (2) energy-dependent unresolved resonance parameters.

The current ENDF-6 format does not include provision for an uncertainty on the nuclear radius. Due to this limitation, the calculated uncertainties in the averaged cross-sections in the unresolved resonance region tend to be small, as discussed by Kawano and Shibata [22]. However, the nuclear radius is usually held fixed while performing a resonance analysis and the uncertainty in the radius parameter should be reflected (absorbed) by the uncertainties in the resonance parameters themselves.

The covariance of unresolved resonance parameters must be in one energy region, even if energy-dependent unresolved resonance parameters are given in MF=2. This problem would be resolved by applying the retroactive evaluation technique to the unresolved resonance parameters. The energy-independent unresolved resonance parameters are fitted to the simulated cross-sections generated from the energy-dependent parameters.

Those two issues require modifications to the current ENDF-6 format. However, motivation for the new format proposal is not that great, as the current format is still able to accommodate the covariance data in the unresolved region as described above.

4. Results and discussions

Resonance parameter covariance matrices for the gadolinium isotopes for ENDF/BVII were evaluated by Leal [23]. They were compiled into the ENDF-6 format files, and tested by processing with ERRORJ.

The relative uncertainties in the total and elastic cross-sections are shown in Figure 10. The uncertainties in the capture cross-section are very similar to the total cross-section, and omitted from this plot. Figure 11 shows the correlation matrix of ^{155}Gd multi-group total cross-section in the resonance region (up to 100 eV), generated with ERRORJ. Regions with negative correlation coefficient are shown by the solid-line boxes. If the covariance in the resonance region is evaluated based on the averaged cross-section data, the correlation matrix may have positive elements only, due to systematic (normalisation) errors in the experimental data used. Negative correlations occur because of the introduction of the physics of resonances into the data analysis.

The first three resonances of ^{155}Gd are at 0.0268 eV, 2.008 eV and 2.568 eV, shown by arrows in Figure 12. Below the first resonance the cross-section has a simple 1/v shape, so that those cross-sections should be almost fully correlated. The resonance analysis tells us that the cross-sections between the first and second resonances must be anti-correlated to the first resonance region.

The correlation matrices for the elastic scattering and capture cross-sections are shown in Figures 13 and 14. The correlation matrix of capture is similar to the total cross-section in Figure 11. The cross-correlation between different reaction channels can be given by the RPCM. Figure 15 shows the correlation matrix between the elastic and capture channels generated by ERRORJ. Such cross-correlation is especially important at thermal energy. For fissile materials like ^{235}U and ^{239}Pu, we expect a strong correlation between the fission and the total cross-sections at thermal energy, as the fraction of fission in the total absorption is very large. For the fertile and non-fissioning materials, the total and capture cross-sections may be strongly correlated. When using the RPCM, such a physical property is automatically taken into account.

Leal, *et al*. [24] presented a method to generate covariance data for ^{233}U resonance parameters using SAMMY. The ^{233}U covariance data were processed with ERRORJ to produce COVERX formatted data, and benchmark calculations were performed with TSUNAMI. It was shown that the contribution of ^{233}U resonance parameter uncertainties to k_{eff} is about 0.5% for the ^{233}U thermal system (u233-sol-therm015).

5. Concluding remarks

We have discussed several important issues concerning the covariance evaluation in the resolved and unresolved resonance regions, including data processing. For existing resonance parameters, we showed that the retroactive technique is a powerful method for generating resonance parameter covariance

matrices (RPCM). The retroactive method has been implemented in the SAMMY code, and examples were shown for the covariance data of gadolinium isotopes.

Resonance parameter covariance matrices tend to be large; it was shown that the compact format drastically reduces the file size. This new format was approved by the CSEWG in 2004, and it is now a part of the official ENDF-6 format. The compact format enables storage of the full RPCM in the evaluated nuclear data library within a reasonable file size.

To process the Reich-Moore resonance parameter covariance to produce multi-group cross-section covariance data, two processing codes are currently available – ERRORJ and PUFF. Both codes are also able to read the compact format. We presented the multi-group cross-section covariance of ^{155}Gd.

REFERENCES

[1] Larson, N.M., *Updated Users' Guide for SAMMY: Multilevel R-matrix Fits to Neutron Data Using Bayese' Equation*, ORNL/TM-9179/R6, Oak Ridge National Laboratory (2003).

[2] Ishikawa, M., "Development of a Unified Cross-section Set ADJ2000 Based on Adjustment Technique for Fast Reactor Analysis", *J. Nucl. Sci. Technol*., Suppl.2, 1073 (2002).

[3] Ishikawa, M., "Recent Application of Nuclear Data to Fast Reactor Core Analysis and Design in Japan", *Proc. Int. Conf. Nuclear Data for Science and Technology*, Santa Fe, New Mexico, USA, 26 Sept.-1 Oct. 2004, p. 1405 (2005).

[4] WPEC/Subgroup 2 (Co-ordinator H. Vonach), *Generation of Covariance Files for Iron-56 and Natural Iron*, Nuclear Energy Agency, OECD (1996).

[5] Shibata, K., A. Hasegawa, O. Iwamoto, S. Chiba, M. Sugimoto, N. Odano, T. Kawano, Y. Nakajima, T. Murata, H. Matsunobu, S.Y. Oh, K. Yokoyama, K. Sugino, M. Ishikawa, K. Kosako, N. Yamano, Y. Kanda, "JENDL-3.2 Covariance File", *J. Nucl. Sci. Technol*., Suppl. 2, 40 (2002).

[6] Kawano, T., K. Shibata, *J. Nucl. Sci. Technol*., 39, 807 (2002).

[7] Leal, L.C., H. Derrien, N.M. Larson, R.Q. Wright, "R-matrix Analysis of ^{235}U Neutron Transmission and Cross-sections in the Energy Range 0 to 2.25 keV", ORNL/TM-13516, Oak Ridge National Laboratory (1997); *Nucl. Sci. Eng*., 131, 230 (1999).

[8] Shibata, K., *J. Nucl. Sci. Technol*., 42, 130 (2005).

[9] Larson, N.M., "Compact Covariance Matrix", in *ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6*, BNL-NCS4494505-Rev., Cross-section Evaluation Working Group, Brookhaven National Laboratory, NY, USA (2005).

[10] MacFarlane, R.E., D.W. Muir, *The NJOY Nuclear Data Processing System Version 91*, LA-12740-M (1994); *The NJOY Nuclear Data Processing System Version 99* (1999).

[11] Reich, C.W., M.S. Moore, *Phys. Rev*., 111, 929 (1968).

[12] Kosako, K., "Covariance Data Processing Code: ERRORJ", *Proc. of the Specialists Meeting on Reactor Group Constants*, J. Katakura, Ed., JAERI, Tokai, Japan, 22-23 February 2001, JEARI-Conf 2001-009, p. 30, Japan Atomic Energy Research Institute (2001); K. Kosako and N. Yamano, *Preparation of a Covariance Processing System for the Evaluated Nuclear Data File, JENDL (III)*, JNC TJ9440 99-003, Japan Nuclear Cycle Development Institute (1999) [in Japanese].

[13] Chiba, G., M. Ishikawa, "Revision and Application of the Covariance Data Processing Code, ERRORJ", *Proc. Int. Conf. Nuclear Data for Science and Technology*, Santa Fe, New Mexico, USA, 26 Sept.-1 Oct. 2004, p. 468 (2005).

[14] Dunn, M.E., *PUFF-III: A Code for Processing ENDF Uncertainty Data Into Multigroup Covariance Matrices*, Oak Ridge National Laboratory, NUREG/CR-6650 ORNL/TM-1999/235 (2000).

[15] Wiarda, D., M.E. Dunn, N.M. Greene, N.M. Larson, L.C. Leal, "New Capabilities for Processing Covariance Data in the Resonance Region", *PHYSOR 2006* [to be published].

[16] Kobayashi, K., S. Lee, S. Yamamoto, T. Kawano, *Nucl. Sci. Eng*., 146, 209 (2004).

[17] Kawano, T., K. Shibata, *Covariance Evaluation System*, JAERI-Data/Code 97-037, Japan Atomic Energy Research Institute (1997) [in Japanese].

[18] Mughabghab, S.F., R.E. Chrien, *Phys. Rev*., 180, 1131 (1969).

[19] Mughabghab, S.F., "Atlas of Neutron Resonances", Academic Press (2006).

[20] Leal, L.C., H. Derrien, J.A. Harvey, K.H. Guber, N.M. Larson, R.R. Spencer, *R-matrix Resonance Analysis and Statistical Properties of the Resonance Parameters of ^{233}U in the Neutron Energy Range from Thermal to 600 eV*, ORNL/TM-2000/372, Oak Ridge National Laboratory (2001).

[21] Chiba, G., “Resonance Self-shielding in Covariance Processing”, *Proc. Workshop of Perspectives on Nuclear Data for the Next Decade*, CEA/BRC, France, 26-28 Sept. 2005 [to be published].

[22] Kawano, T., K. Shibata, “Evaluation of Covariance Matrices for Resolved and Unresolved Resonance Regions”, *Proc. of the 11th Int. Symp. on Reactor Dosimetry*, Brussels, Belgium, 18-23 Aug. 2002, J. Wagemans, H.A. Abderrahim, P. D’hondt, C. De Raedt, Eds.,World Scientifics, p. 631 (2003).

[23] Leal, L. (2006) [private communication].

[24] Leal, L., G. Arbanas, N. Larson, H. Derrien, D. Wiarda, *Nuclear Data Covariance Generation in the Resonance Region*, Talk at CSEWG & USNDP Meeting, Brookhaven National Laboratory, USA, 8-11 Nov. 2005.

FIGURES

Figure 1. Procedure to obtain resonance parameters

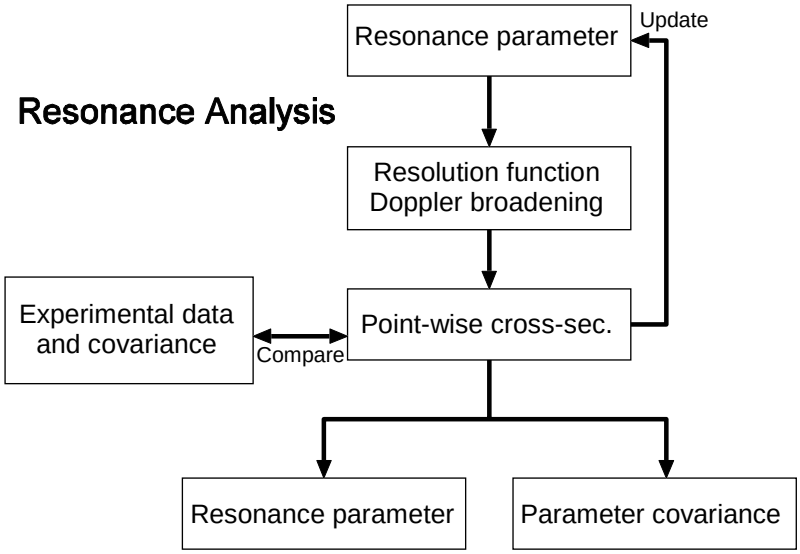


Figure 2. Retroactive method

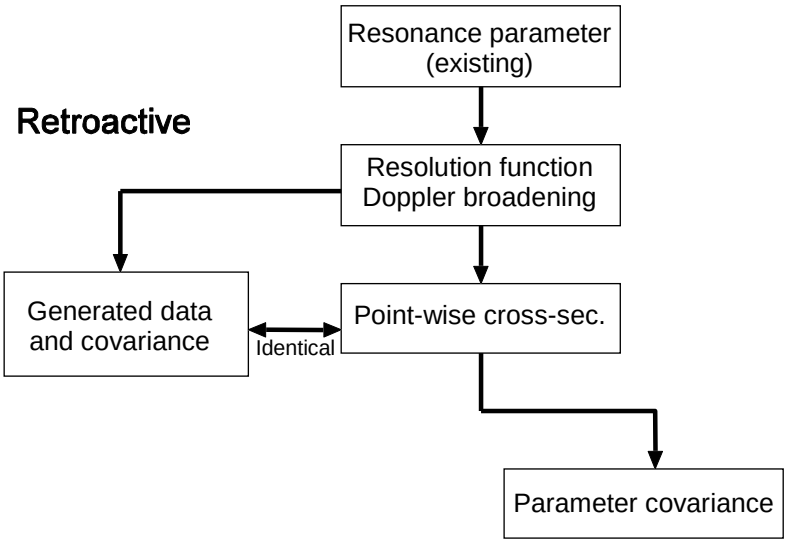


Figure 3. Sensitivity of the capture width of the first resonance to the capture cross-sections for ^{156}Gd

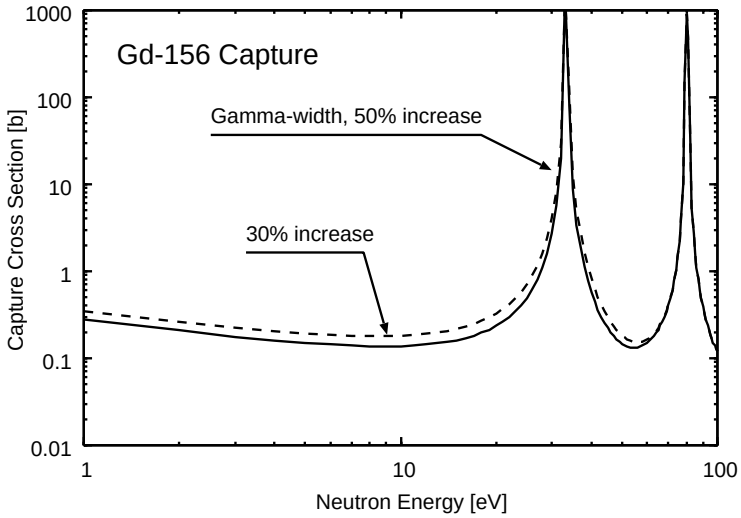


Figure 4. Calculated uncertainties in the ^{156}Gd capture cross-sections, assuming the simulated capture data have 10% uncertainties with 50% correlation

The arrows show the location of resonances

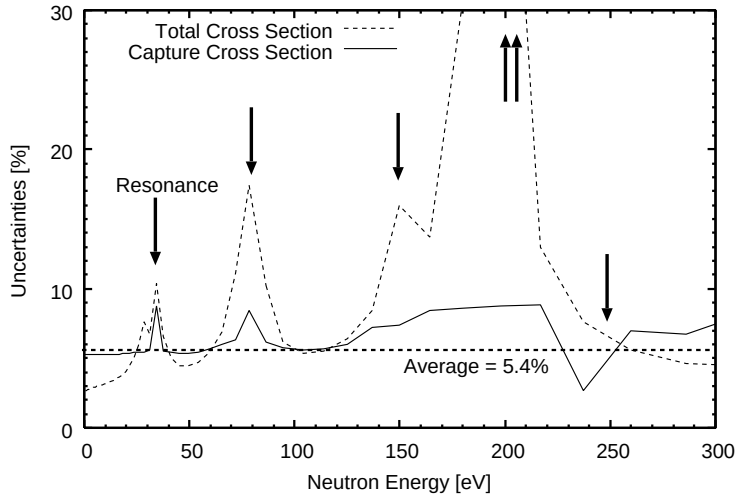


Figure 5. Calculated uncertainties in the ^{156}Gd total cross-sections, assuming the simulated total cross-section data have 10% uncertainties with 50% correlation

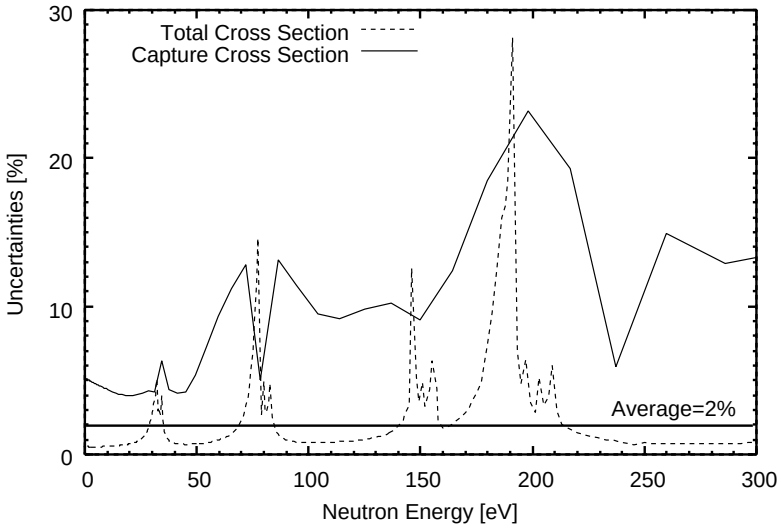


Figure 6. Calculated uncertainties in the ^{156}Gd capture and total cross-sections

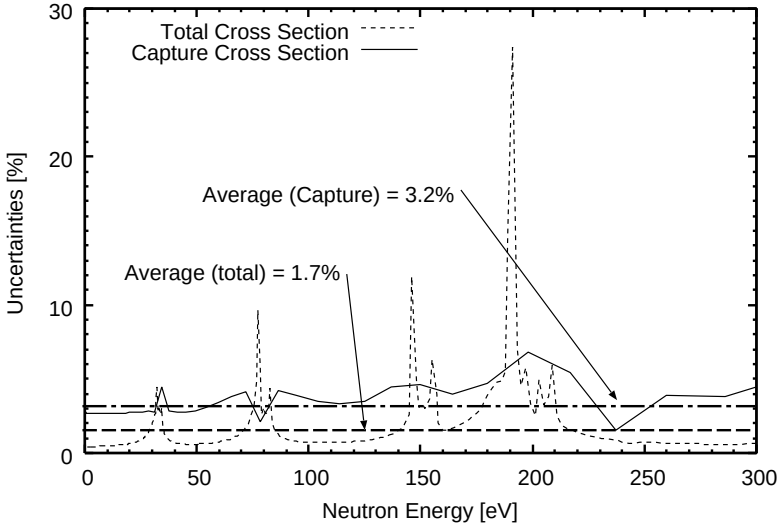


Figure 7. Generated ^{155}Gd capture cross-sections using SAMMY

The dotted and dashed curves are the 20% uncertainty band

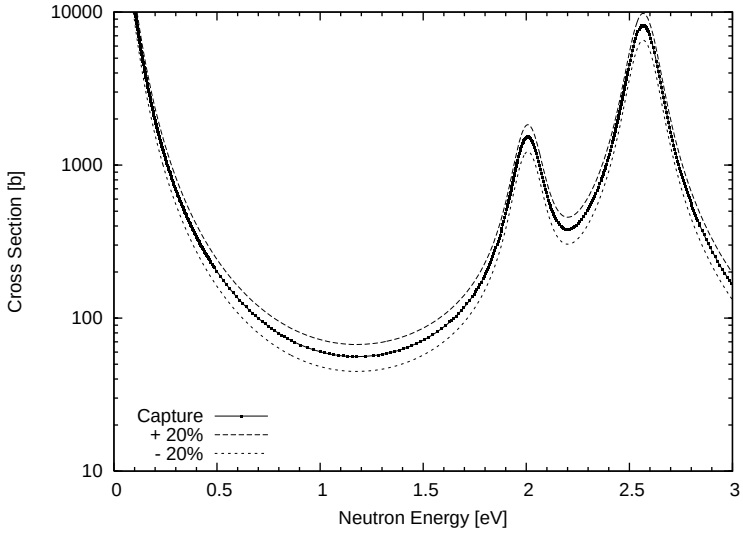


Figure 8. ENDF-6 formatted ^{155}Gd resonance parameter covariance generated by SAMMY

```
  64155.0   1.535920+2          0          0          1          0643432151    1
  64155.0   1.000000+0          0          0          1          0643432151    2
 1.000000-5 1.833000+2          1          3          0          1643432151    3
      1.5   7.900000-1          0          1          0          0643432151    4
 1.535920+2                     0          0          1          0643432151    5
                                3          0      38778         92643432151    6
0.026799999       2.0   1.040000-4 1.080000-1                     643432151    7
2.007999999       1.0   3.706666-4 1.100000-1                     643432151    8
2.568000000       2.0   1.744000-3 1.110000-1                     643432151    9
3.616000000       1.0   4.400000-5 1.300000-1                     643432151   10
   ......

175.5999999       2.0   2.080000-3 1.098000-1                     643432151   96
178.0000000       1.0   9.733333-3 1.098000-1                     643432151   97
180.3999999       1.0   1.466667-2 1.098000-1                     643432151   98
 1.875531-7 .3376958-9-2.264001-7 .7678523-9 .0042410-9 2.186969-8643432151   99
 .0196131-9-.0722565-9 1.476097-8 1.785823-9-.0036186-9-5.272415-9643432151  100
-.0217329-9-.0853346-9 1.741534-9-.0046285-9-.0457875-9 .4604478-9643432151  101
 .0003844-9-.0071501-9-.8064558-9 .0359892-9-.0248011-9-.5288035-9643432151  102
-.0759183-9-.0364101-9-.4262018-9-.0668140-9-.1325805-9-.5289678-9643432151  103
   ......

 8.837309-9 1.220777-8-7.495823-7 1.732927-8-1.512111-7-2.818956-9643432151 6467
 3.366244-9-2.203100-8 3.179969-5 3.093391-7 8.139690-8-4.179741-6643432151 6468
 6.019313-6-3.344716-8 6.208129-7 3.055970-8-2.288672-7 1.823992-5643432151 6469
```

Figure 9. The ENDF-6 resonance parameter covariance of ^{157}Gd in the compact format

```
 6.415700+4 1.555760+2          0          0          1          0644032151    1
 6.415700+4 1.000000+0          0          0          2          0644032151    2
 1.000000-5 3.066000+2          1          3          0          1644032151    3
      1.5   8.000000-1          1          2          1          4644032151    4
 6.415700+4                     3          0        720         60644032151    5
0.030874750       2.0   4.633883-4 1.072601-1                    644032151    6
0.004709259             4.046326-5 1.809663-3                    644032151    7
2.825350651       2.0   3.445999-4 9.710919-2                    644032151    8
0.070088626             8.111083-6 1.940976-3                    644032151    9
16.24198188       1.0   3.992890-4 9.102763-2                    644032151   10
   ......

300.9014716       1.0   5.518277-2 1.016247-1                    644032151  122
0.007512823             8.754985-4 1.692468-3                    644032151  123
306.4155768       2.0   2.815115-3 1.000446-1                    644032151  124
0.013196548             5.442585-5 1.975326-3                    644032151  125
        0.0         0.0          0        180        314        314644032151  126
    2    1  99                                                   644032151  127
    3    1 -99  0                                               644032151  128
    5    4  52                                                   644032151  129
    8    7  11                                                   644032151  130
    9    7   2                                                   644032151  131
   10    7  -1  4  1                                            644032151  132
   11    1  -1 -1 -1           1 -2    -9                       644032151  133
   12    3  -3            5 -2 -1   -64                        644032151  134
   13   12   1                                                   644032151  135
   14    1  -1 -1 -1                    1  4  1 -2              644032151  136
   15    3  -2           -1          -3 -9 -5-72                644032151  137
   16   13   2  1  2                                            644032151  138
   17   11   3  1 -2 -1-12-15                                   644032151  139
   18   13  -2 -3-11-12  1                                      644032151  140
   19   15   1        1                                         644032151  141
   20   11   3        3 -3     2 -1 -1                          644032151  142
   ......
```

Figure 10. Uncertainties in the multi-grouped cross-sections of ^{155}Gd generated by ERRORJ

The solid line is for the total and dashed line is for the elastic scattering cross-sections

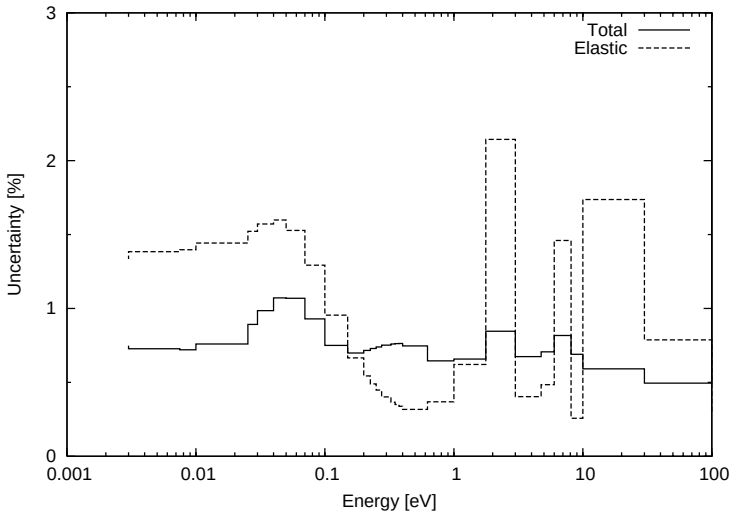


Figure 11. Correlation matrix of ^{155}Gd total cross-sections in the resonance region, generated by ERRORJ

The regions surrounded by the solid-line boxes have negative correlations

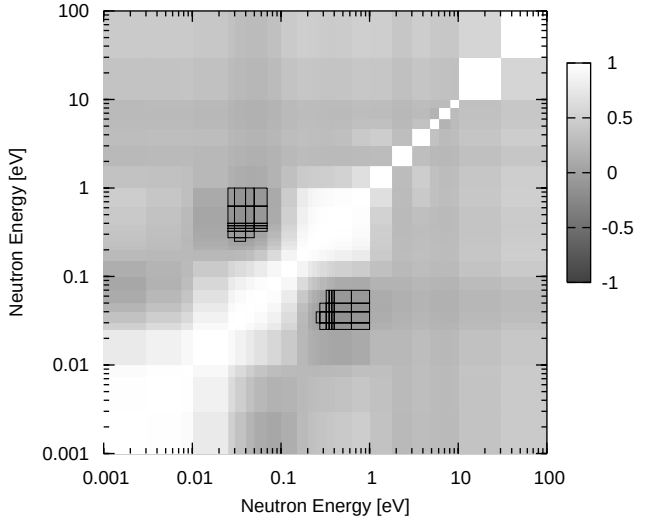


Figure 12. Zoomed plot of Figure 11, in the energy range 0.01-5 eV

Locations of three resonances of ^{155}Gd are shown by the arrows

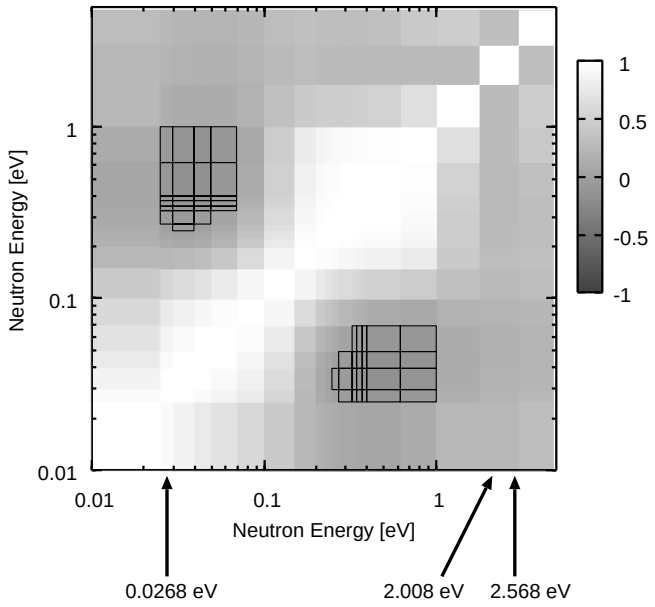


Figure 13. Correlation matrix of ^{155}Gd elastic scattering cross-sections in the resonance region

The regions surrounded by the solid-line boxes have negative correlations

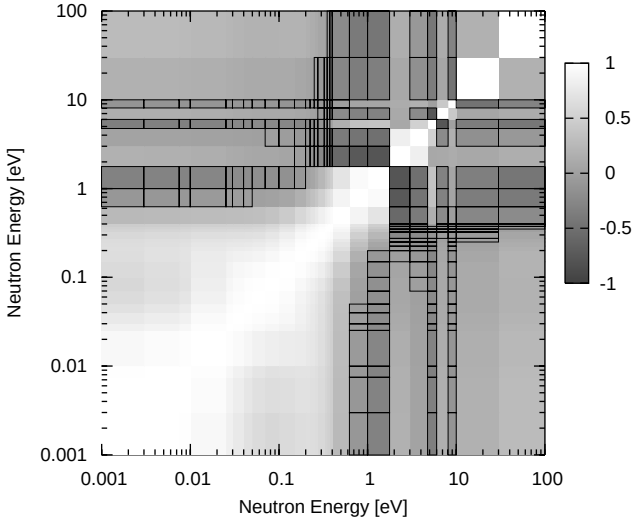


Figure 14. Correlation matrix of ^{155}Gd capture cross-sections in the resonance region

The regions surrounded by the solid-line boxes have negative correlations

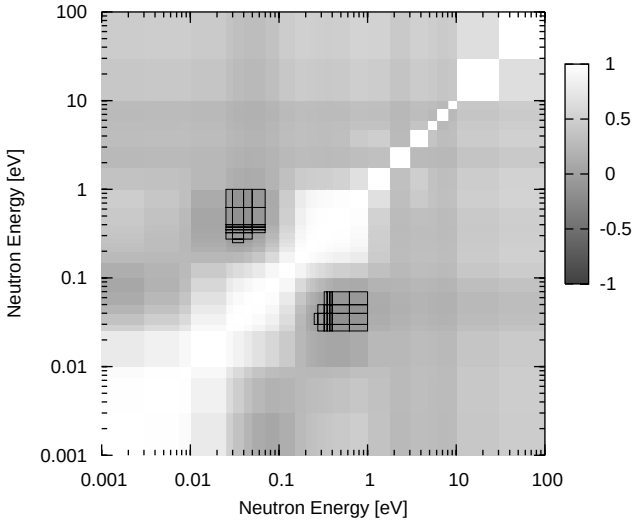
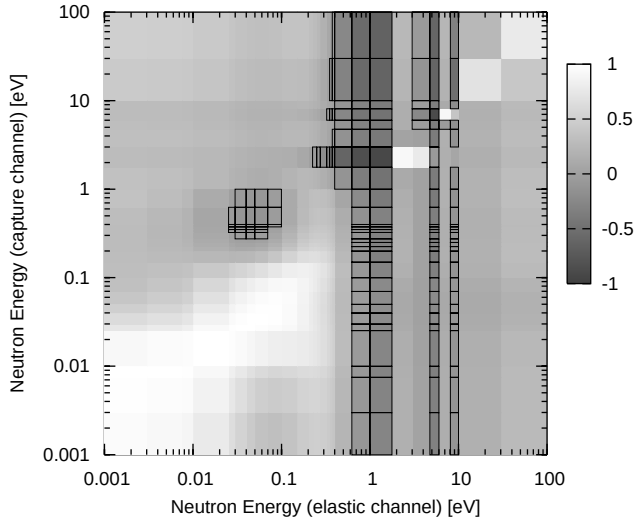


Figure 15. Correlation matrix of ^{155}Gd between elastic and capture reactions in the resonance region

The horizontal axis is the energy of elastic scattering, and the vertical axis is the capture energy. The regions surrounded by the solid-line boxes have negative correlations.



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