ERRORJ - Covariance Processing Code System for JENDL

Version 2 (Manual)

September, 2003

O-arai Engineering Center Japan Nuclear Cycle Development Institute 本資料の全部または一部を複写・複製・転載する場合は、下記にお問い合わせください。 〒319-1184 茨城県那珂郡東海村村松4番地49 核燃料サイクル開発機構 技術展開部 技術協力課 電話: 029-282-1122 (代表) ファックス: 029-282-7980 電子メール: jserv@jnc.go.jp

Inquiries about copyright and reproduction should be addressed to: Technical Cooperation Section, Technology Management Division, Japan Nuclear Cycle Development Institute 4-49 Muramatsu, Tokai-mura, Naka-gun, Ibaraki - Ken 319-1184, Japan

© 核燃料サイクル開発機構 (Japan Nuclear Cycle Development Institute) 2003

ERRORJ – Covariance Processing Code System for JENDL Version 2

Gou Chiba*

Abstract

ERRORJ is the covariance processing code system for Japanese Evaluated Nuclear Data Library (JENDL) that can produce group-averaged covariance data to apply it to the uncertainty analysis of nuclear characteristics. ERRORJ can treat the covariance data for cross sections including resonance parameters as well as angular distributions and energy distributions of secondary neutrons which could not be dealt with by former covariance processing codes. In addition, ERRORJ can treat various forms of multi-group cross section and produce multi-group covariance file with various formats.

This document describes an outline of ERRORJ and how to use it.

*: Reactor Physics Research Group, System Engineering Technology Division,

O-arai Engineering Center, JNC, Japan

ERRORJ -JENDL のための共分散処理システム Version 2

千葉 豪*

要旨

ERRORJ は Japanese Evaluated Nuclear Data Library(JENDL)のための共分散処理シス テムであり、核特性計算値の不確かさの評価に用いるためのエネルギー群で平均化された共分 散データを作成する。ERRORJ は従来の共分散処理コードでは不可能であった、共鳴パラメ ータを含む断面積、並びに二次中性子の角度およびエネルギー分布の共分散の処理が可能であ る。加えて、ERRORJ はさまざまな形式の多群断面積の読み込みおよび多群共分散の出力が 可能である。

このドキュメントは、ERRORJ の概要とその使用法を述べたものである。

* 大洗工学センター システム技術開発部 中性子工学グループ

Contents

List of Figures

1. Introduction

It is important to evaluate uncertainty of nuclear characteristics in the reactor core analysis field. For such kind of analysis, covariance data in nuclear data files are essential.

To apply the covariance data for the uncertainty analysis, group-averaged covariance data are necessary. The original ERRORJ code was developed to obtain the group-averaged covariance data by K. Kosako. [1][2]. ERRORJ can treat the covariance data for cross sections including resonance parameters, angular distributions and energy distributions of secondary neutrons which could not be dealt with by former covariance processing codes, ERRORR in NJOY [3] or PUFF-2 [4].

Original manual of ERRORJ was written in Japanese by K. Kosako [1]. This manual is a translation of the original manual with a little modification in processing angular distributions of secondary neutrons. In chapter 2, we described the outline of development of ERRORJ. Special techniques implemented to ERRORJ are described in chapter 3 and how to use ERRORJ are in chapter 4. In chapter 5, several examples are shown. Summary is described in chapter 6.

2. Development of ERRORJ

ERRORJ was developed based on ERRORR module in NJOY94.105 [3]. Thus, all the functions of ERRORR are available in ERRORJ. ERRORJ produces a COVFIL format file storing multi-group covariance data. The COVFIL format file can be converted to a COVERX format file by a conversion program which is named NJOYCOVX in the ERRORJ system. The COVERX format has been proposed as a standard file of multi-group covariance data in the FORSS system [5]. The calculation flow of ERRORJ is shown in Fig. 1.

ERRORJ version 1 and NJOYCOVX were developed by K. Kosako in 1999.

In 2002, a calculation routine processing the average cosine of elastic scattering angle was modified to calculate relative covariance correctly and version 2 was developed by G. Chiba of Japan Nuclear Cycle Development Institute. Other modifications have been carried out because several small errors were found in the ERRORJ program source.

The features of ERRORJ are as follows:

- (a) Newly-developed method is implemented to treat the covariance data of the general resolved and unresolved resonance parameters. In the ERRORR module, there are several limitations in treatment of the resonance parameters.
- (b) It is possible to process the average cosine of the elastic scattering angle and fission spectrum.
- (c) Various forms of multi-group cross section can be read.
- (d) Output files with various formats are produced by NJOYCOVX (COVERX format file, correlation matrix file, and relative error and standard deviation file).

On the other hand, ERRORJ has some limitations as follows:

- (a) It is impossible to treat the covariance data of the general resolved resonance parameters under the condition, NLRS>0 (long-range covariance contribution).
- (b) The general Adler-Adler resolved resonance parameters cannot be dealt with.

Fig.1 Calculation flow of the covariance data processing system

3. Methods added to ERRORR module

3.1 Newly developed method for processing resonance parameters

It is impossible to apply the method for processing the covariance of compatible resolved resonance parameters, which was developed in PUFF-2, into processing the covariance of general resolved and unresolved resonance parameters. Thus, a new method, named 1% sensitivity method, was developed. The procedure is described below. In ERRORJ, the PUFF-2 method is also available as "area sensitivity method". Comparison between these two methods was carried out by K. Kosako [1][2].

- (a) At first, two point-wise resonance cross sections are calculated. One is a basic resonance cross section $\sigma(E)$ and the other is $\sigma_i(E)$ which is obtained with 1% changed resonance parameter p_i .
- (b) Group averaged cross sections, σ_{g} and $\sigma_{i,g}$, are calculated.
- (c) Sensitivity coefficient of resonance parameter to group averaged cross section, $S_{i,e}$, is calculated as below.

$$
S_{i,g} = \frac{\left(\frac{\sigma_{i,g}}{\sigma_g} - 1\right) \cdot \sigma_g \cdot 100}{p_i}.
$$

(d) Group averaged covariance, $\cos \theta$, is calculated with the sensitivity coefficients and covariance

of the resonance parameters, $cov_{i,i}$, as below.

$$
covg = \sum_{i,j} cov_{i,j} \cdot S_{i,g} \cdot S_{j,g} .
$$

(e) Above procedure is carried out at each *l* value (neutron orbital angular momentum; NLS).

This method can treat a resonance existing over a few energy groups, negative resonance energy, unresolved resonance energy region, and total and elastic scattering cross sections. However, it takes very long calculation time. Current version doesn't include the function to treat a long-range covariance contribution and the Adler-Adler resolved resonance parameters.

3.2 Processing average cosine of elastic scattering angle

ERRORJ can treat the covariance of average cosine of elastic scattering angle, $\overline{\mu}$. The procedure is described below.

- (a) Legendre expansion coefficients of the elastic scattering cross section in a union group structure are prepared from the angular distribution of elastic scattering(MF=4/MT=2).
- (b) Covariance of $\overline{\mu}$ in the laboratory system is obtained from covariance given in MF=34.

$$
cov(\overline{\mu}_g, \overline{\mu}_g) = cov(a_{1,g}^{Lab}, a_{q,g'}^{Lab}) = cov(\sum_m U_{1m} a_{m,g}^{CM}, \sum_l U_{1l} a_{l,g'}^{CM})
$$

where $a_{l,g}^{Lab}$ and $a_{l,g}^{CM}$ are the 1-th order coefficient of Legendre expansion of elastic scattering in the laboratory system and the center mass system, respectively. **U** is a transformation matrix from the center mass system to the laboratory system. If **U** is not defined in the nuclear data file, a module named "Matrixin" is used to calculate **U** . The module was prepared by T. Nakagawa of Japan Atomic Energy Research Institute [6].

Conventionally, covariance of the first order coefficient is only defined. Thus,

$$
cov(\overline{\mu}_g, \overline{\mu}_{g'}) = U_{11} U_{11} cov(a_{1,g}^{CM}, a_{1,g'}^{CM}).
$$

(c) Covariance in a user group structure is calculated as below.

$$
\text{cov}(\overline{\mu}_G,\overline{\mu}_{G^\circ})=\sum_{g\in G, g^\circ\in G^\circ}\text{cov}(\overline{\mu}_g,\overline{\mu}_g^\circ)\cdot\frac{\phi_g\sigma_g^{el}}{\phi_G\sigma_G^{el}}\cdot\frac{\phi_g\cdot\sigma_g^{el}}{\phi_G\cdot\sigma_{G^\circ}^{el}}
$$

Present ERRORJ cannot treat covariance of the higher order coefficient. Therefore, users should set input value [legerd] to 1. Results are given as MT=251. It is not necessary to prepare the group-averaged $\overline{\mu}$ in a user group structure because it can be calculated in ERRORJ.

4. How to use ERRORJ

4.1 How to run

These files are necessary to run ERRORJ.

- (a) Input file
- (b) Evaluated nuclear data file including covariance data
- (c) Cross section data file (GENDF or PENDF or one prepared by users).

ERRORJ produces a standard output file and a covariance file in COVFIL format, which includes the multi-group cross section and relative covariance data. The standard output file named "output" is automatically updated.

Relationship between the tape number and the file name is the same as the NJOY code. ERRORJ uses tape10-19 as scratch files, therefore users should not use the tape numbers. Tape1-9 are also not used.

To transform a covariance file from the COVFIL format to the COVERX format, a utility program NJOYCOVX is used. Users should name a covariance file in COVFIL format "cvf.+nuclide name(NN)". For example, if users want to process U-238, the file name must be "cvf.u238". In addition, users should prepare a directory named "exc-d" to contain correlation matrix files before running NJOYCOVX.

NJOYCOVX needs one parameter, which is nuclide name, as below.

/home/user1/errorj/njoycovx/njoycovx_ld u238

In this example, NJOYCOVX realizes that "cvf.u238" is the file which should be transformed to a file in the COVERX format. Files created by NJOYCOVX are

- (a) multi-group covariance file in the COVERX format, "cvx.(NN)",
- (b) relative standard deviation file, "rsd.(NN)",
- (c) multi-group cross section and relative standard deviation file, "rxs.(NN)",
- (d) multi-group cross section and correlation matrix file, "corr.matrix",
- (e) correlation matrix in each reaction, "mt ###-###", which is made in "exc-d" directory.

An example of the shell script to run ERRORJ is shown in Fig. 2.

```
#! /bin/csh 
# 
set NUCL=cr0 
set MAT=2400 
rm tape* output input 
cp /home/endf/cov/${NUCL} tape20 
ln –s ../njoy-ex/gendf.${NUCL} tape22 
# 
cat>input <<EOF 
  0 
  6 
  *errorr* 
  20 0 22 24 0 / 
 $MAT 21 1 1 / 
  0 33 1 / 
  *errorr* 
  20 0 22 23 24 0 / 
  $MAT 21 1 1 / 
  0 34 1 1 / 
  *stop* 
EOF 
# 
/home/usr1/errorj/src2/errorj_ld < input 
if ( -e tape23 ) then 
    if ( -z tape23 ) exit 
else 
    exit 
endif 
cp tape23 cvf.${NUCL} 
# 
(continue)
```
Fig.2 Example of shell script (1/2)

(continued) if (-d exc-d) then rm –f exc-d/* else mkdir exc-d endif /home/usr1/errorj/njoycovx/njoycovx_ld \${NUCL} mv corr.matrix cor.\${NUCL} rm –fR excd-\${NUCL} mv exc-d excd-\${NUCL} exit

Fig.2 Example of shell script (2/2)

4.2 Detail description about input file

The input manual of ERRORJ is described in the program source. It is shown in Fig. 3. In this section, detail information about the input file is described.

[nout] in card1 is the number of a tape in which multi-group covariance created by ERRORJ is written. If users set [nout] to 23, the multi-group covariance is written in tape23. [nin] is used for reading the existing multi-group covariance file and adding a new multi-group covariance data.

[irelco] in card2 is an option to define a form of covariance matrix, absolute (irelco=0) or relative (irelco=1). The ERRORJ system determines that multi-group covariance in the COVERX format is relative form, thus users should set [irelco] to 1.

[mfcov] in card7 is an option to determine covariance file to be processed.

- (a) mfcov=31; processing covariance of the average number of neutrons per fission $(MF=31)$ (reaction type is restricted, MT=452, 455 and 456)
- (b) mfcov=33; processing covariance of the neutron cross section (MF=33) and resonance parameters (MF=32)
- (c) mfcov=34; processing covariance of the angular distribution of the secondary neutron (MF=34)(reaction type is restricted, MT=2)
- (d) mfcov=35; processing covariance of the energy distribution of the secondary neutron (MF=35)(reaction type is restricted, MT=18)

Fig.3 Input manual (1/5)

Fig.3 Input manual (2/5)

Fig.3 Input manual (3/5)

Fig.3 Input manual (4/5)

Fig.3 Input manual (5/5)

5. Results of processing covariance data in JENDL

Covariance data in JENDL-3.2 [7] and JENDL-3.3 [8] were processed by ERRORJ. Some of the obtained relative standard deviations for Fe-56, Mn-55, U-233, U-235, U-238 and Pu-240 cross sections are shown in Fig. 4.1 \sim 4.9. Resonance parameters were processed using 1% sensitivity method.

It can be observed that the relative standard deviation is very small in the resonance energy region of the uranium-235 capture cross section, for which the covariance data are not defined in JENDL-3.3.

Fig. 4.1 Group-averaged covariance data for elastic scattering cross section of Fe-56 (Fe-Nat. in JENDL-3.2)

Fig. 4.2 Group-averaged covariance data for elastic scattering cross section of Mn-55

Fig. 4.3 Group-averaged covariance data for a number of neutron emitted per fission of U-233

Fig. 4.4 Group-averaged covariance data for capture cross section of U-233

Fig. 4.5 Group-averaged covariance data for fission cross section of U-235

Fig.4.6 Group-averaged covariance data for capture cross section of U-235

Fig. 4.7 Group-averaged covariance data for elastic scattering cross section of U-238

Fig. 4.8 Group-averaged covariance data for elastic scattering cross section of Pu-240

Fig. 4.9 Group-averaged covariance data for capture cross section of Pu-240

6. Summary

The ERRORJ code was developed to process the covariance data. ERRORJ has new functions for processing the covariance data for cross sections including resonance parameters as well as angular distributions and energy distributions of secondary neutrons which could not dealt with by former covariance processing codes. In future, ERRORJ should be updated to treat the covariance data of angular and energy distributions, the resolved resonance parameter of Adler-Adler form and long-range covariance contribution.

Acknowledgements

Development of ERRORJ was carried out by K. Kosako of Sumitomo Atomic Energy Industries, LTD. The author respects his great work. The author also respects MacFarlane R.E. and Muir D.W. of Los Alamos National Laboratory who developed ERRORR routine which is a base of the development of ERRORJ.

References

- [1] Kosako K. and Yamano N.: "Preparation of a Covariance Processing System for the Evaluated Nuclear Data File, JENDL, (III)", JNC TJ 9440 99-003 (1999) [in Japanese].
- [2] Kosako K.: "Covariance Data Processing code: ERRORJ", p.30-34, JEARI-Conf 2001-009 (2001).
- [3] MacFarlane R.E. and Muir D.W.: "The NJOY Nuclear Data Processing System version 91", LA-12740-M (1994).

[4] Smith, III J.D.: "Processing ENDF/B-V Uncertainty Data into Multigroup Covariance Matrices", ORNL/TM-7221 (1980).

[5] Drischler J.D.: "The COVERX Service Module of the FORSS System",ORNL/TM-7181 (ENDF-291) (1980).

[6] Nakagawa T.: private communication (2002).

[7] Nakagawa T. et al.: "Japanese Evaluated Nuclear Data Library Version 3 Revision-2: JENDL-3.2," J. Nucl. Sci. technol. **32**, 1259 (1995).

[8] Nakagawa T. et al.: "Japanese Evaluated Nuclear Data Library Version 3 Revision-3: JENDL-3.3," J. Nucl. Sci. technol. **39**, 1125 (2002).

[9] Rose P.F. and Dunford C.L. : "ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6," BNL-NCS 44945 Rev. 10/91 (1991).

Appendix A:

File format of multi-group cross section (iingxs>0)

Format of multi-group cross section, which is prepared by users, is categorized into three groups. These are ENDF type, block type and column type. Users can select a format to be used by setting [IINGXS] in the input file. In the multi-group cross section file, data should be written with ascending MT order. Units of cross section and energy are barns and eV, respectively.

A.1 ENDF type

Data should be written with ascending energy order.

```
(a) MF=3(TAB1) [IINGXS=1]
[0,0,0 / HL] TEXT 
[MAT,3,MT/0.0, 0.0, 0, 0, 0, 0 ]CONT 
[MAT,3,MT/0.0, 0.0, 0, 0, NR, NP / E / SIG ] TAB1 
[MAT, 3, 0 / 0.0, 0.0, 0, 0, 0, 0] SEND
```
In TAB1 record, lower energy boundary of the group, E, and cross section, SIG, are written iteratively at (NP-1) times. At last, upper energy boundary and zero are written. After all MT cross sections have been described, FEND record should be written.

[MAT, 0, 0/ 0.0, 0.0, 0, 0, 0, 0, 0] FEND

Interpolation mode should be set to 1 because multi-group cross section is described.

(b) MF=1, MF=3 (TAB1) [IINGXS=2]

Energy boundary should be described at first. Except it, this format is the same as IINGXS=1 format.

[MAT,1,451/ 0.0, 0.0, 0, 0, NP, 0/ E] LIST [MAT, 1, 0/0.0, 0.0, 0, 0, 0, 0] SEND [MAT, 0, 0/0.0, 0.0, 0, 0, 0, 0] FEND NP is the total number of groups plus 1.

(c) MF=3(LIST) [IINGXS=3] [0,0,0/ HL] TEXT [MAT,3,MT/ 0.0, 0.0, 0, 0, NP, NL/ SIG] LIST [MAT, 3, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND

NP is the number of multi-group cross section to be inputted and NL is the group number from which input starts. For example, when the number of groups is 20 and users want to input cross section from group 15 to 19, users set NL and NP to 15 and 5.

A.2 Block type

(a) Energy and reaction-wise blocks [IINGXS=11] READ(*) NGN READ(*) (E(i),I=1,NGN+1) READ(*) MT, NG READ(*) (CRS(I,MT),I=1,NG)

CRS is multi-group cross sections. NGN is the total number of groups. E(1) is the highest(lowest) energy boundary when NGN is positive(negative). NG is the same as NGN about an order of cross section. IF NG is not equal to NGN, cross sections from group 1 to NG (NG $>$ 0) or from NGN to NGN-NG+1 (NG<0) are read.

(b) Reaction-wise blocks [IINGXS=12]

READ(*) MT,NG

READ(*)(CRS(I,MT),I=1,NG)

This format is the same as IINGXS=11 case except for information about energy.

(c) MT, NG and cross section blocks [IINGXS=13] READ(*) NMT $READ(*)$ (MT(i), $I=1, NMT$) $READ(*)$ (NG(i), $I=1, NMT)$ $DO j = 1$, NMT $READ(*)$ (CRS(I,j),I=1,NG(j)) ENDDO

NMT is the total number of reactions. Treatment of NG and NGN is the same as IINGXS=11 case.

(d) MT and cross section blocks with descending energy order [IINGXS=14]

READ(*) NMT $READ(*)$ (MT(i), $I=1, NMT$) DO j = 1, NMT $READ(*)$ (CRS(I,j), I=1, NGN)

ENDDO

Cross section should be written with descending energy order.

(e) MT and cross section blocks with ascending energy order [IINGXS=15]

It is the same as IINGXS=14 case except for energy order.

A.3 Column type

```
(a) With energy [IINGXS=21] 
READ(*) NMT 
READ(*) NGN, (MT(i),I=1,NMT) 
DO j = 1, NGN
  READ(*) E(j), (CRS(I,j), I=1, NMT)
ENDDO 
READ(*) E(NGN+1) 
  NGN is the same as IINGXS=11 case.
```
(b) Reaction-wise with descending energy order [IINGXS=22] READ(*)NMT $READ(*)$ (MT(i),I=1,NMT) $DO j = 1$, NGN $READ(*)$ (CRS(I,j), I=1, NMT) ENDDO Cross section should be written with descending energy order.

(c) reaction-wise with ascending energy order [IINGXS=23]

This format is the same as IINGXS=22 case except for energy order.