

Experience with Covariance Matrix Processing

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Outline

- **ZZ-COV-15GROUP-2005** - Covariance Data Review
- Sensitivity-Based Global Assessment of Nuclear Data Requirements (**GANDR**)
- Covariance Data Processing Code: **ERRORJ**

NEA-1730: ZZ-COV-15GROUP-2005 - Covariance Data Review

Processing of available covariance data into 15 energy groups for
intercomparison and use (GEN-IV, ADS)

FzK, ANL (M. Salvatores, G. Palmiotti)

CONTENT:

ENDF/B-V: H-1, Li-6, B-10, C-12, N-14, O-16, Pb.

ENDF/B-VI.8: Li-7, F-19, Na-23, Si-0, Cr-52, Fe-56, Fe-57, Pb-206, Pb-207,
Pb-208, Bi-209, Th-232, U-235 (nu-bar), U-238 (nu-bar, few inelastic levels),
Pu-240

JEFF-3.0: Be-9, Si-28, Fe-56, Ni-58

JENDL-3.3: Zr-90, U-238, Pu-239, Pu-241

IRDF-2002: Li-6(n,t), B-10(n, α), F-19(n,2n), Al-27(n, α), Fe56(n,p), Ni-
58(n,2n) &(n,p), Zr-90(n,2n), Th-232(n,f)&(n, γ), U-235(n,f), U-238(n,f)&(n, γ),
Np-237(n,f), Pu-239(n.f), Am-241(n,f)

Available Cross-Section Covariance Data

ENDF/B-V

- Nuclides: H-1, Li-6, Li-7, Be-9, B-10*, C-0, N-14, O-16, F-19, Na-23, Al-27, Si-0, Sc-45, Ti-46, Ti-47, Ti-48, Cr-0, Mn-55, Fe-0, Fe-54, Fe-56, Fe-58, Co-59, Ni-0, Ni-60, Cu-63, Cu-65, In-115, I-127, Au-197, Pb-0, Th-232, U-235, U-238, Np-237*, Pu-239, Pu-240, Pu-241*, Am-241.

ENDF/B-VI.8

- Nuclides: Li-7, C-0, F-19, Na-23, Si-0, Si-28, Si-29, Si-30, Ti-46, Ti-47, Ti-48, V-0, Cr-50, Cr-52, Cr-53, Cr-54, Mn-55, Fe-54, Fe-56, Fe-57, Fe-58, Co-59, Ni-58, Ni-60, Ni-61, Ni-62, Ni-64, Cu-63, Cu-65, Y-89, Nb-93, In-0, In-115, Re-185, Re-187, Au-197, Pb-206, Pb-207, Pb-208, Bi-209, Th-232, U-235, U-238, Pu-240, Pu-242, Am-241

JEFF-3.0

- Nuclides: H-3, C-0, Be-9, F-19, Si-28, V-0, Cr-50, Cr-53, Cr-54, Mn-55, Fe-54, Fe-56, Co-59, Ni-58, Ni-60, Ni-61, Ni-62, Ni-64, Cu-63, Cu-65, Y-89, Nb-93, Re-185, Re-187, Au-197, Bi-209, Th-232, (U-238)

JENDL-3.3

- Nuclides: H-1, B-10, B-11, O-16, Na-23, Ti-48, V-0, Cr-52, Mn-55, Fe-56, Co-59, Ni-58, Ni-60, Zr-90, U-233, U-235, U-238*, Pu-239, Pu-240, Pu-241*

IRDF-2002

- Nuclides: Li-6(MT=105), B-10(107), F-19(16), Na-23 (16, 102), Mg-24(103), Al-27(103, 107), P-31(103), S-32(103), Sc-45(32-151, 33-102), Ti-46(16, 103), Ti-47(103, 40-5), Ti-48(103, 40/5), Ti-49(40/5), V-51(107), Cr-52(16), Mn-55(102), Fe-54(16, 103, 107), Fe-56(103), Fe-58(102), Co-59(1, 16, 102, 107), Ni-58(16, 103), Ni-60(103), Cu-63(1, 2, 16, 102, 107), Cu-65(16), Zn-64(103), As-75(16), Y-89(16), Zr-90(16), Nb-93(1, 2, 4, 16, 102), Rh-103(40/4=51), Ag-109(40/102), Cd-100(102), In-115(40/4, 40/16, 40/102), I-127(16), La-139(102), Pr-141(16), Tm-169(16), Ta-181(102), W-186(102), Au-197(1, 16, 102), Hg-199(40/4), Pb-204(40/4), Th-232(18, 102)*, U-235(18), U-238(18, 102), Np-237(18), Pu-239(18), Am-241(18)

Multigroup covariance data libraries

- **ZZ-COVFILS**: 30-Group Neutron Cross-Section Covariance Library from **ENDF/B-V** (in BOXER format)
- **ZZ-COVFILS-2**: 74-Group Covariance Data for Fusion Reactors (**ENDF/B-V**)
- **ZZ-VITAMIN-J/COVA**: Covariance Matrix Library based on **JEF-1**, **ENDF/B-IV** and **-V** data; includes processing and verification codes
- **ZZ-VITAMIN-J/COVA/EFF2**: **EFF-2.3** covariance matrices for 18 materials, detector response function covariance data from **IRDF 90.2**
- **ZZ-VITAMIN-J/COVA/EFF3**: **EFF-3** covariance matrices for Be-9, Si-28, Fe-56, Ni-58, Ni-60; includes also processing and verification utilities
- **ERROR-J**: processing code and **JENDL-3.2** & **-3.3** covariance matrices

GANDR - Sensitivity-Based Global Assessment of Nuclear Data Requirements

- IAEA Nuclear Data Section Project (D. W. Muir)
- Computerized tool to **assess the impact of new experimental information on evaluated cross sections and integral parameters**. Ranking of competing proposals for new nuclear data measurements.
- Based on sensitivity and uncertainty analysis
- **Global evaluation of data covariances needed, taking into account of all high-quality differential and clean integral data (ZOTTVL).**

Specialist's meeting of reactor constants
Tokai, Feb. 22 - 23, 2001

共分散データ処理コード

Covariance Data Processing Code:
ERRORJ

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Background

- the progress of reactor constant adjustment for fast reactor in JNC

- evaluation research of covariance data for JENDL-3.2
 - === general resolved resonance format (Breit-Wigner and Reich-Moore)
 - === unresolved resonance format

- adoption of covariance data for dominant nuclides in next JENDL-3.3

Covariance Data in ENDF-6

- MF=30: Data covariances obtained from parameter covariances and sensitivities
- MF=31: Covariances of the average number of neutrons per fission
- MF=32: Covariances of resonance parameters
- MF=33: Covariances of neutron cross sections
- MF=34: Covariances of angular distributions of secondary particles
- MF=35: Covariances of energy distributions of secondary particles
- MF=40: Covariances for production of radioactive nuclei

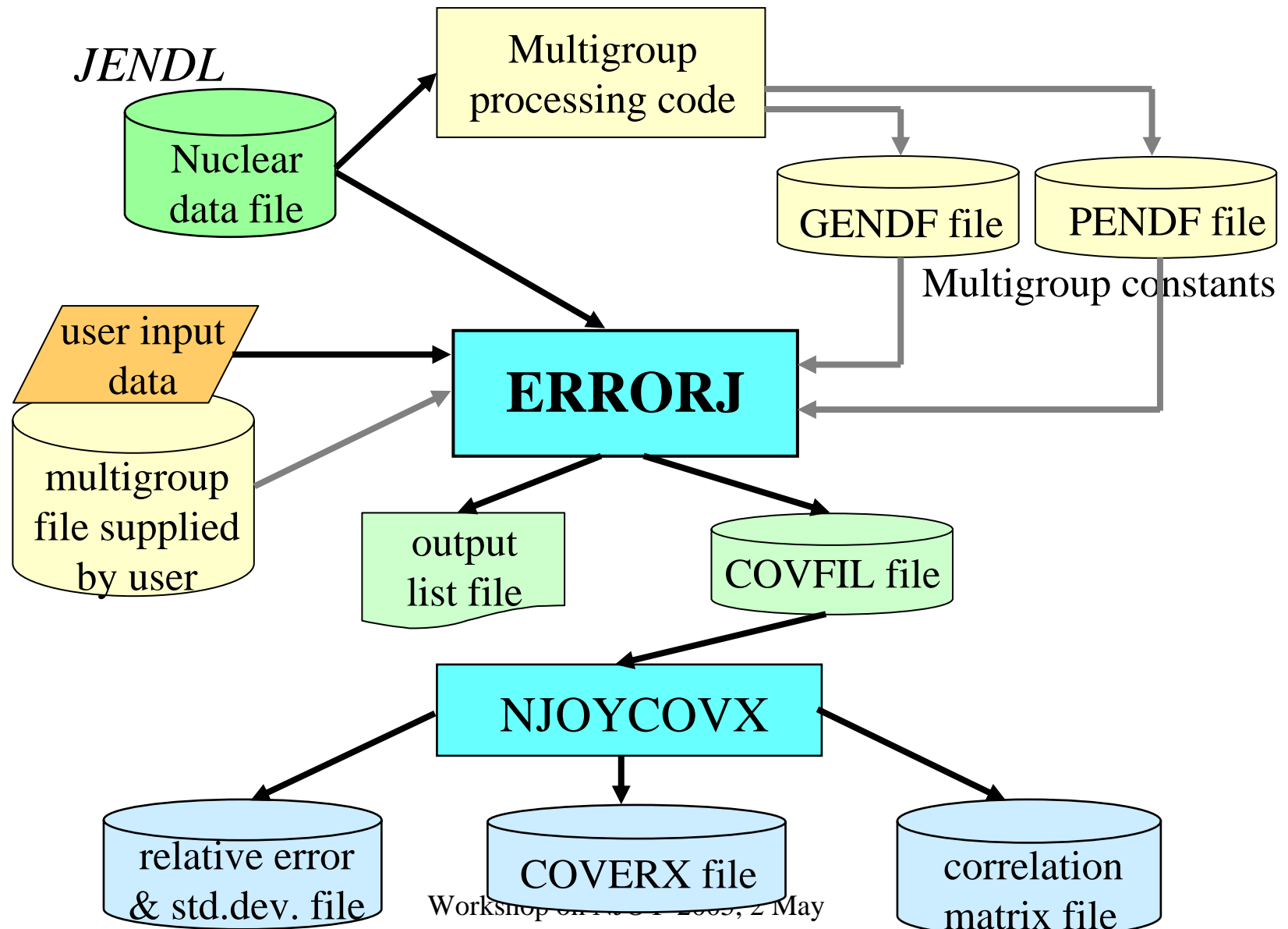
Development of *ERRORJ*

- adoption of the ERRORR module of NJOY94.105 as main body in the system
- production of the file format conversion program, NJOYCOVX, from a COVFIL format file
- adoption of the COVERX format for a standard multigroup covariance data file (commonality with the FORSS system)
- production of the utility programs:
viewcvx ---- viewer of a COVERX format file
editcvx ---- editor and merger of COVERX files

Features of ERRORJ

- Expanded processing for the covariances of resolved and unresolved resonance parameters
- Processing for $\bar{\mu}$ and fission spectrum
- Input of multigroup constants with various forms
 - === user input data
 - === files with various formats
 - === GENDF format file
 - === internal calculation of cross sections (use PENDF)
- Output files with various formats by NJOYCOVX
 - === COVERX format file
 - === correlation matrix (summary and partial) files
 - === relative error and standard deviation file

Calculation Flow of ERRORJ



Processing of R.P. Covariance

Resolved resonance parameter (LRU=1)
Unresolved resonance parameter (LRU=2)

● Area sensitivity method

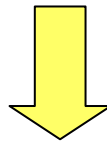
- development for PUFF-2, and adoption in NJOY
- available for fission and radiative capture of Breit-Wigner resolved resonance parameters
- unavailable for total and elastic scattering, other resolved, and unresolved resonance parameters
- assumption as that a resonance isn't extended over few energy groups

radiative capture of single level Breit-Wigner

$$\sigma_{\gamma} = \frac{\pi}{k^2} g \frac{\Gamma_n \Gamma_{\gamma}}{(E - E_r)^2 + \frac{\Gamma_t^2}{4}} \quad \Rightarrow \quad \frac{\partial A_{\gamma}}{\partial \Gamma_n} = \frac{2\pi^2}{k^2} g \frac{\Gamma_{\gamma}}{\Gamma_t} \left(1 - \frac{\Gamma_n}{\Gamma_t} \right)$$

sensitivity coefficient for
neutron width

For elastic scattering, Reich-Moore resolved and unresolved resonance parameters, calculation of resonance area (A) is very difficult.



development of new method

● 1% sensitivity method

- The sensitivity coefficient is obtained from the variation of resonance cross section when a resonance parameter is changed with 1 %.
- The point-wise resonance cross section is used, and the sensitivity coefficient is calculated with group-averaged variation.
- A resonance is extended over few energy groups.
- A negative resonance energy is available.
- $NLRS > 0$ (long-range covariance contribution) and Adler-Adler resolved are unavailable.
- Long calculation time is necessary.

U-238 total

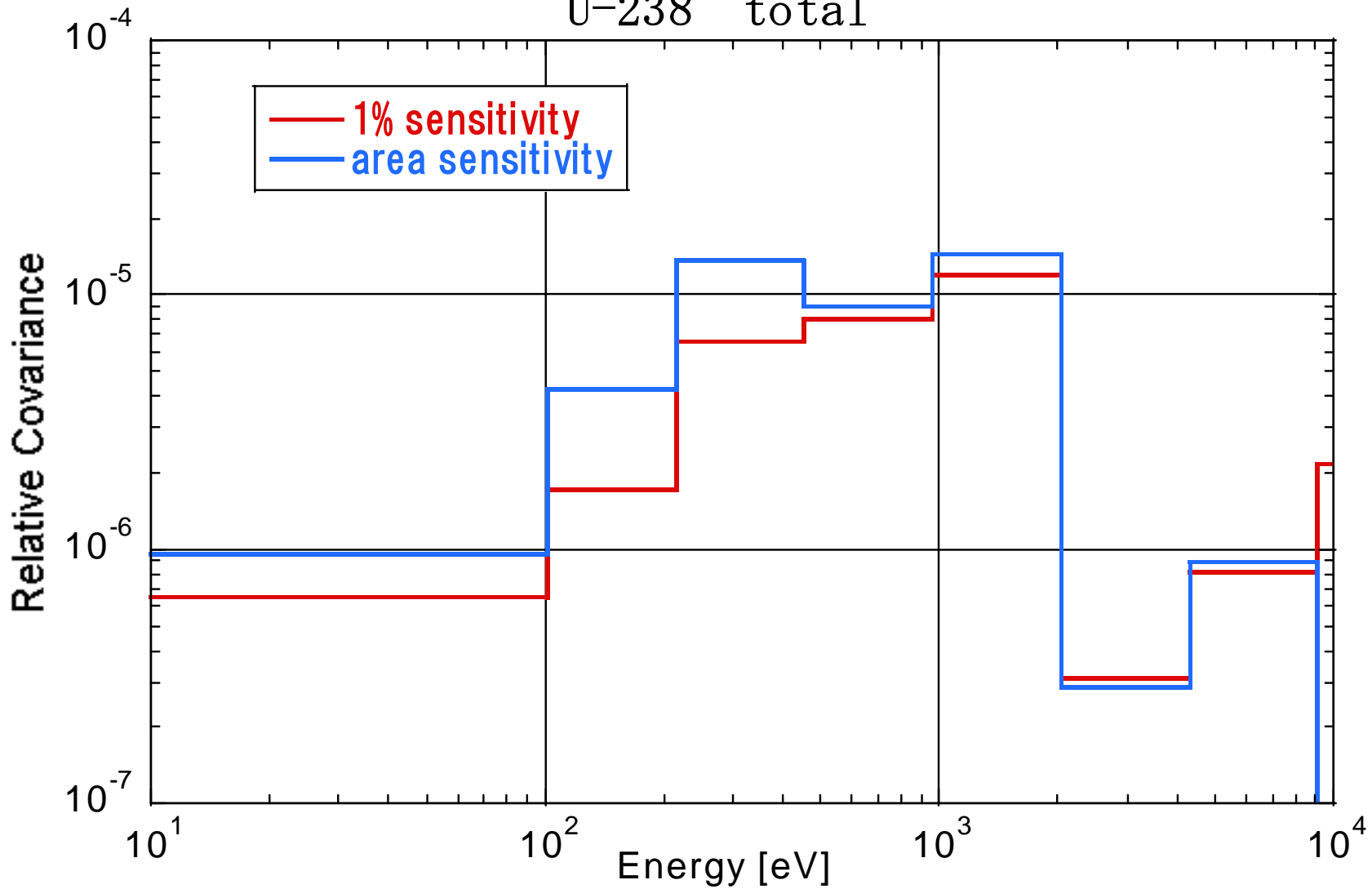


Fig. 2.1 Relative covariance of U-238 total cross sections by resolved resonance parameter of JENDL-3.2 produced by ERRORJ with 19-groups.

U-238 fission

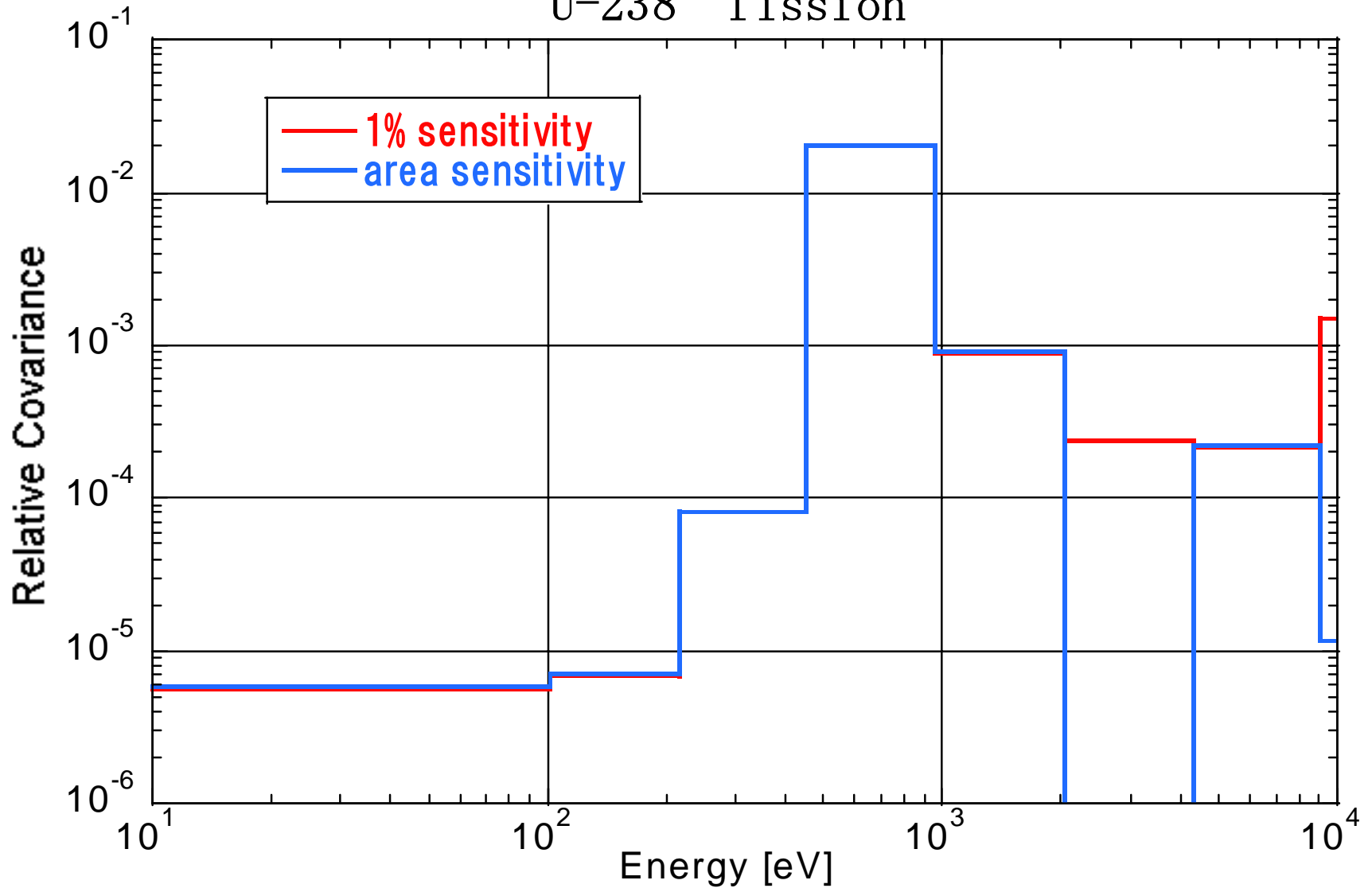


Fig. 2.3 Relative covariance of U-238 fission cross sections by resolved resonance parameter of JENDL-3.2 produced by ERRORJ with 19-groups.

Processing of $\bar{\mu}$ and χ

- $\bar{\mu}$: average cosine of the scattering angle for elastic

MF=3/MT=251: $\bar{\mu}$ (multigroup constants)

MF=3/MT=2: elastic scattering cross sections

MF=34/MT=2: covariance of P_1 component

- χ : fission energy spectrum

MF=5/MT=18: fission energy spectrum

MF=35/MT=18: covariance of χ

Covariances of other angular and energy distribution aren't processed.

fission spectrum, χ

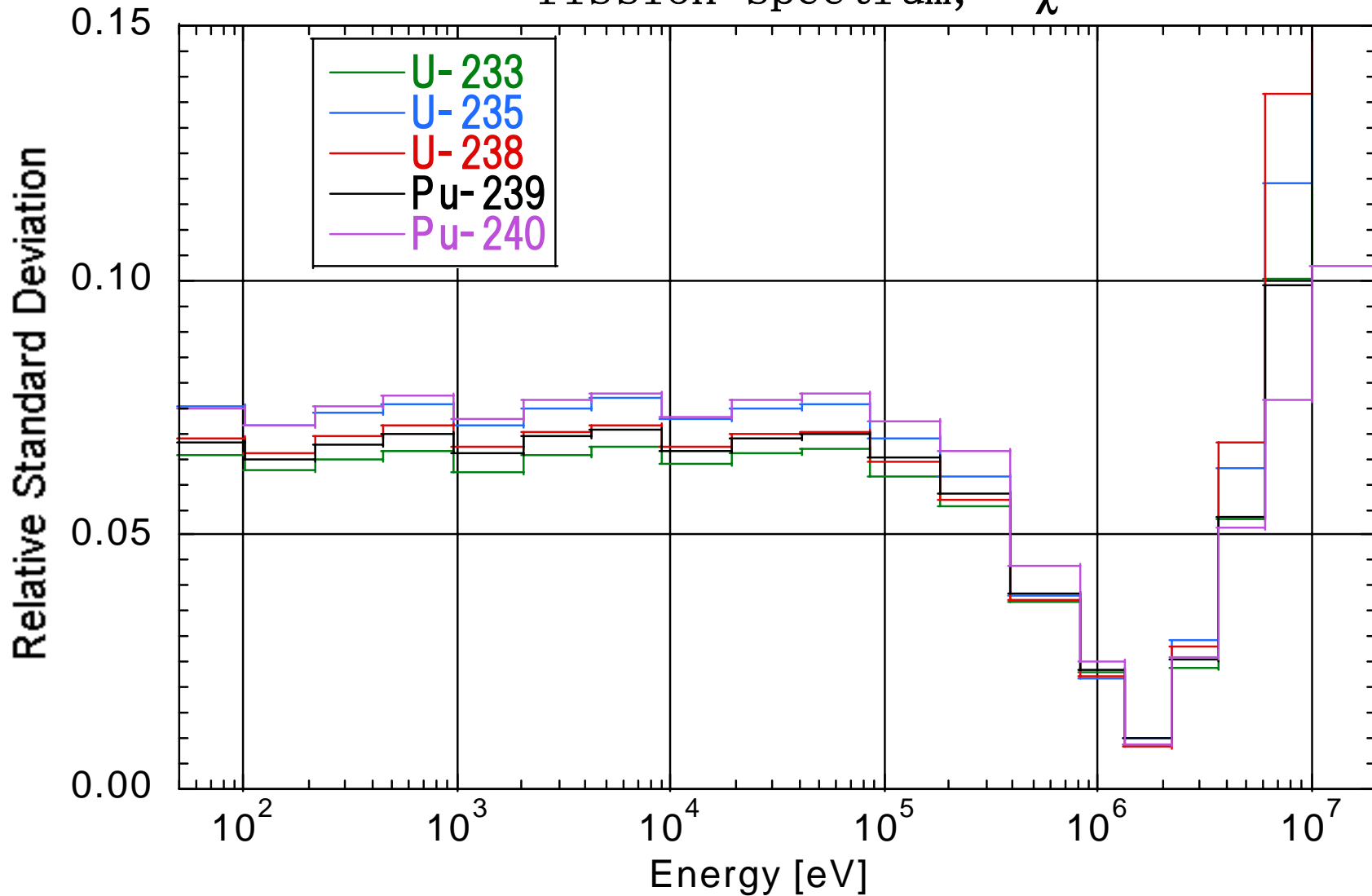


Fig. 5.14 Relative standard deviation by incident energy from 10^5 eV to 500 keV of fission spectra (χ) of JENDL-3.2 produced by ERRORJ with 19-groups.

Summary

- production of the ERRORJ system for processing of JENDL covariance data
- 1% sensitivity method for processing of resonance parameters
- processing of $\bar{\mu}$ and χ
- various input files and output files
- **ERRORJ processed all covariance data** evaluated for JENDL-3.2 in the Covariance Evaluation Working Group.

Reference

「評価済核データファイルJENDL用
共分散処理システムの整備」

“ Preparation of a Covariance Processing System for
the Evaluated Nuclear Data File, JENDL ”

PNC PJ9037 97-001 (1997)

PNC TJ9037 98-001 (1998), published

JNC TJ9440 99-003 (1999), published

This work was supported by Power Reactor and Nuclear
Fuel Development Corporation (JNC).

New features in ERRORJ-ver.2.2

- Non-diagonal elements of covariance matrices are calculated in the resonance energy range
- High speed calculation options
- Effect of resonance self-shielding can be considered (σ_0)