Processing covariances for WPEC/SG46 TAR Exercise

O. Cabellos

Universidad Politécnica de Madrid (UPM), Madrid, Spain

E-mail: oscar.cabellos@upm.es

Outline

- *Legacy Work WPEC/SG26 (2005-2008)*
- *WPEC/SG46 (2019-2021)*
- *Target Accuracy Requirements: Necessity of "Expert Judgment"*
- *Methodology: The inverse problem*
- *TAR Benchmark Specifications*

  https://oecd-nea.org/download/wpec/sg46/
- ***Processing Covariances***
- *New reactor systems in WPEC/SG46: ASTRID, ESFR-SMART, JSFR750 and ALFRED*
- ***Preliminary Results**: Uncertainty Quantification*
- ***Preliminary TAR Results for ENDF/B-VIII.0***

❑ WPEC/SG46 (2019-2021)

https://oecd-nea.org/download/wpec/sg46/

- **WPEC/SG46** is again a new **bridge** between ND evaluators and end-users in the utilisation of integral experiments
- WPEC/SG46 to provide **updated target accuracies for nuclear data uncertainty reduction**
  - *"It is essential to **verify the status of design target accuracies** and their potential evolution (reactor operation and fuel cycle parameters)"*
  - *New reactors concepts are presently explored besides Gen-IV, MA burners, and ADS: MSR, SMR, micro reactors, and test reactors*
- **TAR WPEC/SG46 methodology** based on:
  - *New covariance data matrices: ENDF/B-VIII.0, JEFF-3.3 and JENDL-4.0u*
  - *Using correlations in energy, reactions and isotopes*
  - *Energy structure: "**7 energy groups (based on physical considerations)"***
- *"The **HPRL** will certainly benefit from an update, to motivate and focus new experiments and to meet potential new requirements"*

❑ Methodology: The inverse problem

https://oecd-nea.org/download/wpec/sg46/

❑ The "inverse problem":

- To define the TAR on design parameters: R_n^T
- To find out **the required reduction in the cross-section uncertainties:** Δx_i

$$To\ minimize: \left(\sum_i \frac{\lambda_i}{\Delta x_i^2}\right) \quad i = 1, \dots, K$$

λ_i: cost parameter related with each cross−section

Δx_i: uncertainty cross−section (i.e. standard deviation)

K: total number of reactions-energy groups whose uncertainty is to be determined

- **ISOTOPES:** ^{10}B, ^{16}O, ^{52}Cr, ^{56}Fe, ^{58}Ni, ^{235,238}U, ^{239,240,241}Pu , ^{206,207,208}Pb,^{23}Na + others (e.g. ^{35}Cl)?
- **REACTIONS:** σ_{cap}, σ_{fiss}, ν , σ_{el}, σ_{inel}, PFNS and elastic-P1 + others (e.g. (n,p), n(alpha))?
- **ENERGY Groups:** 7g

The **objective function** is constrained to:

correlation terms

1) $\Delta x_{i0} \geq \Delta x_i \geq 0; i = 1 \dots K$

2) $\sum_i S_{ni}^2 \cdot \Delta x_i^2 + \sum_{ii'} \boldsymbol{S_{ni}} \cdot \Delta x_i \cdot \boldsymbol{corr_{ii'}} \cdot \Delta x_{i'} \boldsymbol{S_{ni}^+} \leq (R_n^T)^2; n = 1 \dots N$

- S_{ni}: sensitivity coefficient for the integral parameter R_n
- $corr_{ii'}$: correlation between i and i′
- R_n^T : target accuracies on the N-integral parameters

❑ Methodology: The inverse problem

https://oecd-nea.org/download/wpec/sg46/

❑ Who is involved in TAR exercise?

$$\textit{To minimize}: \left(\sum_i \frac{\lambda_i}{\Delta x_i^2}\right)_{i=1,\dots,K}$$

- ❑ **ND Differential measurement experts**
  - Cost parameters assigned to isotopes, reactions, and/or energy group

The objective function is constrained to:

1) $\Delta x_{i0} \geq \Delta x_i \geq 0; i = 1 \dots K$

- ❑ **ND Processing**
  - **AMPX/NJOY codes**
  - **Issues to be solved:**
    - MF34/O16-P_1 for JENDL
    - MF34/235U and 238U in ENDF/B-VIII.0
  - **Limitations in NJOY:** unique Ein value for MF35/PFNS
  - **Correlations between MATs-MTs-Energy** to be processed and used

- ❑ **ND Evaluators**
  - Uncertainties for all MATs/MTs
  - Credible uncertainties
  - Mathematically "positive definite" for full covariance data

- ❑ **Lower uncertainty**
  - Standards?

2) $\sum_i S_{ni}^2 \cdot \Delta x_i^2 + \sum_{ii'} S_{ni} \cdot \Delta x_i \cdot corr_{ii'} \cdot \Delta x_{i'} \, S_{ni}^+ \leq (R_n^T)^2; n = 1 \dots N$

- ❑ **Reactor Designers**
  - Safety margins
  - Licensing

- ❑ **Reactor Physicists**
  - Reactor Model
  - Sensitivity Profiles

- ❑ **TAR Solving**
  - Assumptions
  - Inverse method + others ML/AI?
  - **Note:** TAR calculations performed by UPM using the solver DONLP2 (Spelluci P., 1998)

Ref.: Spellucci, P. "*An SQP method for general nonlinear programs using only equality constrained subproblems*". Math. Program. 82, 413–448 (1998)

❑ TAR Benchmark Specifications:

https://oecd-nea.org/download/wpec/sg46/

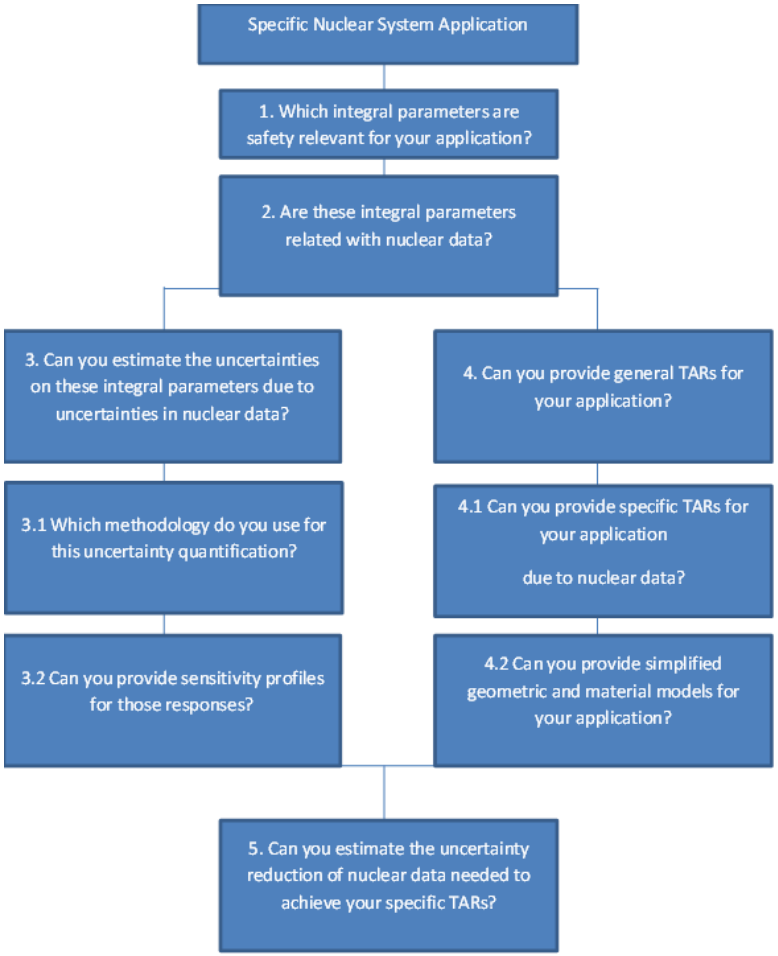
❑ Benchmark Specifications: WPEC/SG46 Exercise on Target Accuracy Requirement (TAR)

WPEC/SG46, May 2021

Table 1. Energy group structure

Group #	Lower Energy (eV)	Upper Energy (eV)	
1	2.23130 10^{6}	1.96403 10^{7}	Above Threshold fertile
2	4.97871 10^{5}	2.23130 10^{6}	Above Threshold inelastic
3	6.73795 10^{4}	4.97871 10^{5}	Continuum to URR
4	2.03468 10^{3}	6.73795 10^{4}	URR
5	2.26033 10^{1}	2.03468 10^{3}	RRR
6	5.40000 10^{-1}	2.26033 10^{1}	EPITHERMAL
7	1.40000 10^{-5}	5.40000 10^{-1}	THERMAL

Figure 1. Procedure for any specific application to participate in WPEC/SG46 exercise on TAR



https://oecd-nea.org/download/wpec/sg46/materials/documents/WPEC_SG46_TAR_Exercise-v2_HM41-OC_GP-OC-v1.pdf

❑ Processing Covariances

- *ND covariances processed with NJOY2016.63*
- *Processed ND:*
  - *MF31*
  - *MF32/MF33*
  - *MF34*
  - *MF35*
- *Energy structure 7g- weighting IWT8 (for fast reactors)*
- *Ein for MF35: 1.0E+5eV*
- *Formats: BOXER, ERROR (and COVERX)*

See MATERIALS at: https://oecd-nea.org/download/wpec/sg46/materials/

❑ Processing Covariances

❑ Processing issues with NJOY2016.63 (LANL GitLab)

- **Discrepancy between NJOY2016 and NJOY99 for JENDL4 MF34 processing in O16**
  Issue #210 · njoy/NJOY2016 · GitHub
- ERRORR covout subroutine only outputs the first subsubsection covariance matrix
  Issue #205 · njoy/NJOY2016 · GitHub
  NJOY2016/ERRORR is now capable of reading MF34 for ENDF/B-VIII.0 mubar for 235U and 239Pu
- NJOY2016/MF35 may be improved: definition of a weighting function instead of only one Ein value
- Need of definite positive for “full” covariance matrices

❑ Working on progress

- AMPX –NJOY processing and comparison

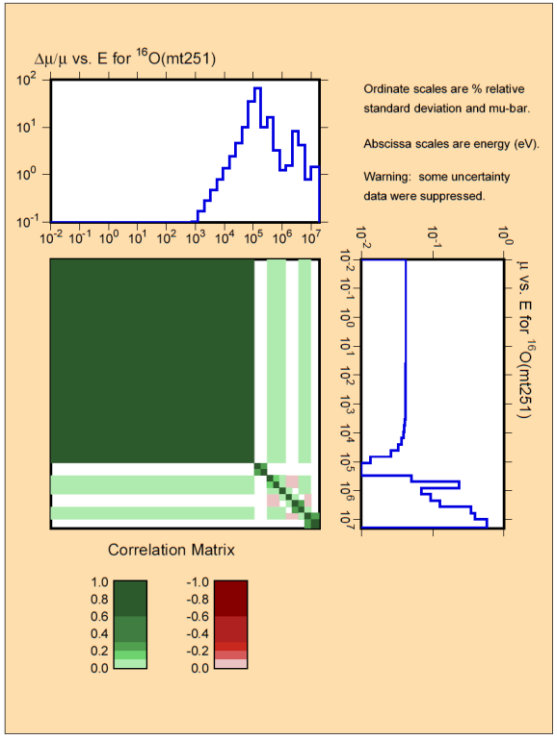
  (**see presentation by A. Jiménez-Carrascosa in JEFF-Nov2021 Processing Session**)

❑ Processing Covariances

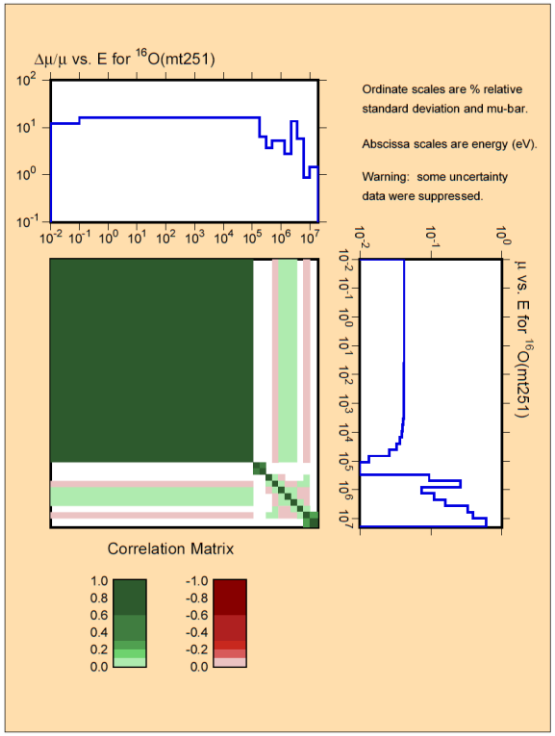
❑ Processing issues with NJOY2016.63 (LANL GitLab)

– **Discrepancy between NJOY2016 and NJOY99 for JENDL4 MF34 processing in O16**

Issue #210 · njoy/NJOY2016 · GitHub



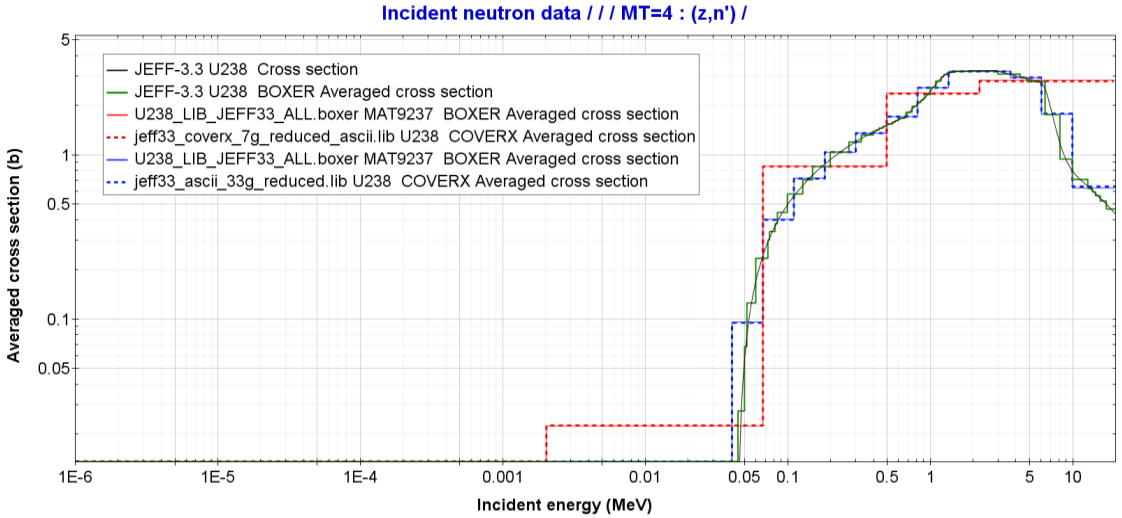
❑ O-16 mu-bar covariance processed by NJOY99

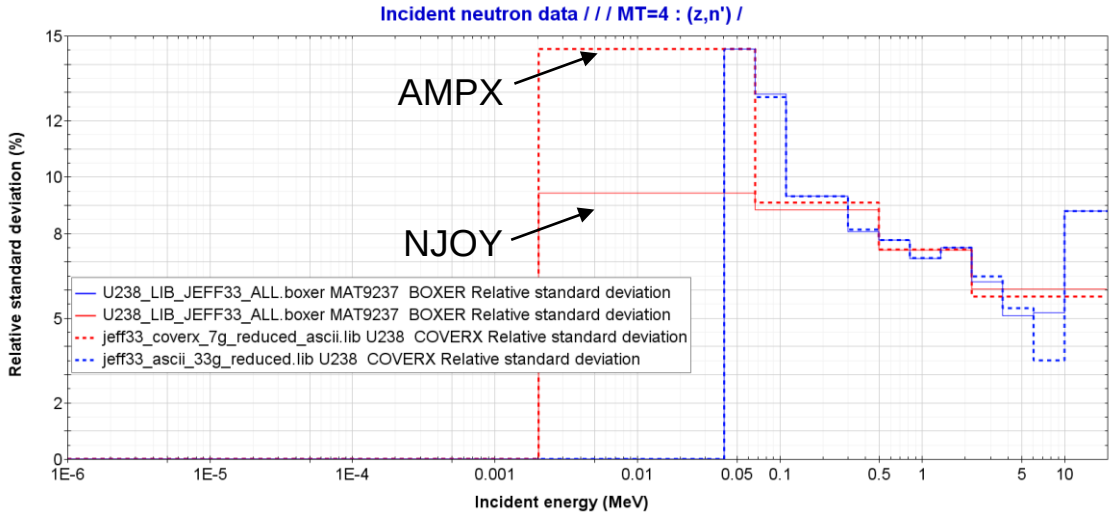


❑ O-16 mu-bar covariance processed by NJOY2016

❑ Processing Covariances

❑ AMPX –NJOY issue processing the relative standard deviation in 7g?

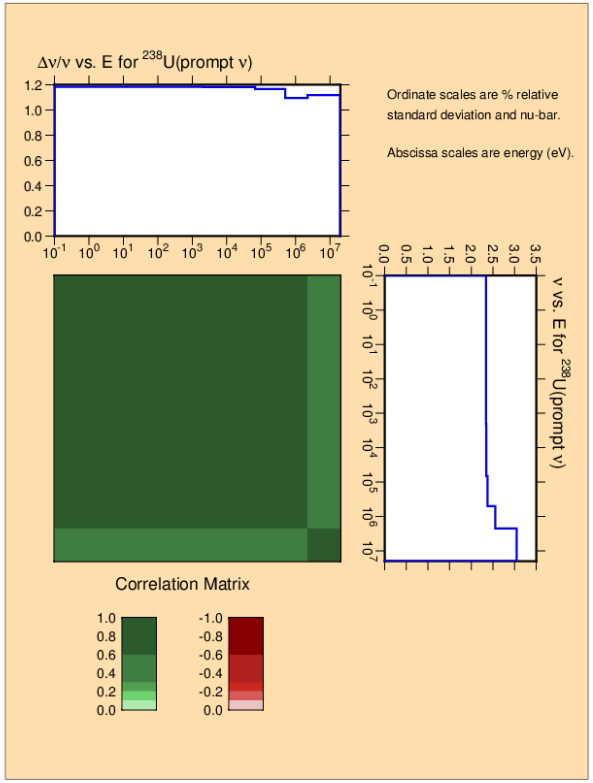




- Reported by email, Nov. 17, 2021

❑ Processing Covariances

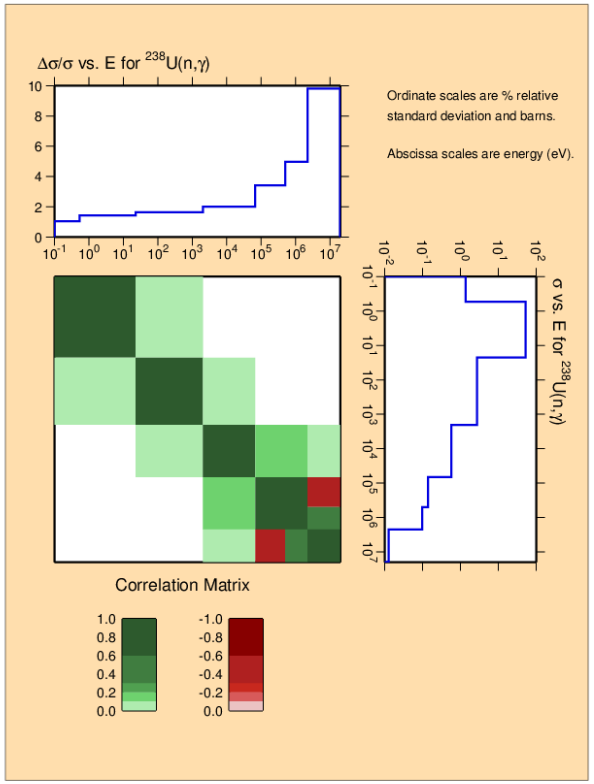
❑ MF31

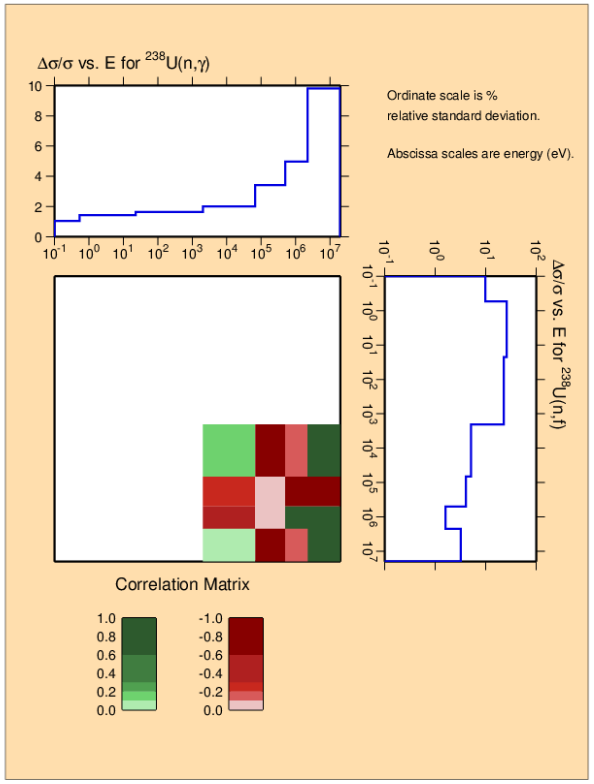



```
groupr /
21 24 0 31/
  9237 1 0  8 0 1 1 1 /
'GENDF-   7g' /
300.0
1.E10
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
3/
3 452 nubar_t/
3 455 nubar_d/
3 456 nubar_p/
5 455 nubar_spc/
0/
0/
errorr
21 0 31 41 /
  9237 1 2 1 1 /
1  300.0 / Just only one temperature
0 31 /
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
covr
 41 0 81 /
 1/
 /
 /
  9237 0 0 0 /
viewr
81 82
covr
 41 71 /
 4 1
'LIB_JEFF33          ' /
'BOXER format'/
  9237 0 0 0 /
stop
```

❑ Processing Covariances

❑ MF32/33

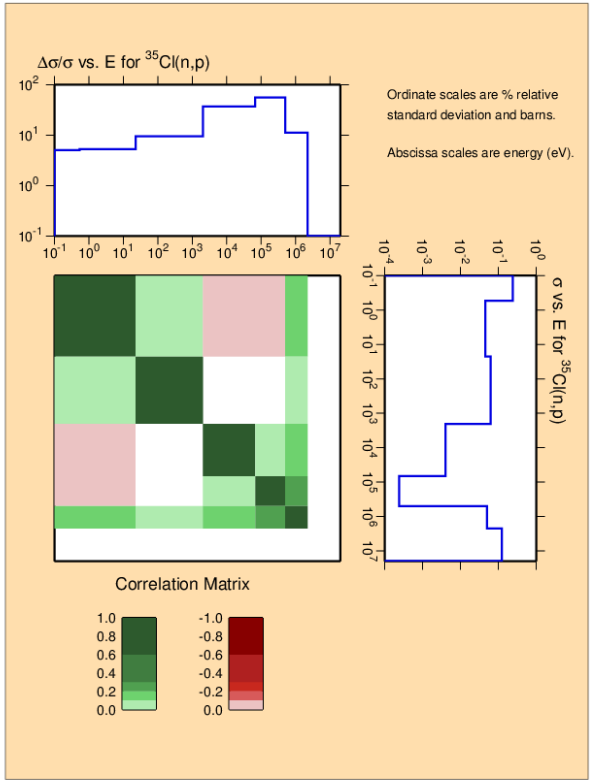





```
groupr /
21 24 0 31/
  9237 1 0  8 0 1 1 1 /
'GENDF-   7g' /
300.0
1.E10
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
3/
3 18/
3 251/
3 452 nubar_t/
3 455 nubar_d/
3 456 nubar_p/
5 455 nubar_spc/
0/
0/
errorr
21 0 31 77 /
  9237 1 2 1 1 /
1  300.0 / Just only one temperature
0 33 /
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
covr
 77 0 81 /
 1/
 /
 /
  9237 0 0 0 /
viewr
81 82
covr
 77 78 /
 4 1
'LIB_JEFF33          ' /
'BOXER format'/
  9237 0 0 0 /
stop
```

❑ Processing Covariances

❑ Evaluated without MF33 (only MF32)




```
groupr /
21 24 0 31/
  1725 1 0  6 0 1 1 1 /
'GENDF-   7g' /
300.0
1.E10
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
3/
3 251/
0/
0/
errorr
999/
21 88/
1    / MT1
2    / MT2
102  / MT102
600  / MT600
0/
errorr
88 0 31 77 /
  1725 1 2 1 1 /
1  300.0 / Just only one temperature
0 33 /
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
covr
 77 0 81 /
 1/
 /
 /
  1725 0 0 0 /
viewr
81 82
covr
 77 78 /
 4 1
'LIB_ENDFB-VIII.0     ' /
'BOXER format'/
  1725 0 0 0 /
stop
```

- NJOY2016 input for Cl35-ENDF/B-VIII.0

- NJOY21 does not need the intermediate error module

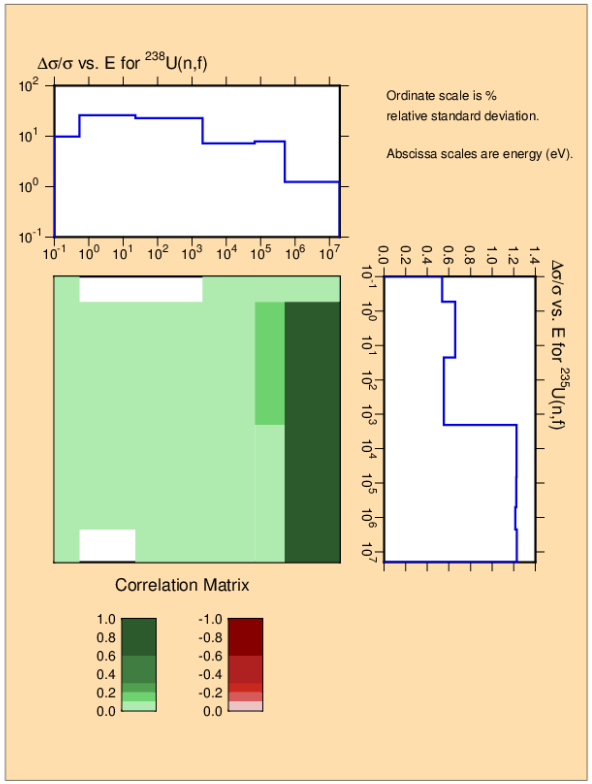
❑ Processing Covariances

❑ Processing correlations between materials (MAT)

Library	
ENDF/B-VII.1	9228(U235) MT18 – 9237(U238) MT18 9228(U235) MT18 – 9237(U238) MT102 9228(U235) MT18 – 9437(PU239) MT18
ENDF/B-VIII.0	9237(U238) MT18 – 9437(PU239) MT18 9237(U238) MT102– 9437(PU239) MT18 9228(U235) MT18 – 9237(U238) MT18 9228(U235) MT18 – 9237(U238) MT102 9228(U235) MT18 – 9437(PU239) MT18
JEFF-3.3	None
JENDL-4.0u	9440(PU240)MT18 – 9443(PU241) MT18 9437(PU239)MT18 – 9443(PU241) MT18 9437(PU239)MT18 – 9440(PU240) MT18 9237(U238) MT18 – 9443(PU241) MT18 9237(U238) MT18 – 9440(PU240) MT18 9237(U238) MT18 – 9437(PU239) MT18 9228(U235) MT18 – 9443(PU241) MT18 9228(U235) MT18 – 9440(PU240) MT18 9228(U235) MT18 – 9437(PU239) MT18 9228(U235) MT18 – 9237(PU239) MT18

❑ Processing Covariances

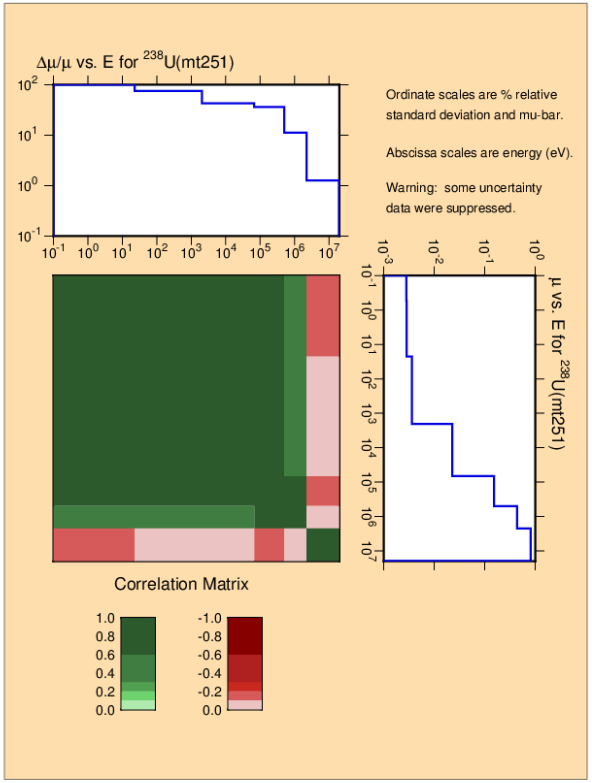
❑ Correlation between MATs




```
moder /
2 99
'  9228 and   9237' /
91      9228  /
92      9237  /
0/
errorr
21 0 99 26 61 /
  9228 1 2 1 1 /
1  300.0 / Just only one temperature
2 33 /
  9237    18 /
0 /
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
covr
 26 0 81 /
 1/
 /
 /
  9228    18  9237    18 /
viewr
81 82
covr
 26 27 /
 4 1
'LIB_ENDFB-VIII.0    ' /
'BOXER format'/
  9228    18  9237    18 /
stop
```

❑ Processing Covariances

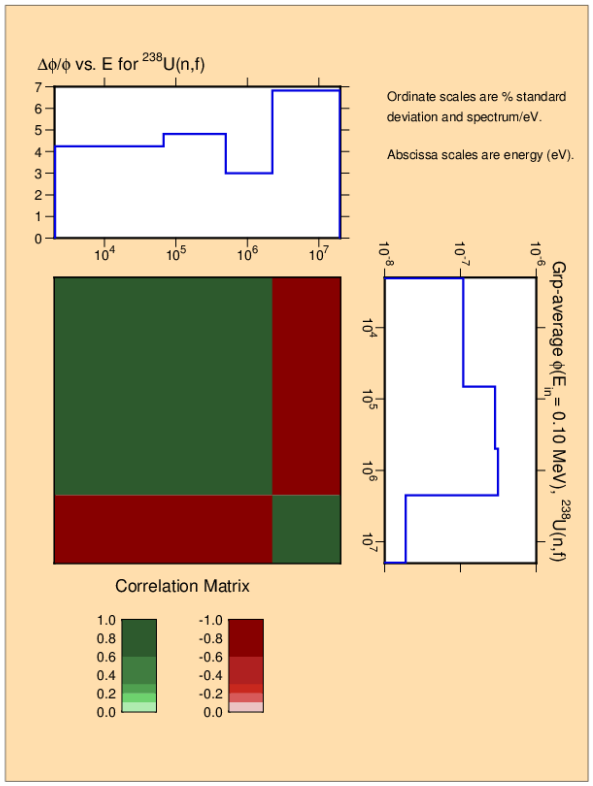
❑ MF34




```
groupr /
21 24 0 31/
  9237 1 0  8 0 1 1 1 /
'GENDF-   7g' /
300.0
1.E10
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
3/
3 251/
0/
0/
errorr
21 0 31 42 /
  9237 1 2 1 1 /
1  300.0 / Just only one temperature
0 34 /
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
covr
 42 0 81 /
 1/
 /
 /
  9237 0 0 0 /
viewr
81 82
covr
 42 72 /
 4 1
'LIB_JEFF33          ' /
'BOXER format'/
  9237 0 0 0 /
stop
```

❑ Processing Covariances

❑ MF35




```
groupr /
21 24 0 31/
  9237 1 0  8 0 1 1 1 /
'GENDF-   7g' /
300.0
1.E10
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
3/
3 18/
3 452 nubar_t/
3 455 nubar_d/
3 456 nubar_p/
5 455 nubar_spc/
5 18 nubar_spc/
0/
0/
errorr
21 0 31 40 /
  9237 1 2 1 1 /
1  300.0 / Just only one temperature
0 35  1 1 -1    1.0000E+05 /
7 /
 1.00000E-05
 5.40000E-01
 2.26033E+01
 2.03468E+03
 6.73795E+04
 4.97871E+05
 2.23130E+06
  1.9640E+07 /
covr
 40 0 81 /
 1/
 /
 /
  9237 0 0 0 /
viewr
81 82
covr
 40 70 /
 4 1
'LIB_JEFF33          ' /
'BOXER format'/
  9237 0 0 0 /
stop
```

❑ Processing Covariances

https://oecd-nea.org/download/wpec/sg46/

❑ Issues in evaluated files

ND Evaluation	Large procesed uncertainties (> 100%)	Lack of ND covariances	Processed null
ENDF/B-VII.1	B10(n,n') – g=2 Cr52(n,alpha) g=2	No MF33 • Pb206(n,p), Pb206(n,alpha) • Pb207(n,p), Pb207(n,alpha) • Pb208(n,p), Pb208(n,alpha) No MF34 • B10 • O16 • Cr52 • Ni58 • U235, U238 • Pu239, Pu240, Pu241 No MF35 • Pu-241	Processed null values • B10(n,alpha) – g=1 • B10(n,n') – g=3 • Ni58(n, alpha) g=3-7 • Ni58(n,p) – g=3-7 • Cr52(n,n') –g=3 • U235(n,n') – g=5 • Na23(n,elasticP1) –g= 7 • U-235(CHI) – g=7 • U-238(CHI) – g=7 • Pu239(CHI) – g=7 • Pu-240(CHI) – g=7

❑ Processing Covariances

https://oecd-nea.org/download/wpec/sg46/

❑ Issues in evaluated files

ND Evaluation	Large procesed uncertainties (> 100%)	Lack of ND covariances	Processed null
ENDF/B-VIII.0	B10(n,n') – g=2 Cr52(n, n,alpha) - g=2 O16(n,n') – g=1 O16(n, elastic-P1) – g=5-7	No MF33 • Fe56 (n,alpha) • Pb206(n,p), Pb206(n,alpha) • Pb207(n,p), Pb207(n,alpha) • Pb208(n,p), Pb208(n,alpha) No MF34 • B10 • Cr52 • Fe56 • Ni58 • Pu240, Pu241 No MF35 • Pu-241	Processed null values • B10(n,alpha) – g=1 • B10(n,n') – g=3-7 • Cr52(n,n') – g=3-7 • Ni58(n,p) – g=3-7 • Ni58(n,alpha) –g=3-7 • Na23(n,elasticP1) - g=7 • Pu239(CHI) – g=7 • Pu240(CHI) –g=7 **Fail NJOY2016.63:** • U235(n,elasticP1) • U238(n,elasticP1) • Pu239(n,elasticP1)

Note: **See Appendix I.**

❑ Processing Covariances

❑ Issues in evaluated files

ND Evaluation	Large procesed uncertainties (> 100%)	Lack of ND covariances	Processed null
JEFF-3.3	B10(n,n') – g=2 U238(n,elasticP1) – g=6,7	No MF31 • Pu240 No MF33 • Pb206(n,p), Pb206(n,alpha) • Pb207(n,p), Pb207(n,alpha) • Pb208(n,p), Pb208(n,alpha) No MF34 • B10 • O16 • Na23 • Cr52 • U235 • Pu239, Pu240 No MF35 • Pu240	Processed null values • B10(n,alpha) –g=1 • B10(n,n') - g=3-7 • Cr52(n,n') - g=3-7 • Ni58(n,alpha) – g=3-7 • Ni58(n,p) –g=3-7 • Fe56(n,alpha) –g=2-7 • U235(n,n') – g=5 • Ni58(n,elasticP1) –g=3-7 • Pu241(n, elasticP1) –g=6-7

Note: **See Appendix I.**

❑ Processing Covariances

❑ Issues in evaluated files

ND Evaluation	Large procesed uncertainties (> 100%)	Lack of ND covariances	Processed null
JENDL-4.0u	-	No MF33 • B10(n,p) • Pb206(n,p), Pb206(n,alpha) • Pb207(n,p), Pb207(n,alpha) • Pb208(n,p), Pb208(n,alpha) No MF34 • B10	Processed null values • B10(n,n') –g=1-3 • Ni58(n,p) –g=1, 3-7 • Ni58(n,alpha) –g=4-7 • Na23(n,elasticP1) – g=7 • Cr52(n,elasticP1) – g=1,6,7 • Ni58(n,elasticP1) – g=7 • Fe56(n,elasticP1) – g=6-7 • U235(n,elasticP1) – g=6-7 • U238(n,elasticP1) – g=6-7 • Pu239(n,elasticP1) – g=6-7 • Pu240(n,elasticP1) – g=6-7 • Pu241(n,elasticP1) – g=6-7

❑ **Discrepancy between NJOY2016 and NJOY99 for JENDL4 MF34 processing in O16**

❑ Processing Covariances

❑ *Formats: BOXER*

- *merged all covariances in a unique BOXER file for each MAT*

```
0 LIB_EN-b-  7 BOXER format          9228   1 9228   1   8 10   8  3   0   8   1
 1.000E-05 5.400E-01 2.260E+01 2.035E+03 6.738E+04 4.979E+05 2.231E+06 1.964E+07
 -1 -1 -1 -1 -1 -1 -1 -1
1 LIB_EN-b-  7 BOXER format          9228   1 9228   1   7 10   7  3   0   7   1
 3.372E+02 7.588E+01 2.497E+01 1.513E+01 1.092E+01 7.304E+00 7.549E+00
 -1 -1 -1 -1 -1 -1 -1
2 LIB_EN-b-  7 BOXER format          9228   1 9228   1   7 10   7  3   0   7   1
 4.725E-03 3.911E-03 1.018E-02 2.067E-02 2.007E-02 2.217E-02 2.905E-02
 -1 -1 -1 -1 -1 -1 -1
4 LIB_EN-b-  7 BOXER format          9228   1 9228   1  24  7  24  4   0   7   0
 1.0000 0.2026 0.0062-0.0589-0.0315 1.0000-0.0462-0.0600 0.0221 1.0000-0.0194
 0.0380 0.7388 0.5038 1.0000 0.8449 0.9323 0.6131 1.0000 0.8705 0.5597 1.0000
 0.5123 1.0000
  -1  -1  -1  -1  -1  -3  -1  -1  -1  -3  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1
  -1  -1  -1  -1
4 LIB_EN-b-  7 BOXER format          9228   1 9228   2  40  7  43  4   0   7   7
 0.1149 0.0217 0.0102 0.0015-0.1064-0.0716-0.0462-0.0005 0.2260 0.4974 0.8987
 0.0079-0.0122-0.0221-0.0084 0.9806 0.8297 0.7678 0.6509 0.0405 0.0742 0.0493
 0.8309 0.9823 0.8125 0.6811 0.1778 0.3263 0.2168 0.8016 0.8569 0.9226 0.5952
 0.0648 0.1188 0.0790 0.5500 0.5795 0.5783 0.6263
  -1  -1  -1  -1   3  -1  -1  -1  -1   3  -1  -1  -1  -1   3  -1  -1  -1  -1  -1
  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1  -1
  -1  -1  -1
...
...
```

- **BOXER is a useful format … to increase precision (as suggested by Ivo Kodeli, JEFF Nov2021, JEFDOC-2059)**

See MATERIALS at: https://oecd-nea.org/download/wpec/sg46/materials/

INDUSTRIALES
ETSII | UPM

❑ Processing Covariances

- *Formats:*

SG33 –> SG7

```
# Date:
# Lab:
# Library: LIB_ENDFB-VIII.0
#
# Data:    U235
 Data: 1000*Correlation( U235   / MF3/MT1    , U235   / MF3/MT1    )
#
# Grp upper E(eV)          X         Rel. unc.    Abs. unc.       X         Rel. unc.    Abs. unc.
#     lowest=  1.E-05
#
#-I2-------E12.4-----------E12.4-------E12.4-------E12.4-------E12.4-------E12.4-------E12.4
   1  1.9640E+07       7.5490E+00  2.9050E-02  2.1930E-01  7.5490E+00  2.9050E-02  2.1930E-01
   2  2.2310E+06       7.3040E+00  2.2170E-02  1.6193E-01  7.3040E+00  2.2170E-02  1.6193E-01
   3  4.9790E+05       1.0920E+01  2.0070E-02  2.1916E-01  1.0920E+01  2.0070E-02  2.1916E-01
   4  6.7380E+04       1.5130E+01  2.0670E-02  3.1274E-01  1.5130E+01  2.0670E-02  3.1274E-01
   5  2.0350E+03       2.4970E+01  1.0180E-02  2.5419E-01  2.4970E+01  1.0180E-02  2.5419E-01
   6  2.2600E+01       7.5880E+01  3.9110E-03  2.9677E-01  7.5880E+01  3.9110E-03  2.9677E-01
   7  5.4000E-01       3.3720E+02  4.7250E-03  1.5933E+00  3.3720E+02  4.7250E-03  1.5933E+00
#
# Grp upper E(eV)         1     2     3     4     5     6     7
#     lowest= 1.E-05      Y     Y     Y     Y     Y     Y     Y
#
#-I2-------E12.4--A-----I6----I6----I6----I6----I6----I6----I6
   1  1.9640E+07  X    1000   512   560   613   504  1000  1000
   2  2.2310E+06  X     512  1000   871   932   739  1000  1000
   3  4.9790E+05  X     560   871  1000   845    38    22   -32
   4  6.7380E+04  X     613   932   845  1000   -19   -60   -59
   5  2.0350E+03  X     504   739    38   -19  1000   -46     6
   6  2.2600E+01  X    1000  1000    22   -60   -46  1000   203
   7  5.4000E-01  X    1000  1000   -32   -59     6   203  1000
#
 Data: 1000*Correlation( U235   / MF3/MT1    , U235   / MF3/MT2    )
#
# Grp upper E(eV)          X         Rel. unc.    Abs. unc.       X         Rel. unc.    Abs. unc.
#     lowest=  1.E-05
#
#-I2-------E12.4-----------E12.4-------E12.4-------E12.4-------E12.4-------E12.4-------E12.4
   1  1.9640E+07       7.5490E+00  2.9050E-02  2.1930E-01  4.1560E+00  3.7550E-02  1.5606E-01
   2  2.2310E+06       7.3040E+00  2.2170E-02  1.6193E-01  4.2500E+00  3.3450E-02  1.4216E-01
   3  4.9790E+05       1.0920E+01  2.0070E-02  2.1916E-01  8.4500E+00  2.5470E-02  2.1522E-01
   4  6.7380E+04       1.5130E+01  2.0670E-02  3.1274E-01  1.1440E+01  2.7260E-02  3.1185E-01
   5  2.0350E+03       2.4970E+01  1.0180E-02  2.5419E-01  1.2120E+01  1.8480E-02  2.2398E-01
   6  2.2600E+01       7.5880E+01  3.9110E-03  2.9677E-01  1.1900E+01  1.2280E-02  1.4613E-01
   7  5.4000E-01       3.3720E+02  4.7250E-03  1.5933E+00  1.3730E+01  2.2530E-02  3.0934E-01
#
# Grp upper E(eV)         1     2     3     4     5     6     7
#     lowest= 1.E-05      Y     Y     Y     Y     Y     Y     Y
#
#-I2-------E12.4--A-----I6----I6----I6----I6----I6----I6----I6
   1  1.9640E+07  X     626   578   580   550    79   119    65
   2  2.2310E+06  X     595   923   857   802   217   326   178
   3  4.9790E+05  X     681   813   982   831    49    74    41
   4  6.7380E+04  X     651   768   830   981    -8   -22   -12
   5  2.0350E+03  X       0     0     0     8   899   497   226
   6  2.2600E+01  X       0     0     0    -1   -46   -72  -106
   7  5.4000E-01  X       0     0     0     2    10    22   115
...
...
```

❑ Conclusion

- ❑ ***Processing Covariances***
- ❑ ***And now*** *… using processed covariances in 7 groups*
  - *First, checking mathematical properties:*
    - *Positive definite, symmetry, correlations in [-1,1]*
    - *Negative eigenvalues (roundoff issues)*

      … minor adjustments needed to perform Cholesky decomposition
  - *Identifying*
    - *large relative uncertainties*
    - *lack of covariances*

  Ref.: *I. Kodeli, "Mathematical verification of JEFF-3.3 and ENDF/B-VIII.0 covariance data, JEFF Nov 2021.*

  Ref.: *Nathan A. Gibson, "Update on Covariance Data Testing Strategy at LANL", CSEWG Nov 2021.*
- ❑ *Applying in*
  - *UQ (sandwich formula and/or Monte Carlo approaches)*
  - *TAR exercise*

Acknowledgments

This work is part of the SANDA project (Supplying Accurate Nuclear Data for energy and non-energy Applications) that has received funding from the European Union's H2020/Euratom under grant agreement No. 847552

❑ Appendix I: Processing Covariances with NJOY2016.63

- *ND covariances processed with NJOY2016.63*
- *Processed ND:*
  - *MF31*
  - *MF32/MF33*
  - *MF34*
  - *MF35*
- *Energy structure 7g- weighting IWT8*
- *Ein for MF35: 1.0E+5eV*
- *Formats: BOXER, ERROR (and COVERX)*

See MATERIALS at: https://oecd-nea.org/download/wpec/sg46/materials/

❑ Processing Covariances

https://oecd-nea.org/download/wpec/sg46/

❑ Issues in evaluated files

ND Evaluation	Large procesed uncertainties (> 100%)	Lack of ND covariances	Processed null
ENDF/B-VII.1	B10(n,n') – g=2 Cr52(n,alpha) g=2	No MF33 • Pb206(n,p), Pb206(n,alpha) • Pb207(n,p), Pb207(n,alpha) • Pb208(n,p), Pb208(n,alpha) No MF34 • B10 • O16 • Cr52 • Ni58 • U235, U238 • Pu239, Pu240, Pu241 No MF35 • Pu-241	Processed null values • B10(n,alpha) – g=1 • B10(n,n') – g=3 • Ni58(n, alpha) g=3-7 • Ni58(n,p) – g=3-7 • Cr52(n,n') –g=3 • U235(n,n') – g=5 • Na23(n,elasticP1) –g= 7 • U-235(CHI) – g=7 • U-238(CHI) – g=7 • Pu239(CHI) – g=7 • Pu-240(CHI) – g=7

❑ Processing Covariances

https://oecd-nea.org/download/wpec/sg46/

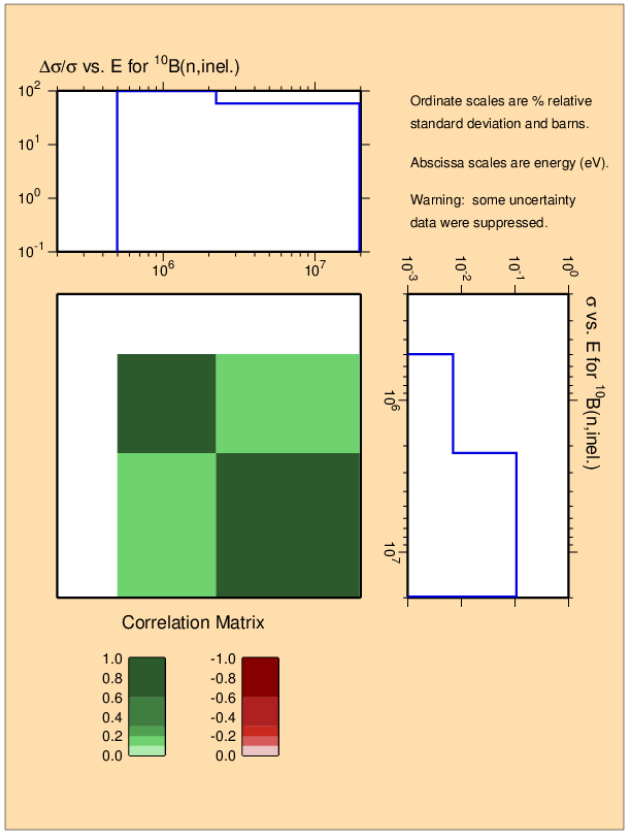
❑ Issues in evaluated files

ND Evaluation	Large procesed uncertainties (> 100%)	Lack of ND covariances	Processed null
ENDF/B-VIII.0	B10(n,n') – g=2 Cr52(n, n,alpha) - g=2 O16(n,n') – g=1 O16(n, elastic-P1) – g=5-7	No MF33 • Fe56 (n,alpha) • Pb206(n,p), Pb206(n,alpha) • Pb207(n,p), Pb207(n,alpha) • Pb208(n,p), Pb208(n,alpha) No MF34 • B10 • Cr52 • Fe56 • Ni58 • Pu240, Pu241 No MF35 • Pu-241	Processed null values • B10(n,alpha) – g=1 • B10(n,n') – g=3-7 • Cr52(n,n') – g=3-7 • Ni58(n,p) – g=3-7 • Ni58(n,alpha) –g=3-7 • Na23(n,elasticP1) - g=7 • Pu239(CHI) – g=7 • Pu240(CHI) –g=7 **Fail NJOY2016.63:** • U235(n,elasticP1) • U238(n,elasticP1) • Pu239(n,elasticP1)

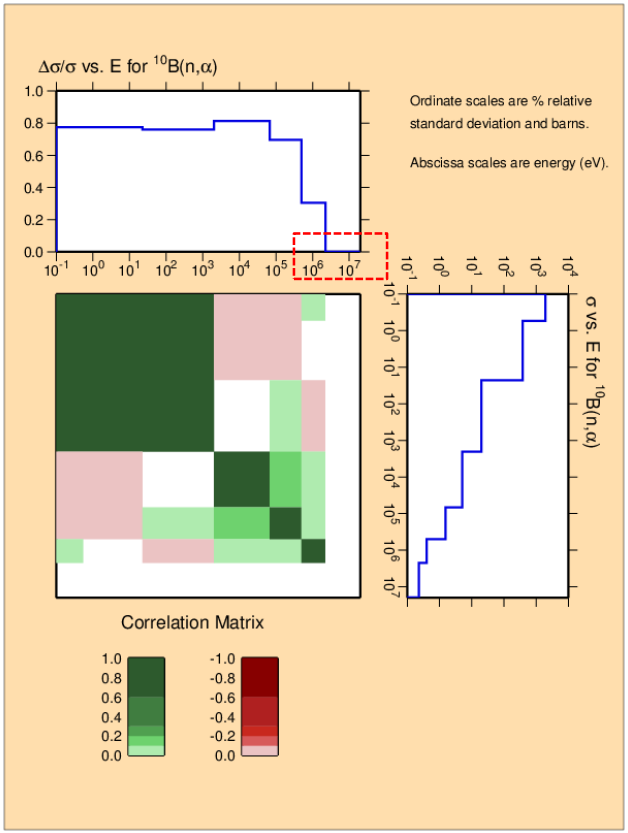
Note: **See Appendix I.**

❑ Appendix I: Processing Covariances with NJOY2016.63

❑ ENDF/B-VIII.0: 10B



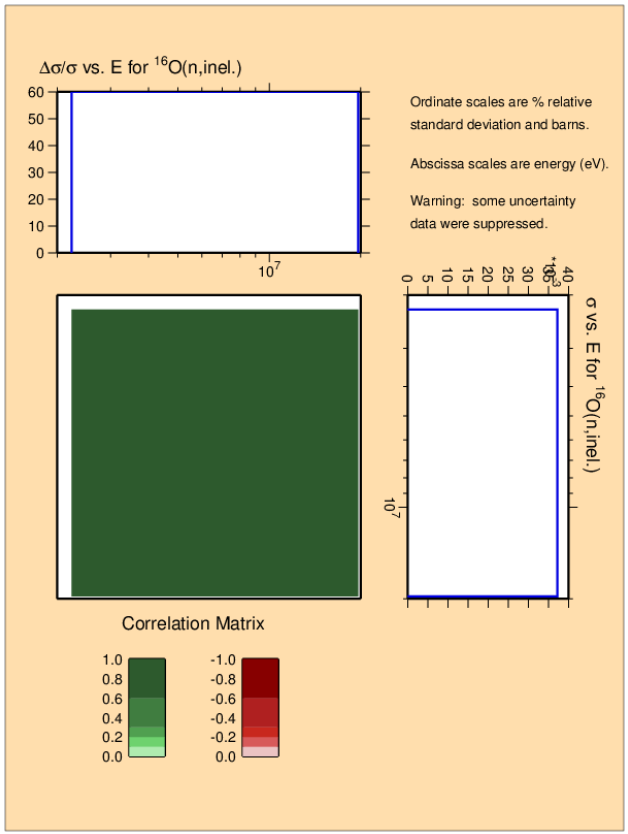
➢ Large processed uncertainties (> 100%)



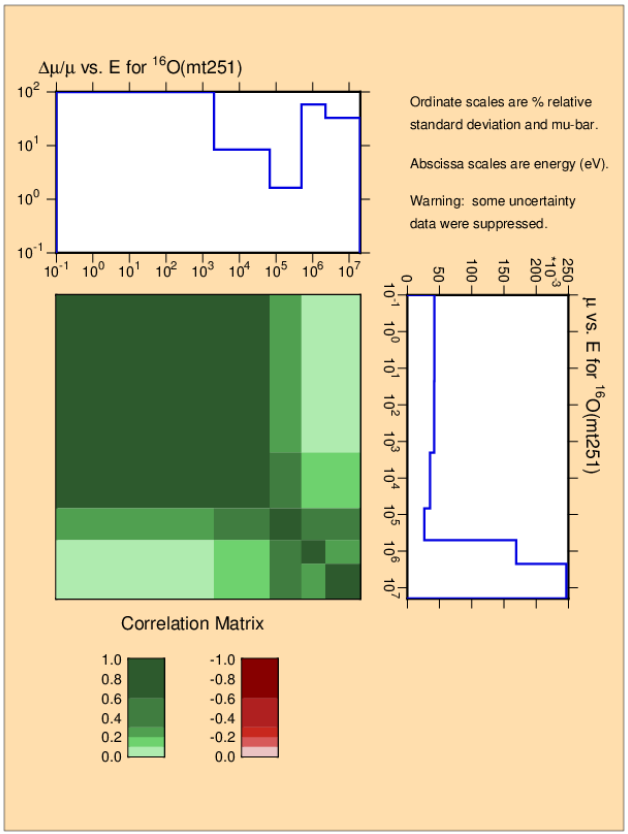
➢ Null processed (E > 2.23 MeV – g=1)

❑ Appendix I: Processing Covariances with NJOY2016.63

❑ ENDF/B-VIII.0: 16O



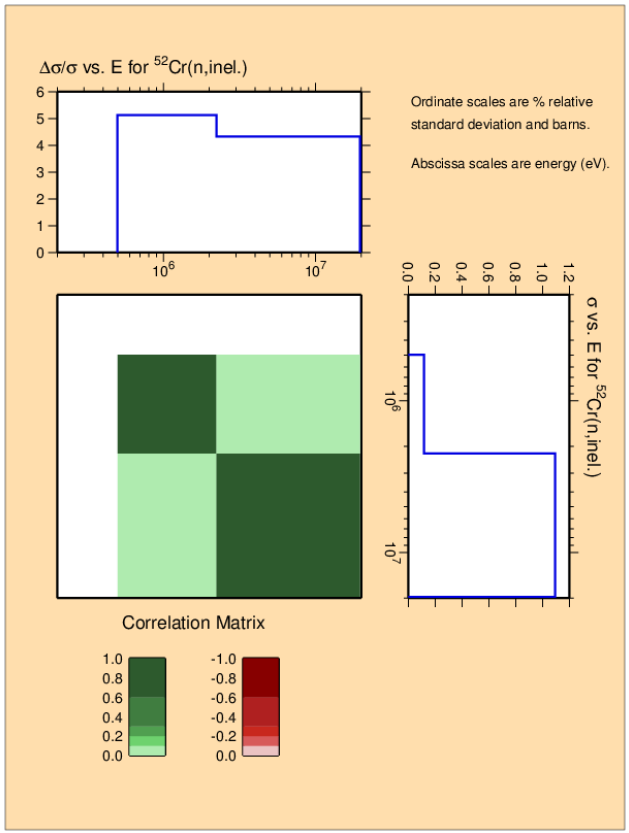
➢ Large processed uncertainties (> 100%)



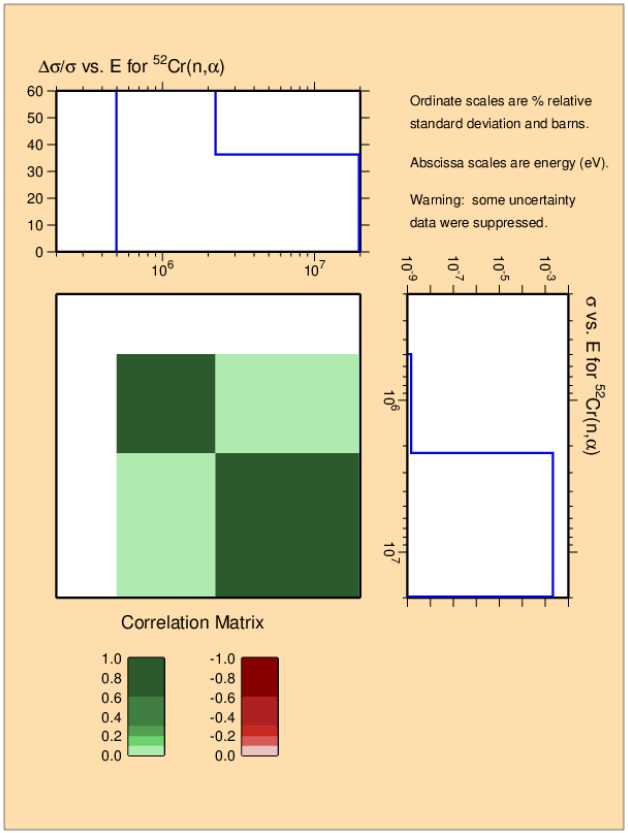
➢ Large processed uncertainties (> 100%)

❑ Appendix I: Processing Covariances with NJOY2016.63

❑ ENDF/B-VIII.0: 52Cr



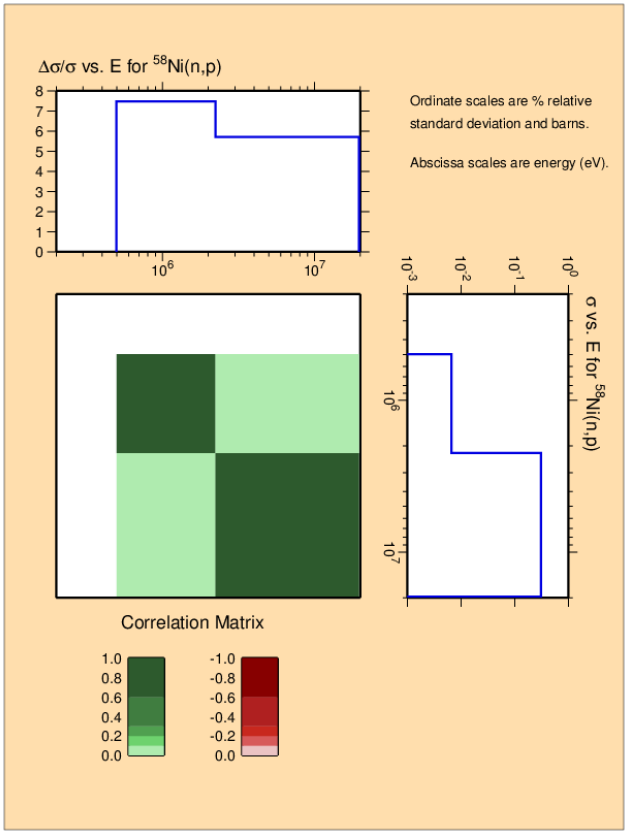
➢ Null processed (E < 497 keV – g=3-7)



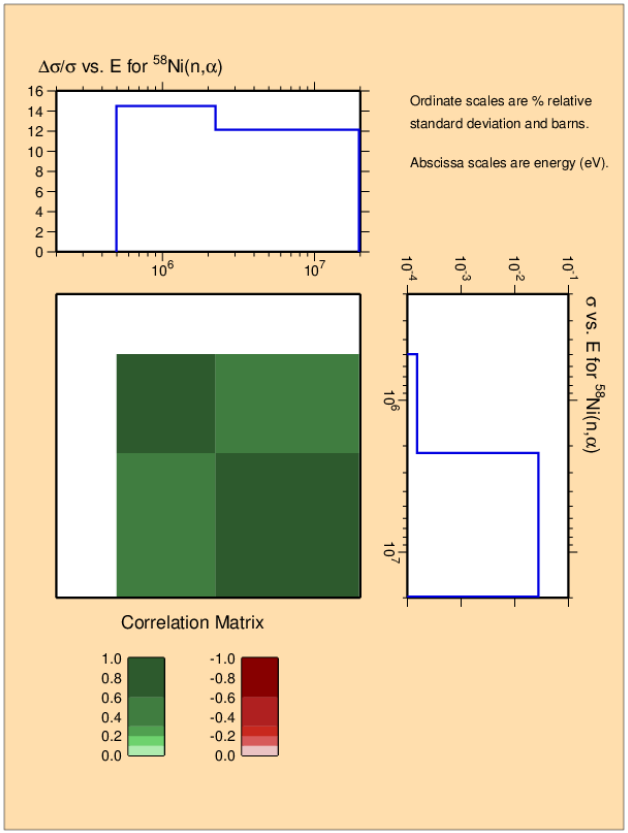
➢ Large processed uncertainties (> 100%)

❑ Appendix I: Processing Covariances with NJOY2016.63

❑ ENDF/B-VIII.0: 58Ni



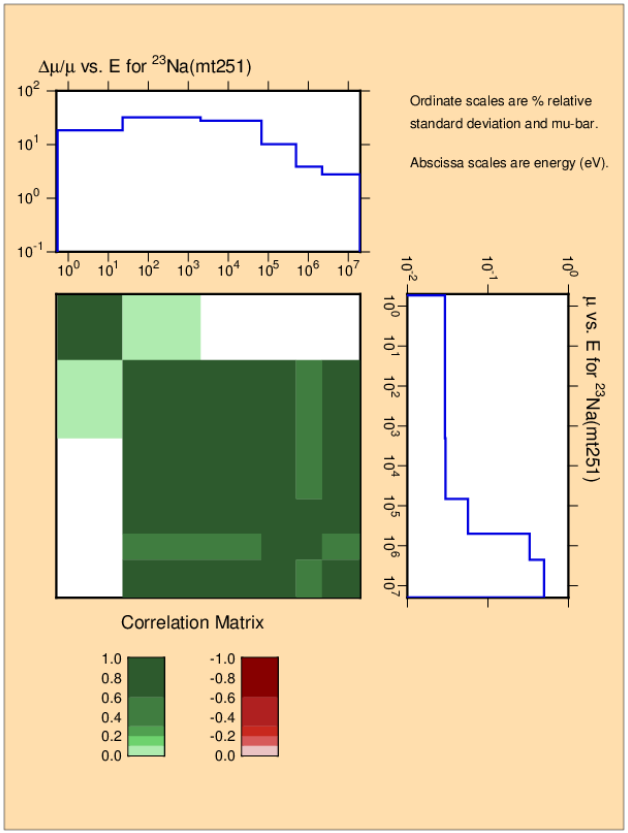
➢ Null processed (E < 497 keV – g=3-7)



➢ Null processed (E < 497 keV – g=3-7)

❑ Appendix I:
Processing Covariances with NJOY2016.63

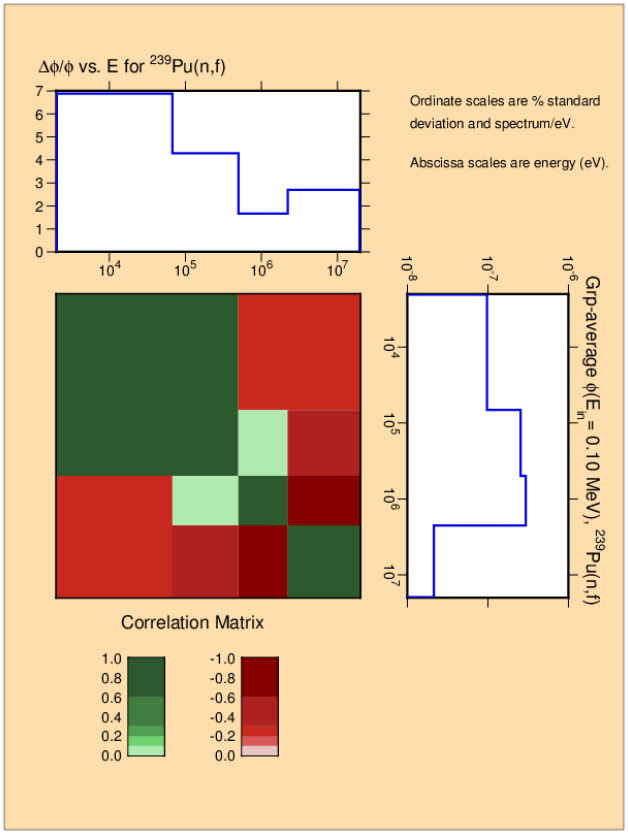
❑ ENDF/B-VIII.0: 23Na



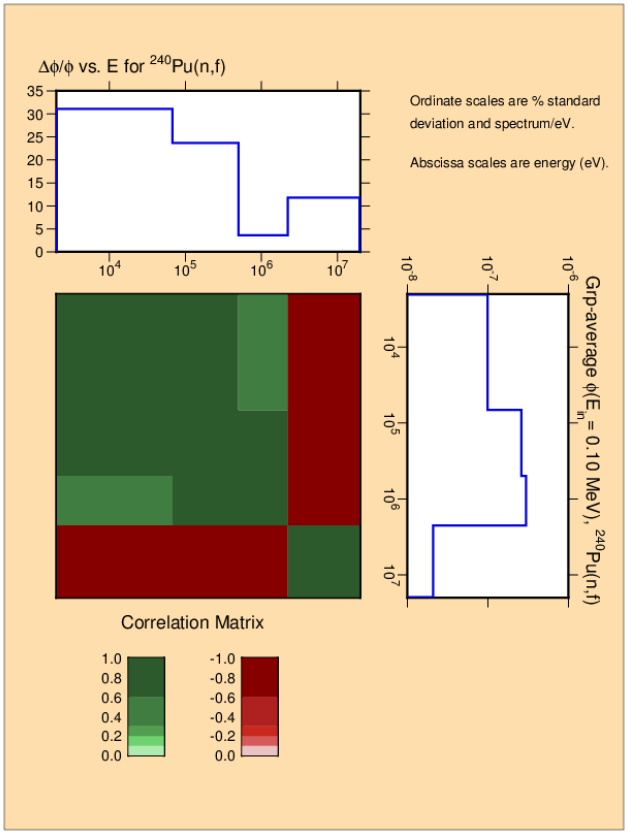
➢ Null processed (E < 0.54 eV – g=7)

❑ Appendix I: Processing Covariances with NJOY2016.63

❑ ENDF/B-VIII.0: 239Pu and 240Pu



➢ Null processed (E < 0.54 eV – g=7)



➢ Null processed (E < 0.54 eV – g=7)

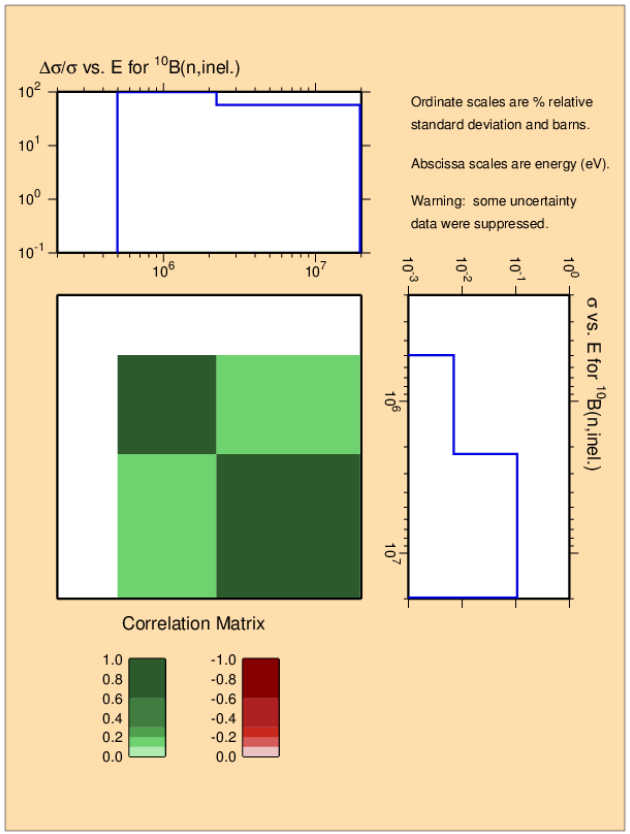
❑ Processing Covariances

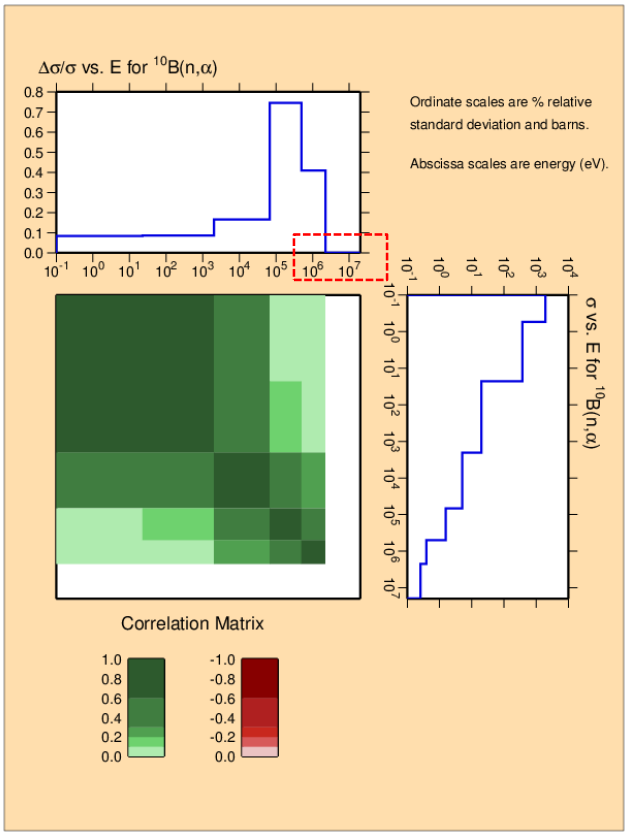
❑ Issues in evaluated files

ND Evaluation	Large procesed uncertainties (> 100%)	Lack of ND covariances	Processed null
JEFF-3.3	B10(n,n') – g=2 U238(n,elasticP1) – g=6,7	No MF31 • Pu240 No MF33 • Pb206(n,p), Pb206(n,alpha) • Pb207(n,p), Pb207(n,alpha) • Pb208(n,p), Pb208(n,alpha) No MF34 • B10 • O16 • Na23 • Cr52 • U235 • Pu239, Pu240 No MF35 • Pu240	Processed null values • B10(n,alpha) –g=1 • B10(n,n') - g=3-7 • Cr52(n,n') - g=3-7 • Ni58(n,alpha) – g=3-7 • Ni58(n,p) –g=3-7 • Fe56(n,alpha) –g=2-7 • U235(n,n') – g=5 • Ni58(n,elasticP1) –g=3-7 • Pu241(n, elasticP1) –g=6-7

❑ Appendix I: Processing Covariances with NJOY2016.63

❑ JEFF-3.3: B10





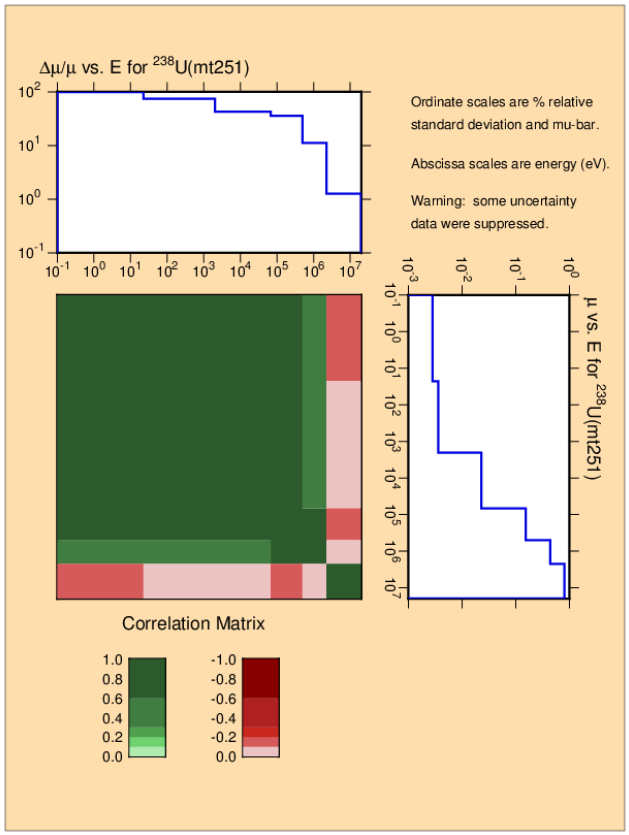
➢ Large processed uncertainties (> 100%)

➢ Null processed (E < 497 keV – g=3-7)

➢ Null processed (E > 2.23 MeV – g=1)

❑ Appendix I: Processing Covariances with NJOY2016.63

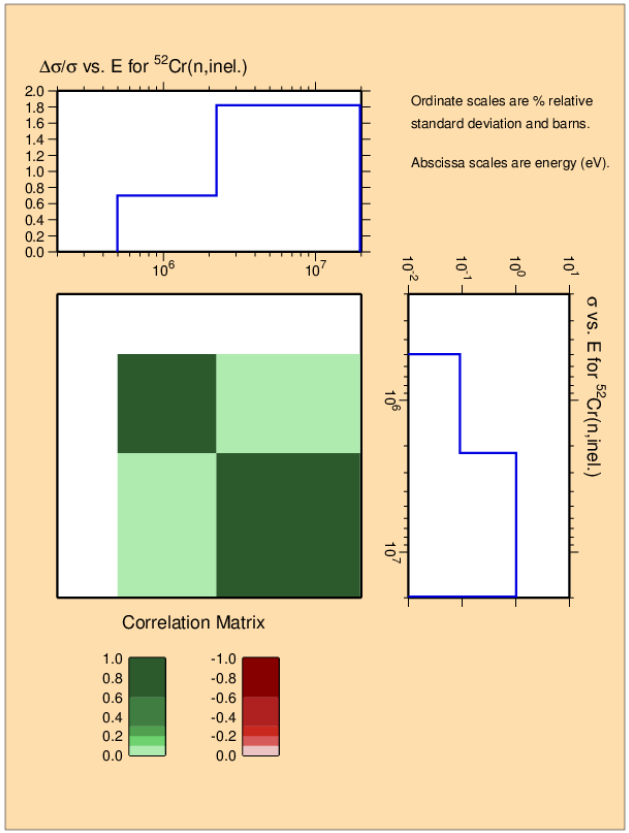
❑ JEFF-3.3: 238U



➢ Large processed uncertainties (> 100%)

❑ Appendix I:
Processing Covariances with NJOY2016.63

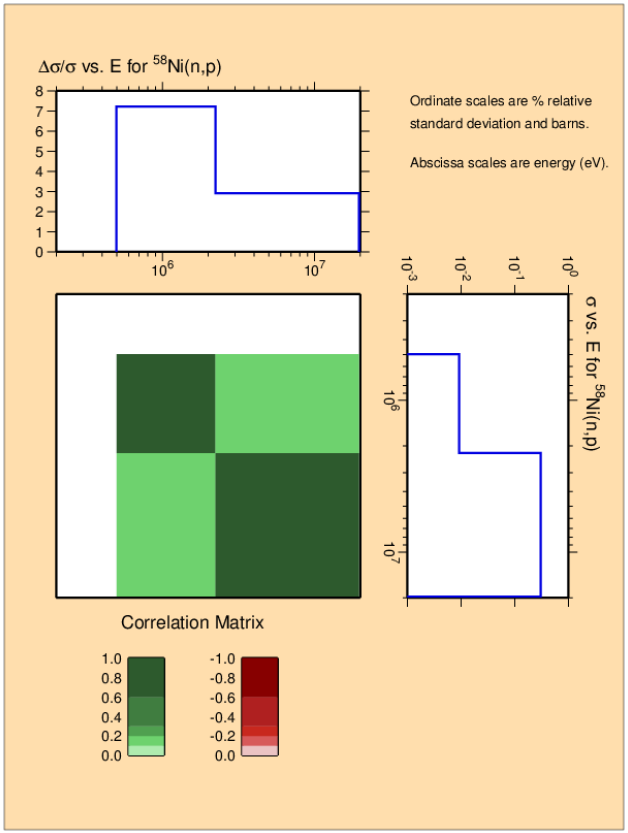
❑ JEFF-3.3: 52Cr



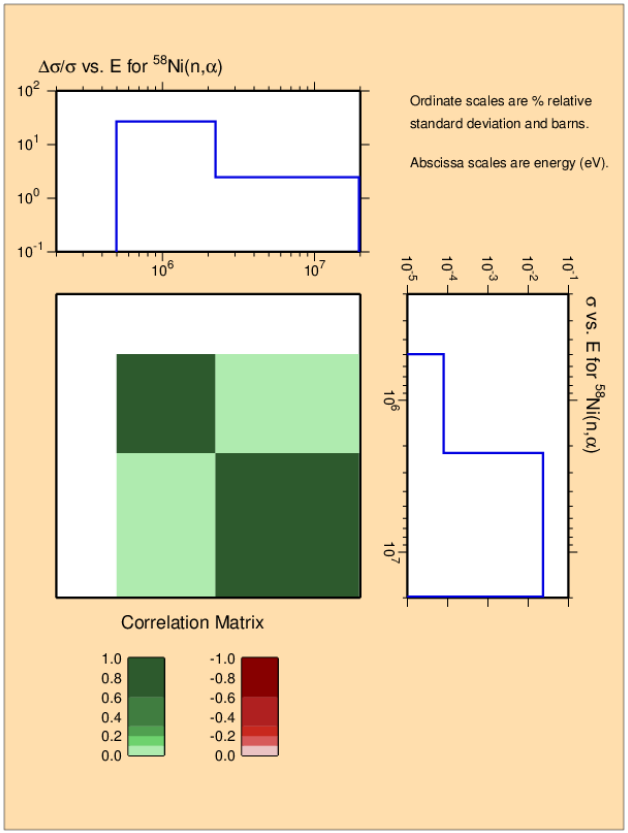
➢ Null processed (E < 497 keV – g=3-7)

❑ Appendix I: Processing Covariances with NJOY2016.63

❑ JEFF-3.3: 58Ni



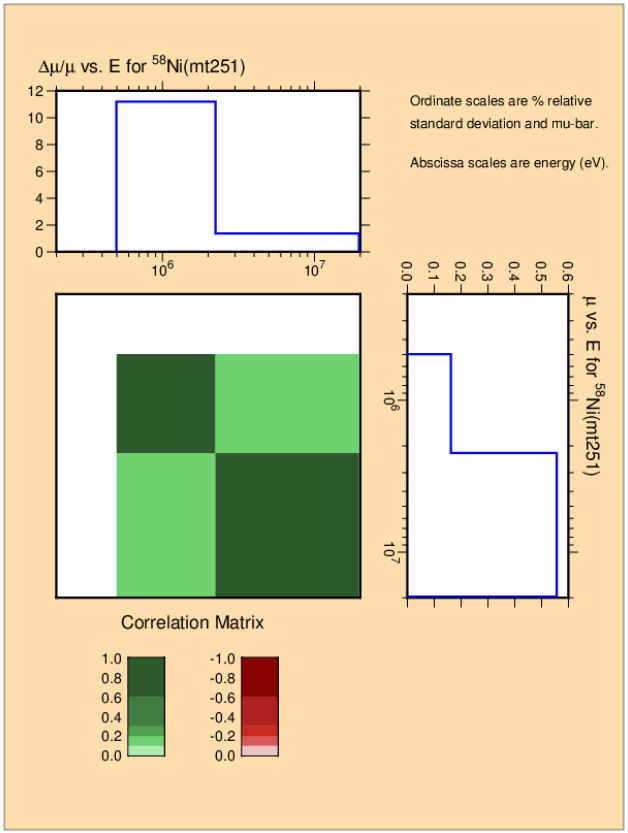
➢ Null processed (E < 497 keV – g=3-7)



➢ Null processed (E < 497 keV – g=3-7)

❑ Appendix I: Processing Covariances with NJOY2016.63

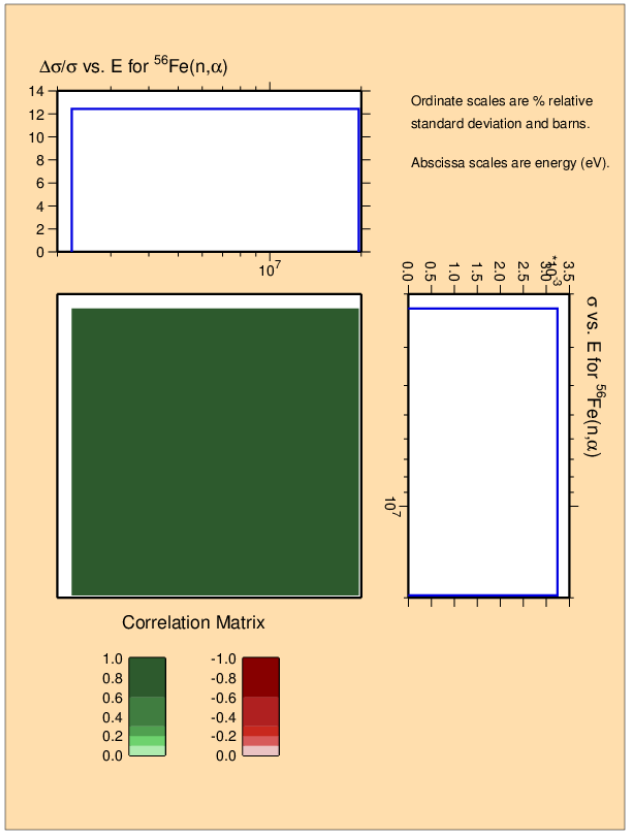
❑ JEFF-3.3: 58Ni



➢ Null processed (E < 497 keV – g=3-7)

❑ Appendix I: Processing Covariances with NJOY2016.63

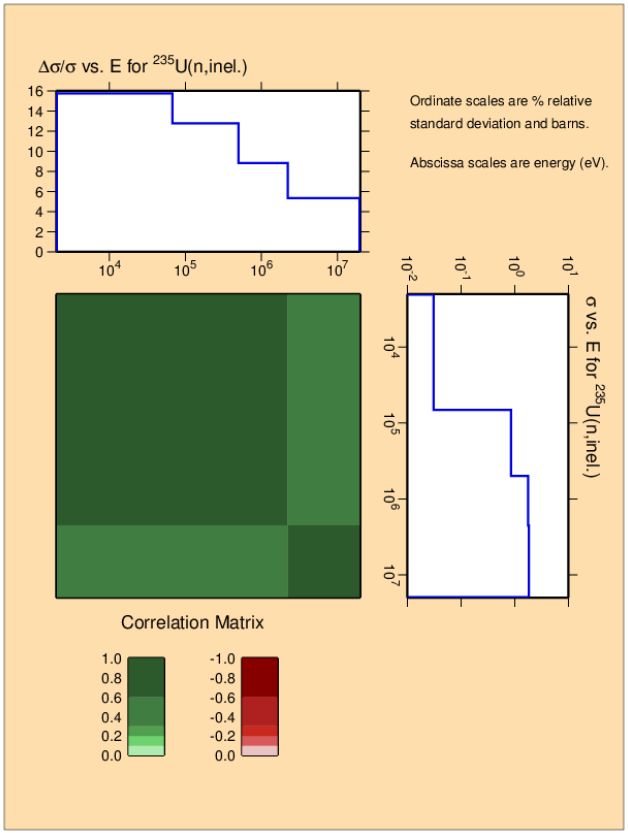
❑ JEFF-3.3: 56Fe



➢ Null processed (E < 2.23 MeV – g=2-7)

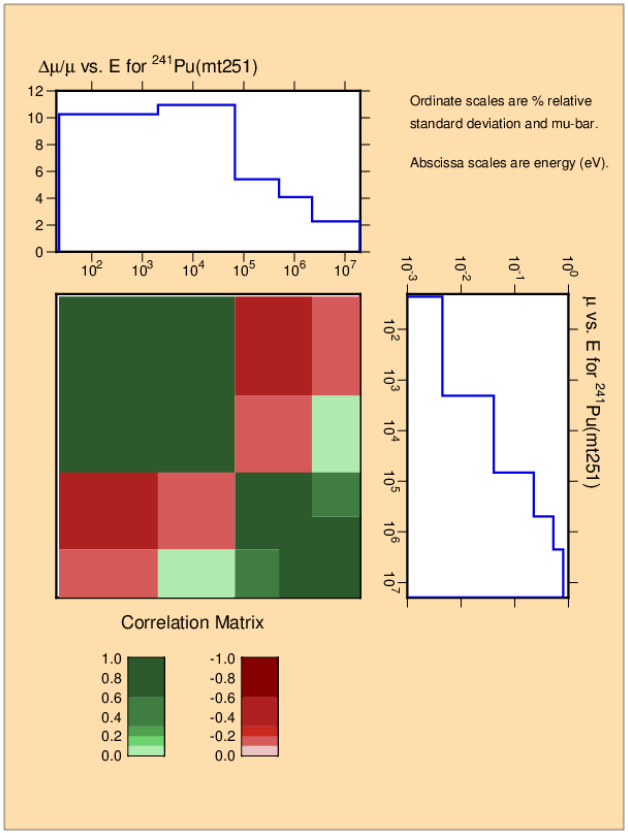
❑ Appendix I: Processing Covariances with NJOY2016.63

❑ JEFF-3.3: 235U



➢ Null processed (E < 2.03 keV – g=5-7)

❑ JEFF-3.3: 241Pu



➢ Null processed (E < 22.6 eV – g=6-7)

❑ Processing Covariances

❑ Issues in evaluated files

ND Evaluation	Large procesed uncertainties (> 100%)	Lack of ND covariances	Processed null
JENDL-4.0u	-	No MF33 • B10(n,p) • Pb206(n,p), Pb206(n,alpha) • Pb207(n,p), Pb207(n,alpha) • Pb208(n,p), Pb208(n,alpha) No MF34 • B10	Processed null values • B10(n,n') –g=1-3 • Ni58(n,p) –g=1, 3-7 • Ni58(n,alpha) –g=4-7 • Na23(n,elasticP1) – g=7 • Cr52(n,elasticP1) – g=1,6,7 • Ni58(n,elasticP1) – g=7 • Fe56(n,elasticP1) – g=6-7 • U235(n,elasticP1) – g=6-7 • U238(n,elasticP1) – g=6-7 • Pu239(n,elasticP1) – g=6-7 • Pu240(n,elasticP1) – g=6-7 • Pu241(n,elasticP1) – g=6-7