A-priori and a-posteriori covariance data in nuclear cross section adjustments: issues and challenges

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Outline

- The following subjects will be discussed:
  - Assessment of adjustments.
  - Definition of criteria to accept new central values of cross sections after adjustments.
  - Avoid compensation among different input data in the adjustments.
  - Validation of the “a priori” and use of the “a posteriori” covariance matrix.
  - Issues related to the presence of negative eigenvalues in the “a priori” covariance matrix.

Adjustment Formulas

$G=(M_{EC} + SM_{\sigma} S^T)$: total integral covariance matrix

$$\chi^2 = (\sigma' - \sigma)^T M_{\sigma}^{-1} (\sigma' - \sigma) + (E - C)^T M_{EC}^{-1} (E - C)$$

The cross sections modifications that minimize the χ^2 and the associated "a posteriori" covariance matrix are:

$$\sigma' - \sigma = M_{\sigma} S^T G^{-1} (E - C)$$

$$M_{\sigma'} = M_{\sigma} - M_{\sigma} S^T G^{-1} S M_{\sigma}$$

The χ^2 after adjustment is computed as:

$$\chi'^2 = (E - C)^T G^{-1} (E - C)$$

Assessment of Adjustments

- The first step is to select a comprehensive set of experiments, possibly complementary in the type of information that they provide.

  - First criterion is given by the representativity factor:

$$f_{re} = \frac{(S_R M_\sigma S_E)}{[(S_R M_\sigma S_R)(S_E M_\sigma S_E)]^{1/2}} \qquad \Delta R'^2 = \Delta R^2 (1 - f_{re}^2)$$

  - The complementarity of the experiments can be established by looking at the correlation factor among the selected experiments (i. e. S_R is replaced by $S_{E'}$ of the experiment E').
  - Experiments can be selected, because they provide information of elemental type to improve specific reactions (e. g. capture in irradiation experiment), or specific energy range of a cross sections (e. g. using particular detectors for spectral indices of threshold reactions).

Parameters for Assessing Adjustments

- **Adjustment Margin:** $AM^i = U^i_\sigma + U^i_{EC} - |(E^i - C^i)|$
- **Individual χ_i measured in sigmas (before adj.):** $\chi^i = \frac{|E^i - C^i|}{\sqrt{U^{i2}_\sigma + U^{i2}_{EC}}}$
- **Diagonal χ_i measured in sigmas (after adj.):** $\chi^{i2}_{diag} = (E^i - C^i)^2\, G^{-1}_{ii}$
- **Initial $\chi^2$and χ_i^2 experiment contribution to χ^2:** $\chi'^{i2}_{con} = \frac{[(E-C)^{\mathrm{T}} G^{-1})_i . (E^i - C^i)]}{N_E}$
- **IS (Ishikawa factor):** $IS^i = \frac{U^i_\sigma}{U^i_{EC}}$
- **$\Delta\, \chi_{i\,E}{}'^2$ contribution to [χ'^2- χ^2] due to change of (E-C):**

$$\Delta\chi'^{i2}_{C} = \frac{-[\Delta(E-C')^T\, M^{-1}_{EC})_i . \Delta\left(E^i - C'^i\right)]}{N_E}$$

- **$\Delta\, \chi_{i\,E}{}'^2$ contribution to [χ'^2- χ^2] due to $\Delta\sigma_i$:** $\Delta\chi'^{i2}_{\sigma} = \frac{-[\Delta\sigma^T\, M^{-1}_\sigma)_i . \Delta\sigma_i]}{N_E}$

Assessment of Adjustments

"A Priori" Analysis

Integral Param.	U^i_σ (%)	U^i_{EC}(%)	$\lvert(E^i - C^i)\rvert / C^i(\%)$	AM_i(%)	EM_i(%)	$\chi^i\,(\sigma)^{a)}$	IS_i
JEZEBEL K_{eff}	0.72	0.20	0.01	0.91	0.19	0.02	3.61
GODIVA $^{239}Pu\ \sigma_{fis}/^{235}U\ \sigma_{fis}$	0.73	1.84	1.42	1.15	0.42	0.72	0.39
PROFIL ^{239}Pu in ^{238}Pu sample	5.80	2.43	27.38	-19.15	-24.95	4.36	2.38
TRAPU2 ^{243}Cm build up	49.19	4.04	107.04	-53.82	-1.03	2.16	13.52

"A Posteriori" Analysis

Integral Param.	U'^i_σ (%)	$\lvert(E^i - C'^i)\rvert / C'^i(\%)$	$\chi^i_{diag}\,(\sigma)^{a)}$	$\Delta\chi'^{i^2}_C$	$\chi^{i^2}_{con}$	$\chi'^{i^2}_{con}$
JEZEBEL K_{eff}	0.17	0.07	0.04	-0.00	0.00	0.00
GODIVA $^{239}Pu\ \sigma_{fis}/^{235}U\ \sigma_{fis}$	0.37	0.27	0.75	-0.00	0.01	0.00
PROFIL ^{239}Pu in ^{238}Pu sample	1.47	1.26	6.42	-4.01	4.71	0.48
TRAPU2 ^{243}Cm build up	3.63	0.62	2.27	-10.01	9.95	0.06

χ^2	χ'^2	$\sum_i \Delta\chi'^{i2}_C$	$\sum_\sigma \Delta\chi'^{i2}_\sigma$
26.73	1.61	-24.36	-0.73

Acceptance of Adjusted Central Values

After an adjustment is performed, are all cross section changes to be accepted (especially when large variations of cross sections are observed)? Several considerations:

- **Sometimes the cross section changes are completely unphysical.**
- **Reject cross sections which variation is larger than one sigma of the "a priori" standard deviation.**
- **Caution has to be taken when large variations are observed in energy ranges that were not the main target of the adjustment.**
- **Caution also has to be exerted, when large variations of the cross sections are produced but the "a posteriori" associated standard deviation reductions are small.**
- **A good check, after adjustment, is to compare against existing validated files. A further action consists to compare the obtained adjusted cross sections against reliable differential data (require interactions with evaluators).**

Acceptance of Adjusted Central Values

Unphysical cross section changes obtained in the adjustment.

Cross Section	Energy Group	Relative Change Due to Adjustment (%)
^{238}Pu σ_{capt}	3	-155.5
^{238}Pu σ_{capt}	10	-108.0
^{238}Pu σ_{capt}	16	-126.3
^{238}Pu σ_{capt}	17	-111.5

Acceptance of Adjusted Central Values

Cross sections with changes after adjustment larger than initial standard deviation

Cross Section	Energy Group	Relative Change Due to Adjustment (%)	Stand. Deviat. Before Adjustment (%)
$^{16}O\ \sigma_{elas}$	6	2.5	2.0
$^{56}Fe\ \sigma_{elas}$	8	14.2	10.5
$^{235}U\ \sigma_{elas}$	5	6.1	5.0
$^{238}U\ \sigma_{fiss}$	4	0.60	0.57
$^{239}Pu\ \sigma_{capt}$	15	12.6	7.9
$^{238}Pu\ \sigma_{capt}$	9	-61.4	31.0
$^{241}Am\ \sigma_{fiss}$	6	-1.8	1.3
$^{133}Cs\ \sigma_{capt}$	9	19.4	14.0
$^{105}Pd\ \sigma_{capt}$	11	32.2	12.7
$^{101}Ru\ \sigma_{capt}$	13	-16.0	9.0
$^{242}Cm\ \sigma_{capt}$	13	184.2	100

Acceptance of Adjusted Central Values

Cross sections with significant changes after adjustment, but small standard deviation variation

Cross Section	Energy Group	Relative Change Due to Adjustment (%)	Stand. Deviat. Before Adjustment (%)	Stand. Deviat. After Adjustment (%)
$^{105}Pd\ \sigma_{capt}$	4	-12.8	25.3	24.8
$^{56}Fe\ \sigma_{elas}$	10	11.4	9.2	8.2
$^{239}Pu\ \sigma_{capt}$	6	10.7	20.5	19.7
$^{238}Pu\ \sigma_{capt}$	6	-23.8	28.0	27.3
$^{240}Pu\ \sigma_{inel}$	5	12.4	32.0	31.0
$^{240}Pu\ \chi$	1	14.2	89.9	89.6
$^{242m}Am\ \sigma_{capt}$	12	10.8	50.0	49.4

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Avoiding Compensations

- In many cases, the adjustment can produce untrustworthy results in terms of adjusted cross sections, when some forms of compensation exist. Compensations can appear in different ways:
  - It is possible that some reactions compensate each other (e. g. ^{239}Pu χ and inelastic), because of missing experiments able to discriminate between the two parameters. There is a need for specific (preferably of elemental type) integral experiments:
    - irradiation experiments (for capture, (n,2n))
    - spectral indices (capture and fission)
    - “flat” adjoint flux reactivity experiments (to separate inelastic from absorption cross section)
    - neutron transmission or leakage experiments (mostly for inelastic cross sections)
    - reaction rate spatial distribution slopes (elastic, and inelastic)

Avoiding Compensations

- Other sources of compensations are missing isotopes in the adjustment and missing reactions in the covariance matrix:
  - fission spectrum
  - anisotropic scattering
  - secondary energy distribution for inelastic cross sections (multigroup transfer matrix)
  - cross correlations (reaction and/or isotopes)
- Underestimation or overestimation of well known reaction standard deviations (e. g. ^{239}Pu fission)

Avoiding Compensations

^{239}Pu σ_{fiss} standard deviations for different covariance matrix: COMMARA-2.0 (COMM.), COMAC, and JENDL-4 (JENDL) (%).

Group	COMM.	COMAC	JENDL	Group	COMM.	COMAC	JENDL	Group	COMM.	COMAC	JENDL
1	0.8	3.1	0.9	12	0.8	3.4	0.8	23	1.3	3.3	1.3
2	0.9	2.5	0.9	13	0.9	3.4	0.8	24	1.6	3.1	1.5
3	0.8	2.3	0.8	14	0.9	3.4	0.8	25	1.8	3.1	1.8
4	0.9	3.2	0.7	15	1.2	3.4	0.8	26	1.6	2.9	1.6
5	0.9	4.2	0.8	16	0.8	3.4	2.4	27	2.6	0.4	2.7
6	0.8	3.7	0.7	17	0.8	3.4	2.5	28	1.7	3.0	1.8
7	0.8	3.4	0.7	18	0.7	3.5	1.7	29	1.0	2.5	1.1
8	0.9	3.3	0.7	19	1.2	2.9	1.2	30	1.5	2.8	1.5
9	0.8	3.4	0.8	20	1.3	3.3	1.3	31	1.8	1.2	1.8
10	1.0	3.4	0.7	21	1.3	2.8	1.3	32	0.8	1.7	0.8
11	0.9	3.4	0.8	22	1.5	3.1	1.5	33	1.1	0.6	1.1

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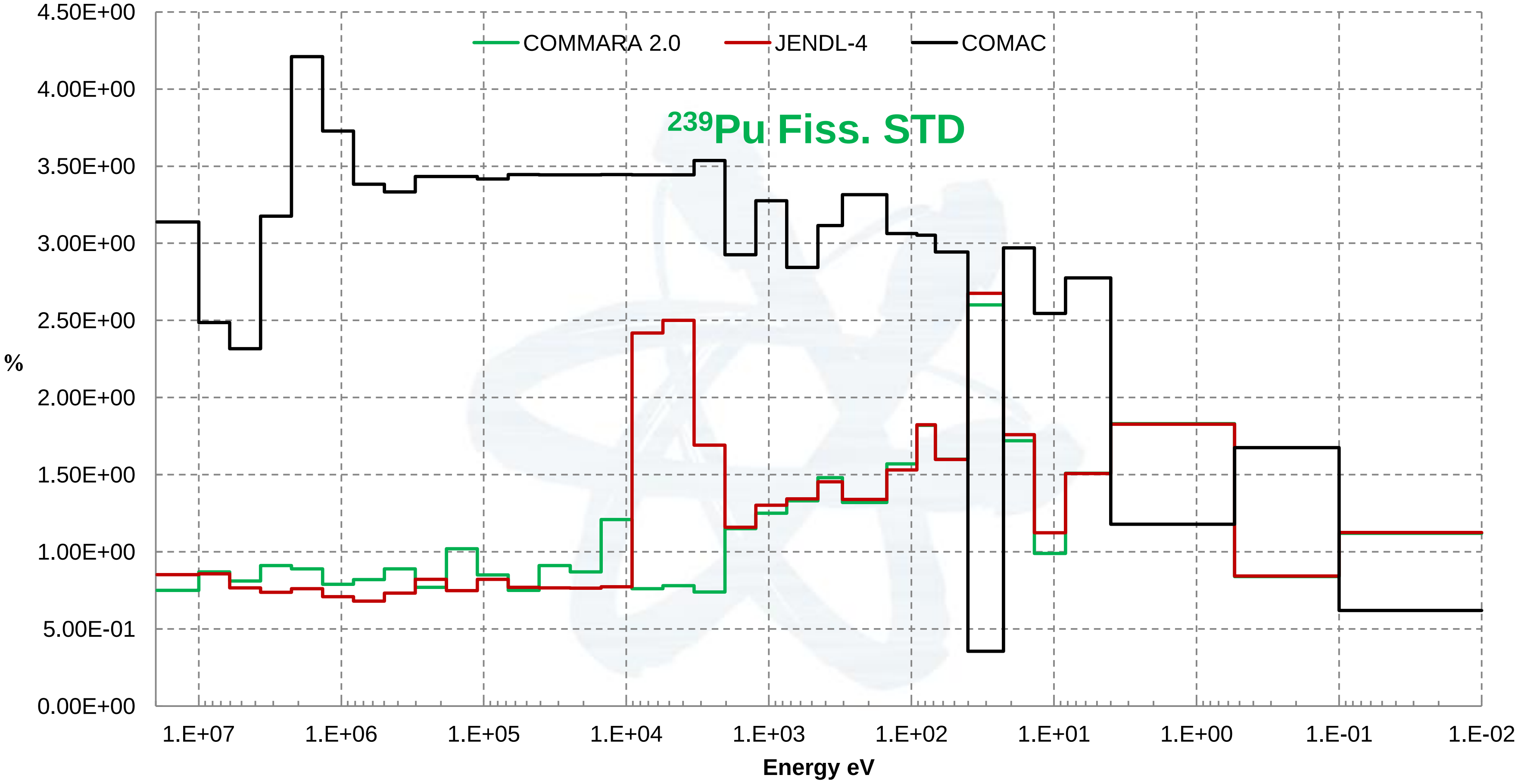
Avoiding Compensations



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Covariance Matrix Validation

If the adjustment assessment has established that: experiments (with reliable experimental uncertainties and correlations) are useful, consistent and complementary, and sources of compensation have been identified and fixed, then we can identify problems with the covariance matrix:

- Presence of large (more than three sigmas) "a priori" individual χ^i for specific experiments.
- An a posteriori χ'^2 significantly larger than one.
- Presence of negative (unphysical) cross section after adjustment.
- Adjustments of cross sections resulting in variations larger than one initial standard deviation.

Covariance Matrix Validation

- Observation of large difference among well-established covariance matrices (e. g. previously shown for the ^{239}Pu fission). This is the most complicated case, as it can generate harmful compensations.
- One particular difficult case is to assess if the standard deviation is too large. Likely, some insight can be gained by looking at the $\Delta\chi'^{i\,2}_{\sigma}$ after adjustment.
- The converse case of determining if the standard deviation is too low could be identified by using an elemental experiment focused on the considered cross section and looking if after adjustment a variation larger than more than one initial standard deviation has been observed

Use of “A Posteriori” Covariance Matrix

- Most of the “a priori” covariance matrix validation criteria turn around standard deviations. The same can be said for the use of the “a posteriori” covariance matrix. Solid conclusions can be made on the standard deviations, but very little can be assumed for the correlations.
- The first consequence of the adjustment is that the “a posteriori” correlation matrix is full. Are the new correlations useful and have they a physical meaning?

  Yes they are useful, and, possibly, they are physical.
- The new created correlations are not too large in magnitude but sufficient to have a significant impact in reducing the “a posteriori’ uncertainty
- The current opinion among experts is that the sensitivity coefficients detect and establish these correlations and, therefore, there is, likely, a physical meaning associated to them.

ABR Ox. K_{eff} Uncertainty (pcm)

COMMARA 2.0

Isotope	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}	χ	P_1^{el}	Total
U238	278	29	112	105	547	0	0	633
PU239	308	223	71	30	79	161	0	428
FE56	170	0	0	172	147	0	44	287
PU240	61	45	82	5	17	24	0	116
NA23	4	0	0	20	80	0	69	107
CR52	21	0	0	38	18	0	0	47
O16	5	0	0	45	2	0	0	46
PU241	10	7	3	0	2	0	0	13
Total	453	229	156	213	578	163	82	834

ADJUSTED No New Correl.

Isotope	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}	χ	P_1^{el}	Total
U238	128	29	91	23	62	0	0	173
PU239	71	149	70	16	37	93	0	206
FE56	141	0	0	138	97	0	44	224
PU240	19	32	62	4	16	23	0	78
NA23	4	0	0	19	59	0	59	86
CR52	21	0	0	38	18	0	0	46
O16	5	0	0	40	2	0	0	41
PU241	2	7	4	0	2	0	0	8
Total	205	156	130	153	136	96	74	374

ADJUSTED Full Correl.

Isotope	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}	χ	P_1^{el}	Total
U238	-56	-12	-17	-20	-43	0	0	-76
PU239	37	43	17	4	7	-30	0	52
FE56	92	0	0	100	41	0	33	146
PU240	11	14	23	3	11	11	0	33
NA23	5	0	0	-9	-12	0	-34	-37
CR52	7	0	0	15	-11	0	0	12
O16	5	0	0	49	2	0	0	49
PU241	-1	6	4	0	2	0	0	7
Total	84	44	22	111	-15	-28	-10	143

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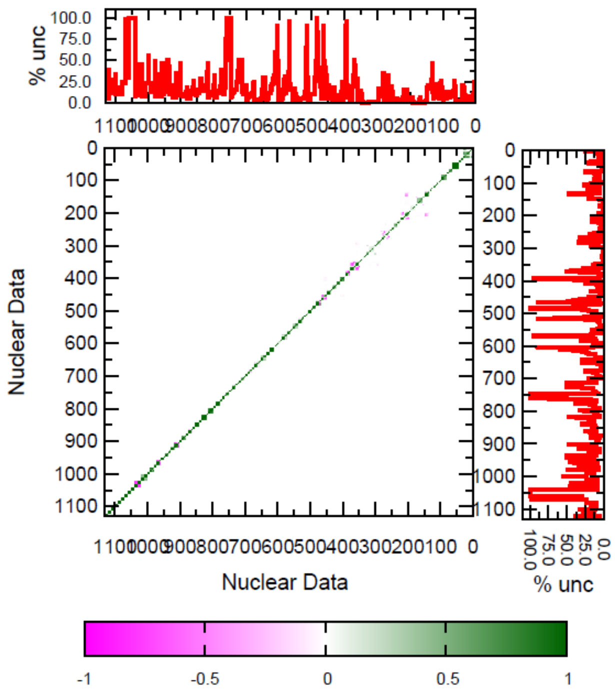
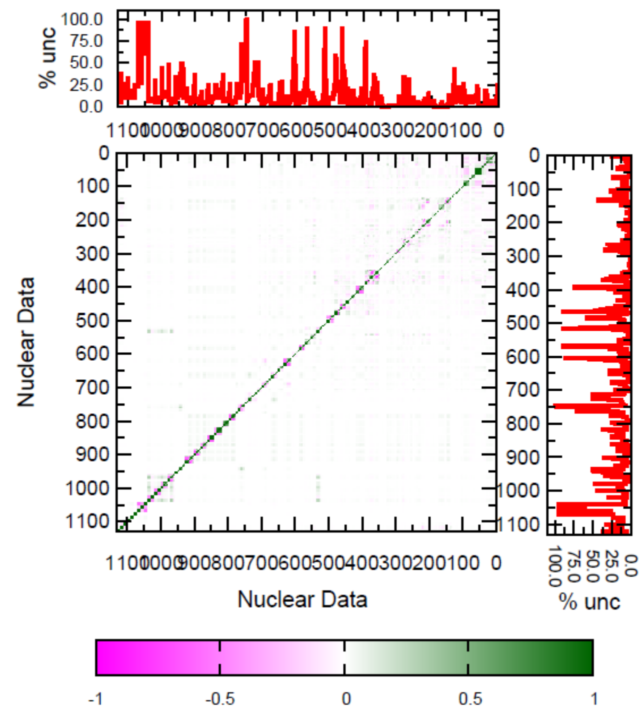
Correlations: ENDF/B-VII.0 Adjustment (87 Experiments)

Nuclear Data Correlation Before Adjustment



Nuclear Data Correlation After Adjustment



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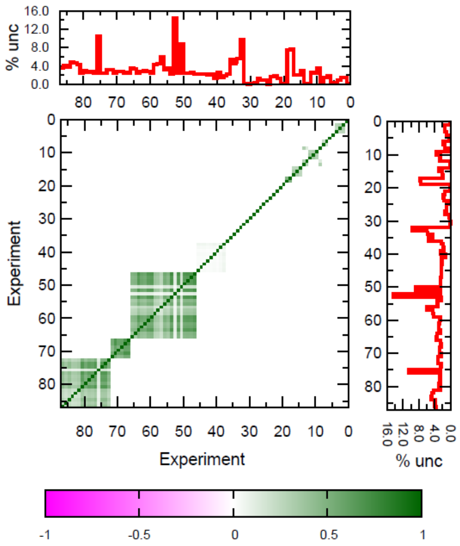
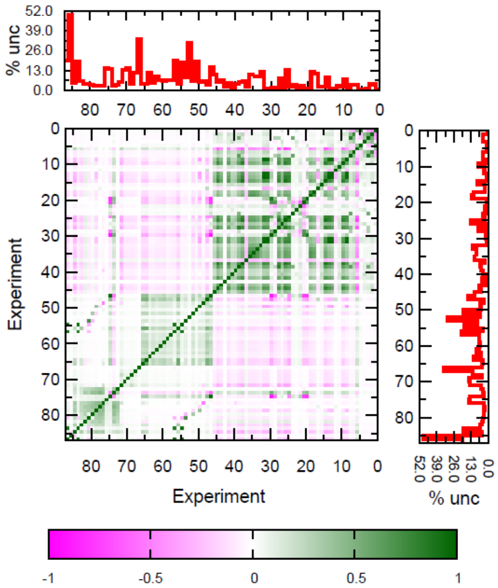
Correlations: ENDF/B-VII.0 Adjustment (87 Experiments)

EXP. CORR. BASED ON INITIAL DATA (MEAS. + CALC.)

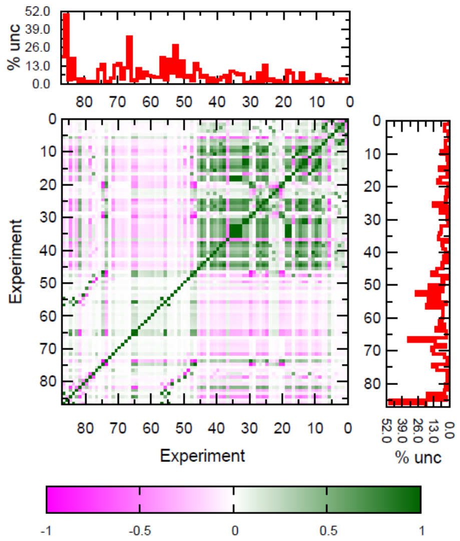


EXP. CORR. BASED ON G MATRIX COVAR.

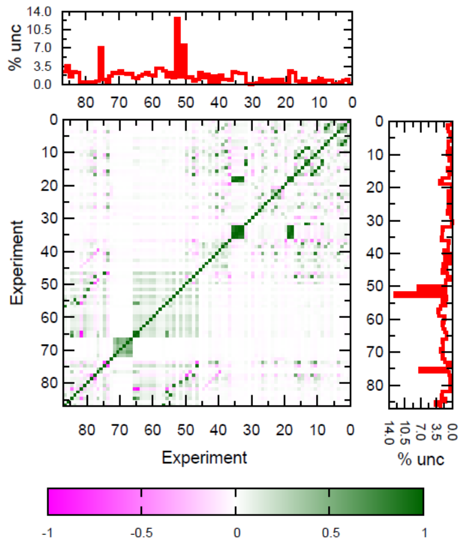


Correlations: ENDF/B-VII.0 Adjustment (87 Experiments)

EXP. CORR. BASED ON INITIAL NUCL. DATA COVAR.

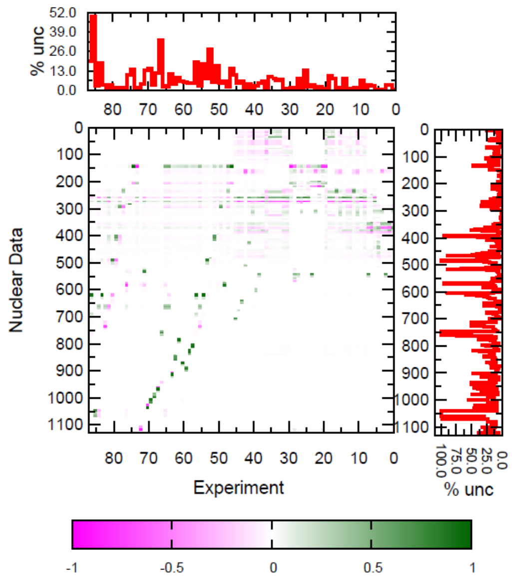


EXP. CORR. BASED ON ADJUST. NUCL. DATA COVAR.

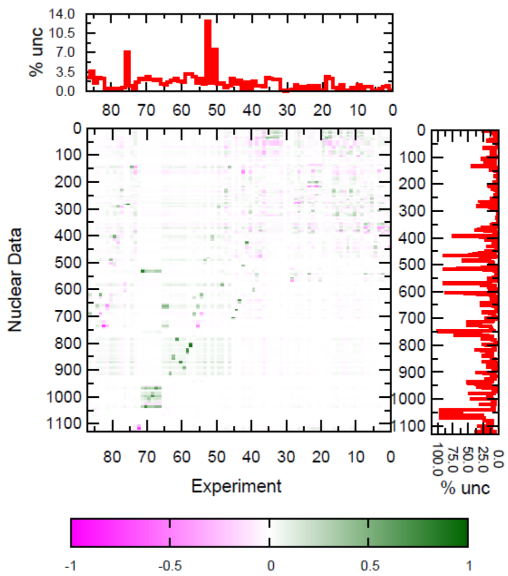


Correlations: ENDF/B-VII.0 Adjustment (87 Experiments)

EXPERIMENTS AND NUCL. DATA CORREL. BEFORE



EXPERIMENTS AND NUCL. DATA CORREL. AFTER



Problems with negative eigenvalues in covariance matrix

- If covariance matrix has zero and/or negative eigenvalues (mostly due to truncations) there are problems:
  - Difficulty in inverting matrices (both original and adjustment one)
  - Many multiplications leads to unphysical values (imaginary values of cross section standard deviations)
- Problem found in big adjustment where 75 zero or negative eigenvalues found (1126 cross sections):
  - Impossible to invert the initial covariance matrix
  - Imaginary values for standard deviations of 7 cross sections (elastic and inelastic ^{235}U)
- Possible remedies:
  - Multiply by a factor all correlations. We had to use 0.8 factor that affects significantly results.
  - Recalculate matrix by replacing with positive eigenvalues:

    $B=VT'V^{-1}$. Slight impact on results.
  - Under study: identification of data responsible for negative values through kernel of eigenvalues, then apply factor only to identified cross sections.

Conclusions

- The role of cross section adjustment has entered a new phase, where the mission is to provide useful feedback not only to designers but directly to evaluators in order to produced improved nuclear data files that will account in a rigorous manner of all experimental information available, both differential and integral.
- Criteria have been established for assessing the robustness and reliability of the adjustment:
  - evaluation of consistency, completeness, usefulness, and complementarity of the set of experiments selected for the adjustment
  - criteria provide information on the reliability of the experimental uncertainties, the correlation among experiments and hints on possible yet undetected systematic errors
  - criteria for accepting the “a posteriori” cross sections
  - identifications and elimination of possible compensation effects coming from missing experiments, isotopes, reactions, and unreliability of the covariance matrix

Conclusions

- **Once the adjustment is deemed to be dependable, many conclusions can be drawn on the reliability of the adopted covariance matrix and feedback, therefore, can be provided mostly on standard deviations and, at a somewhat more limited extent, on the "a priori" correlation values among nuclear data.**
- **Some indications of the use of the "a posteriori" covariance matrix have been provided, even though more investigation is needed to settle this complex subject.**

33 energy group structure (eV).

Group	Upper Energy	Group	Upper Energy	Group	Upper Energy
1	1.96×10^{7}	12	6.74×10^{4}	23	3.04×10^{2}
2	1.00×10^{7}	13	4.09×10^{4}	24	1.49×10^{2}
3	6.07×10^{6}	14	2.48×10^{4}	25	9.17×10^{1}
4	3.68×10^{6}	15	1.50×10^{4}	26	6.79×10^{1}
5	2.23×10^{6}	16	9.12×10^{3}	27	4.02×10^{1}
6	1.35×10^{6}	17	5.53×10^{3}	28	2.26×10^{1}
7	8.21×10^{5}	18	3.35×10^{3}	29	1.37×10^{1}
8	4.98×10^{5}	19	2.03×10^{3}	30	8.32×10^{0}
9	3.02×10^{5}	20	1.23×10^{3}	31	4.00×10^{0}
10	1.83×10^{5}	21	7.49×10^{2}	32	5.40×10^{-1}
11	1.11×10^{5}	22	4.54×10^{2}	33	1.00×10^{-1}