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Comments on the status of modern covariance data based on different fission and fusion reactor studies

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Abstract. Both the availability and the quality of covariance data improved over the last years and many recent cross section evaluations, such as JENDL-4.0, ENDF/B-VII.1, JEFF-3.3T3 etc. include new covariance data compilations. However, several gaps and inconsistencies still persist. Although most modern nuclear data evaluations are based on similar (or even same) sets of experimental data, and the agreement in the results obtained using different cross sections is reasonably good, larger discrepancies were observed among the corresponding covariance data. This suggests that the differences in the covariance matrix evaluations reflect more the differences in the (mathematical) approaches used and possibly in the interpretations of the experimental data, rather than the different nuclear experimental data used. Furthermore, "tuning" and adjustments are often used in the process of nuclear data evaluations. In principle, if adjustments or "tunings" are used in the evaluation of cross-section then the covariance matrices should reflect the cross-correlations introduced in this process. However, the presently available cross-section covariance matrices include practically no cross-material correlation terms, although some evidence indicate that tuning is present. Experience in using covariance matrices of different origin (such as JEFF, JENDL, ENDF, TENDL, SCALE, etc.) in sensitivity and uncertainty analysis of vast list of cases ranging from fission to fusion and from criticality, kinetics and shielding to adjustment applications are presented. The status of the available covariance and future needs in the areas including secondary angular and energy distributions is addressed.

PACS. 07.05.Kf Data analysis: algorithms and implementation; data management (for data analysis in nuclear physics, see 29.85.-c) – 02.50.Cw describing text of that key

1 Introduction

The performance of the new cross-section evaluations, if judged by the agreement with the large set of integral experiments, greatly improved over the last decades. Indeed, using the recent nuclear data evaluations, the calculation-to-experiment (C/E) ratios for the large series of critical integral benchmarks are indeed excellent. For example, the comparison presented in [1] reveals that almost 50% of the calculated k_{eff} values (about 900 out of over 2000 critical benchmarks analysed using ENDF/B-VII.1, JENDL-4.0 and JEFF-3.1.1) lie within one standard deviation (1σ) of the experimental plus MCNP statistical uncertainty. However, such good agreement of C/E is difficult to understand from the mathematical (statistical) point of view. Indeed, much larger dispersion of results is to be expected from the statistical point of view taking into account the calculational uncertainties due to nuclear data, unless (1) the later are very small (highly unlikely), or (2) are correlated with the integral results, suggesting some

adjustment or tuning procedure was used in the evaluation process. Manifestly, these "tunings" are not reflected in the cross-section co-variance matrices, which include practically no cross-material correlation terms. The total uncertainty to cover 68% of the 2000 analysed C/E cases is around 1.8σ of the experimental uncertainty, which would correspond to the average 1σ computational uncertainty of only around 500 pcm, i.e. of a similar order of magnitude as the measurement uncertainties and lower than the typically calculated values.

2 SUS3D and XSUN-2017 computer code package

The SUS3D [2] code was developed in the 1990-ies to allow 1-, 2-, and 3-dimensional cross-section sensitivity and uncertainty calculations. In the past few decades the code was applied to waste range of different nuclear applications, including neutron and gamma ray shielding, criticality, and kinetics. The latest version of SUS3D is part of the XSUN-2017 [3] code package.

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An important factor limiting the use of S/U analysis is the availability and the quality of cross-section covariance data. Several tools and nuclear data libraries were developed to facilitate the access and allow the validation of the data. This will be presented in Sect. 3).

2.1 Examples of applications

The SUS3D code was used since early 1990's for very various applications, such as:

- Reactor pressure vessel surveillance dosimetry [2]: uncertainty in predicted dosimeter reaction rates and pressure vessel exposition, determination of realistic safety margins and consequently the reactor lifetime predictions;
- Fission shielding benchmarks [2]. Sensitivity and uncertainty in the measured reaction rates were calculated for the several benchmarks from the SINBAD database, such as the ASPIS Iron, ASPIS Iron88 and VENUS-3 pressure vessel dosimetry benchmark
- Sensitivity/uncertainty pre- and post-analysis of the fusion shielding benchmarks performed at the Frascati Neutron Generator (FNG) at ENEA Frascati (sensitivity/uncertainty of the measured fast/thermal activation rates and the tritium production in FNG-Bulk Shield benchmark, FNG-Streaming, FNG-SiC, FNG-Tungsten [4], FNG HCPB and FNG-HCLL tritium breeding modules [5], [6] and FNG Copper [7] benchmarks);
- Criticality benchmarks (sensitivity to k_{eff} and β_{eff}): many benchmarks from IRPhE and ICESBEP (KRITZ-2 [8], SNEAK-7A & -7B [9], VENUS-2 etc.), MYRRHA reactor [10] etc.;
- Oil well logging: sensitivity and uncertainty of the Carbon-to-Oxygen C/O gamma-ray ratio [11].

3 Types of covariance matrices

Different data formats for cross section covariances are available in the evaluated files according to the type of nuclear data:

- MF=31: covariance of average number of neutrons per fission ($\bar{\nu}$ - MT=452, 455, 456);
- MF=32: Shape and area of individual resonances;
- MF=33: covariance of neutron cross section;
- MF=34: covariance of angular distribution of secondary neutron (SAD). NJOY processing is available for the reaction MT=251/ P_1 only;
- MF=35: covariance of energy distribution of secondary neutron (SED). NJOY processing is available for the reaction MT=18 only;
- MF=30: Covariances obtained from parameter covariances and sensitivities (no NJOY processing available yet);
- MF=40: Covariances for production of radioactive nuclei.

Several nuclear data processing codes and multi-group covariance data libraries are available from the OECD/NEA Data Bank, such as:

- NJOY-99 /-2012 /-2016 (ERRORR, COVR) [12]: processing of files MF=31-35 (COVFILS format);
- PUFF-IV: Code System to Generate Multigroup Covariance Matrices from ENDF/B-VI Uncertainty Files (COVERX Format);
- SUNJOY/ERRORR34 (part of SUS3D package) [2]: SAD covariance (MF=4 & 34) processing code (COVFILS format);
- ANGELO-LAMBDA [13]: utility programs for interpolation and mathematical verification of the matrices (COVERX and BOXER format input data, COVFILS output format);
- Multigroup covariance data libraries: ZZ-VITAMIN-J/COVA, ZZ-SCALE5.1/COVA and ZZ-SCALE6/COVA-44G (44-group cross section covariance matrix library extracted from SCALE6.0 [14]).

3.1 Uncertainties in prompt and delayed Nu-bar ($\bar{\nu}_p/\bar{\nu}_d$) (MF31)

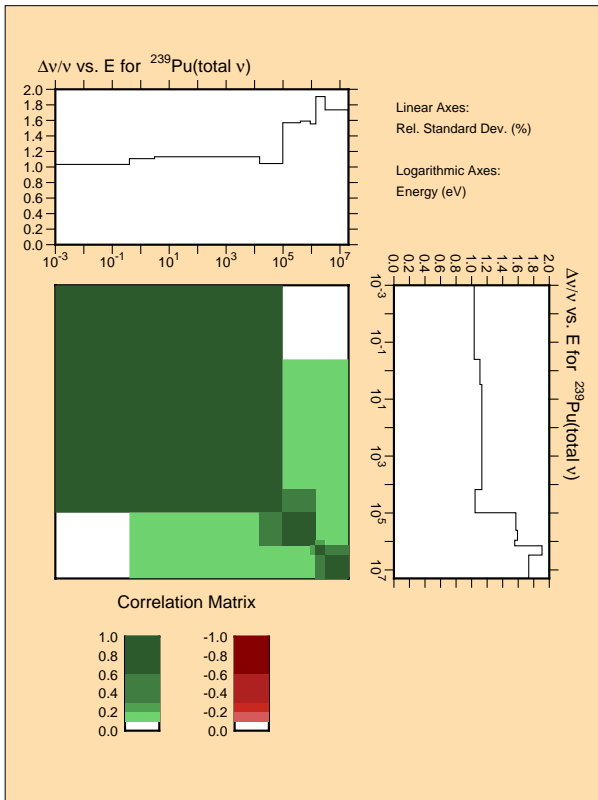
The uncertainties in prompt nu-bar directly influence the uncertainty in k_{eff} and are therefore often among its major contributors. Large differences can be observed among different evaluations, the standard deviations ranging from as low as $\sim 0.1\%$ (most probably unrealistically optimistic) up to $\sim 1\%$. This results in very different uncertainty estimations (see an example in Tab. 1).

Examples of $\bar{\nu}_p$ covariances of ^{239}Pu are shown in Fig 1. The standard deviations passed from $\sim 1\%$ in older SCALE-5.1 and -6.0m libraries to $\sim 0.1\%$ in the recent ENDF/B-VII.1 and JENDL-4.0 evaluations, most probably to accommodate a better C/E agreement for a large series of integral benchmarks, rather than reflecting the uncertainties in differential measurements. Whereas this approach may provide relatively realistic uncertainties in k_{eff} for classes of problems covered by the integral benchmarks, it is likely to lead to biased results of adjustment analysis since preventing any modifications of $\bar{\nu}_p$ and thus freezing the values including the tunings introduced during the evaluations.

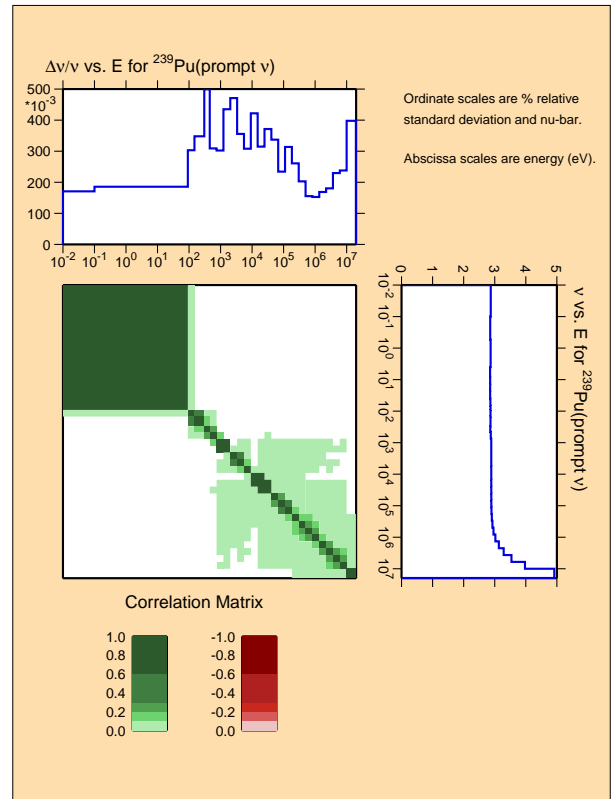
Furthermore, no cross-isotope correlations are included in the available evaluations. Due to their importance for burn-up calculations these correlations were evaluated in [16].

Similarly, the uncertainties in delayed nu-bar were found important for reactor kinetics calculations, such as the uncertainties in effective delayed neutron fraction - β_{eff} . Only JENDL-4.0 [17] evaluation includes the corresponding covariance matrices (see Fig 1), therefore most β_{eff} S/U analyses were based on these data [9]. However, here again no correlations are proposed between delayed nu-bar values of different isotopes even if it is evident that such correlations exist because of the use of similar measurement techniques and theoretical computational model. Missing correlation in evaluated files are likely to result in misleading uncertainty calculations.

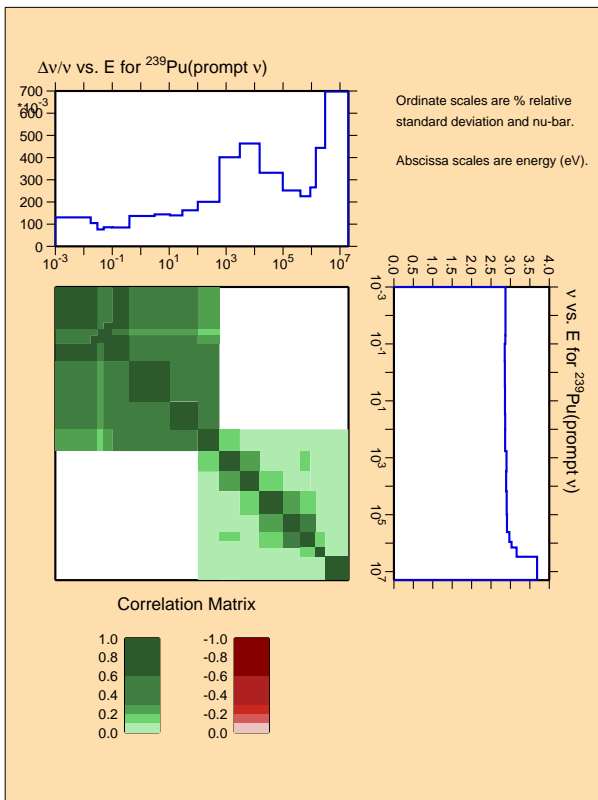
SCALE-6.0m



ENDF/B-VII.1



JENDL-4.0 ν_{prompt}



JENDL-4.0 ν_{delayed}

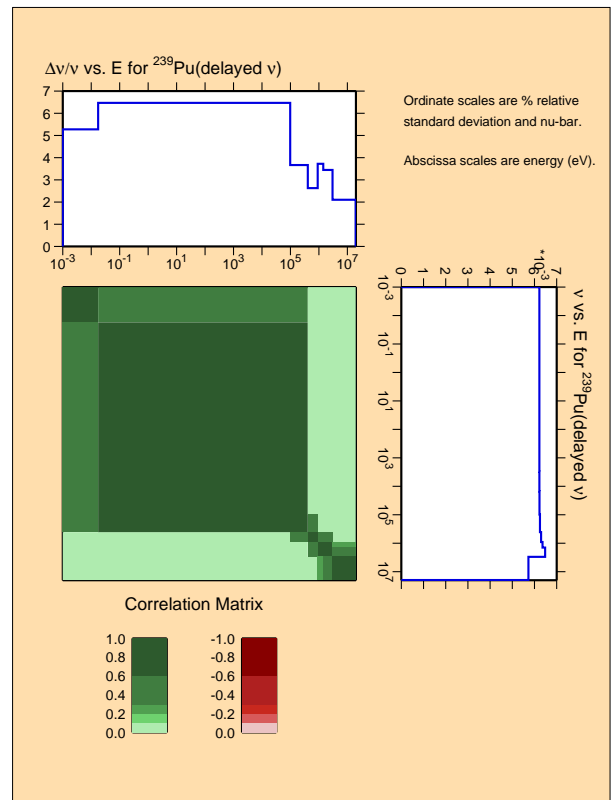
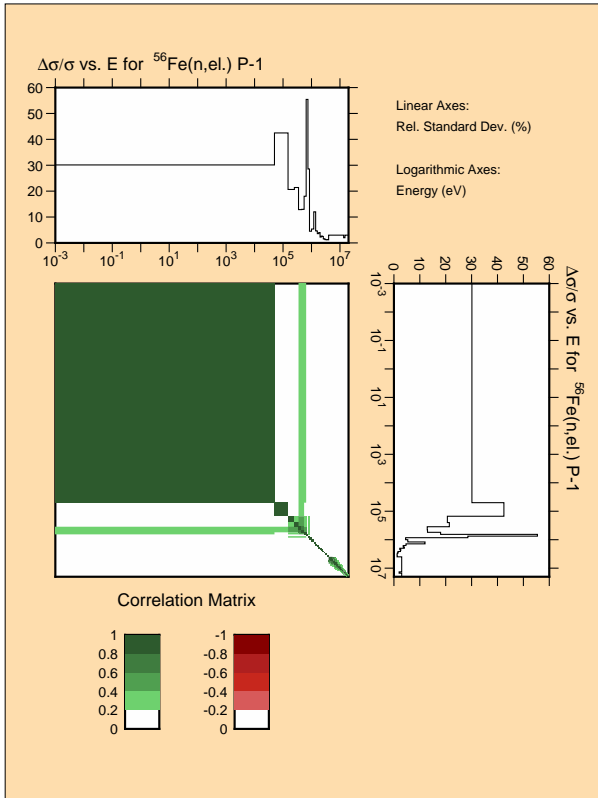
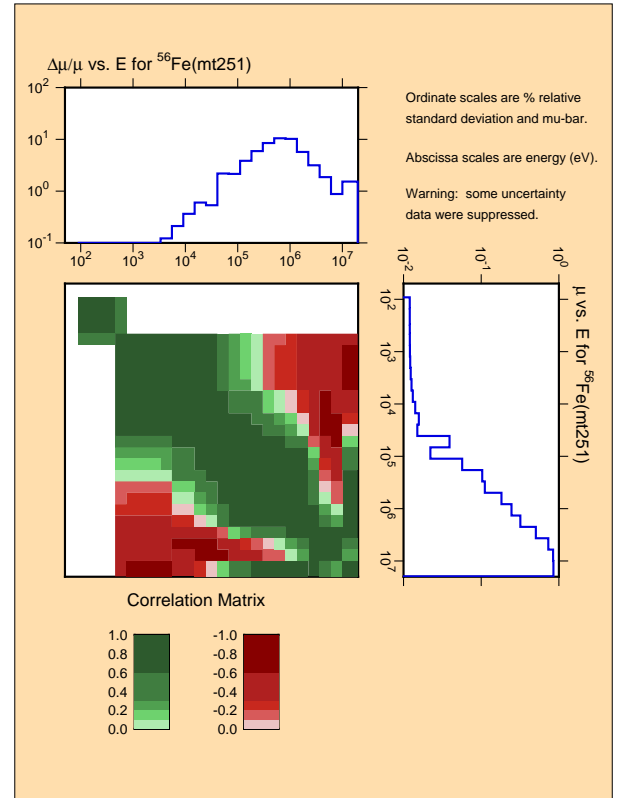


Fig. 1. Covariance matrices of ^{239}Pu for $\bar{\nu}$ from the SCALE-6.0m, ENDF/B-VII.1 and JENDL-4.0 evaluations.

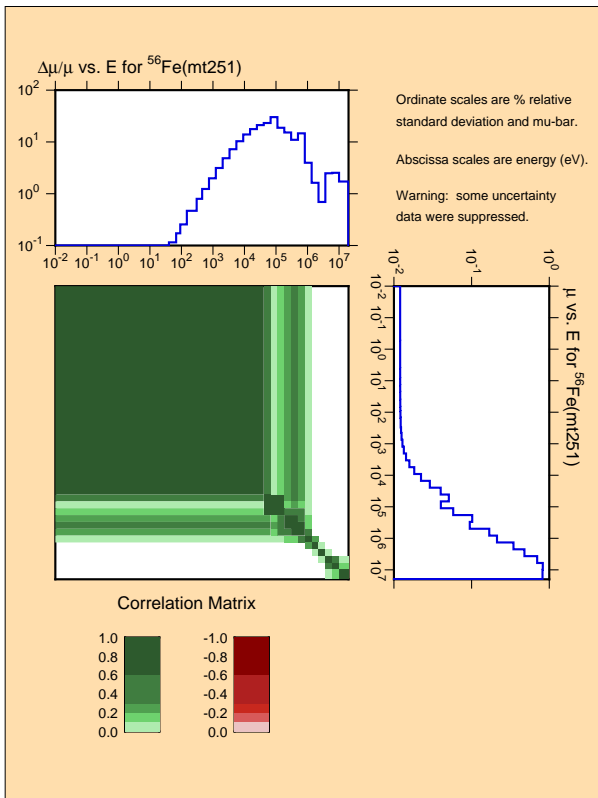
EFF-2.4



JENDL-4.0



ENDF/B-VII.1



TENDL-2015

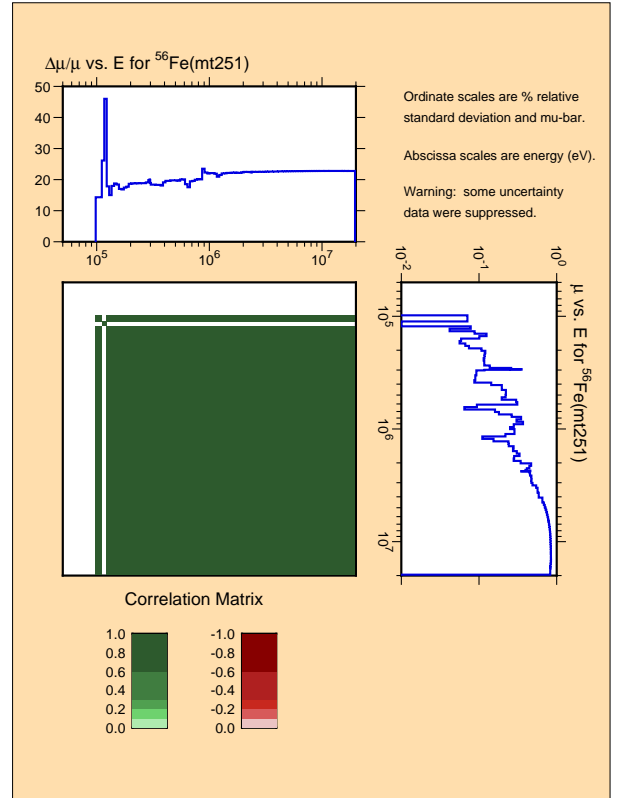


Fig. 2. SAD covariance matrices of ^{56}Fe elastic cross-sections from the EFF-2.4, JENDL-4.0, ENDF/B-VII.1 and TENDL-2015 evaluations.

Table 1. Uncertainties in k_{eff} and β_{eff} calculated using the SUSD3D code. The two values for the β_{eff} uncertainty correspond to the assumption of no / full correlation among the $\bar{\nu}_d$ uncertainties of different actinides.

Benchmark	Covariance evaluation	Uncertainty (%)	
		k_{eff}	β_{eff}
SNEAK-7A	JENDL-4.0	0.61	2.7 / 3.8
	ENDF/B-VII.1	0.77	
	SCALE-6.0m	1.09	
FLATTOP-Pu	JENDL-4.0	0.70	2.6 / 3.3
	ENDF/B-VII.1	0.55	
	SCALE-6.0m	1.20	
JEZEBEL	JENDL-4.0	0.60	2.5 / 2.7
	ENDF/B-VII.1	0.56	
	SCALE-6.0m	1.35	

An attempt to estimate the correlations among the $\bar{\nu}_d$ values of different actinides is described in [18]. The GEF code [19] was used to calculate the variance-covariance of the delayed fission yield data for ^{235}U , ^{238}U and ^{239}Pu actinides as a function of input model parameters and the corresponding uncertainties. Typical values of the correlations coefficients as high as around 0.8 between ^{235}U and ^{239}Pu , and around 0.3 between ^{238}U and ^{239}Pu were observed. It was concluded that this is likely to have considerable impact on the uncertainty propagation calculations, such as those of the effective delayed neutron fraction and the burn-up evolution.

3.2 MF33 covariance matrices

The covariance information of the type MF33 is most widely evaluated and used, also because the processing is in general well established. The main concerns represent the lack of correlations between different isotopes and rather large differences among evaluations in some cases. An example of the use of different copper and iron covariance evaluations is shown in Table 2 and 3, respectively. More details can be found in [7] and [15].

3.3 SAD uncertainties (MF34)

The importance of the uncertainties in the secondary angular distributions (SAD) was demonstrated in several fast neutron applications such as fusion [20], fast reactors etc. and the processing of these data and the S/U methodology is available and tested since decades. In the EFF-2 evaluations in the 1990-ies, the covariance matrices for angular distribution of secondary particles became available for the elastic cross sections for ^{56}Fe , ^{52}Cr , ^{58}Ni and ^{60}Ni [21], [22]. The matrices were prepared in the file MF=34 ENDF/B-6 format in terms of covariances among Legendre coefficients, and energy-dependent correlation was included as well. The evaluations included the terms from P_1 up to P_6 .

In the scope of the European Fusion File (EFF) project in 1995 a procedure was developed to process the SAD covariance matrices into a multi-group form to be used subsequently by the SUSD3D S/U code [23]. The processing code, called ERRORR34, now part of the SUSD3D [2] code package, can process the ENDF/B-6 format files MF=4 and MF=5 (SAD/SED cross-sections), and MF=34 (SAD covariances). Group-collapse strategy similar to the one used in NJOY [12] was adopted, therefore many NJOY-91.91 (ERRORR) subroutines were used. As in the ERRORR module, union groups are first formed as an union of the user's and ENDF/B grids. The SAD partial cross-sections, weighting flux and covariance matrices are defined to produce multi-group values on this grid. The covariance matrices in the user defined energy structure are then calculated from:

$$cov(\sigma_G^l, \sigma_{G'}^{l'}) = \sum_{g, g'} r_{cov}(\sigma_g^l, \sigma_{g'}^{l'}) \frac{\Phi_g \sigma_g^l}{\Phi_G} \frac{\Phi_{g'} \sigma_{g'}^{l'}}{\Phi_{G'}} \quad (1)$$

where:

g refers to the union group, and G to the user defined energy group, σ_G^l represent the l^{th} Legendre polynomial coefficients of the SAD partial cross-sections, in energy group G , $r_{cov}(\sigma_g^l, \sigma_{g'}^{l'})$ is the SAD relative covariance in union group structure, Φ_G is the weighting flux in group G . Finally the relative covariance in the new energy grid is obtained from:

$$r_{cov}(\sigma_G^l, \sigma_{G'}^{l'}) = \frac{cov(\sigma_G^l, \sigma_{G'}^{l'})}{\sigma_G^l \cdot \sigma_{G'}^{l'}} \quad (2)$$

Modifications were subsequently needed also in the SUSD3D code, in order to take into account the full covariance matrix information provided by ERRORR34.

Among the recent nuclear data evaluations, the JENDL-4.0 [17] includes the SAD (MF34) covariances relative to the reaction type MT251 (average scattering cosine) for several important isotopes (Fe, U, Pu, etc.). The recent versions of NJOY (NJOY-99, -2012 and -2016) can also process these data in the multi-group form. Note however that these data (and the NJOY processing) is of course limited to the P_1 Legendre term. MT34/MF251 covariances for few isotopes (^{56}Fe) are likewise included in the ENDF/B-VII.1 [24] evaluation. Even more SAD covariances are available in the TENDL [25] libraries for elastic and some inelastic reactions. The evaluations include also higher than P_1 Legendre terms, however only P_1 can be processed using the recent NJOY (-99 and above) codes. The ERRORR34 code sequence can not be used in these cases since it is based on the older NJOY-91 version and would need to be updated for this purpose.

An example of the EFF-2.4 covariance matrices for ^{56}Fe (processed by the code ERRORR34) is presented in Fig 2), compared to the recent evaluation available in the JENDL-4.0, ENDF/B-VII.1 and TENDL-2015 evaluations and processed using NJOY-99. Note that contrary to the recent evaluations the EFF-2.4 data include the terms P_1 to P_6 .

Table 2. FNG-Cu benchmark: Uncertainty due to transport cross-sections of different origin compared to the C/E values.

Reaction rate & det. position	Uncertainty (%)			C/E
	JEFF-3.2	ENDF/B-VI.8	TENDL-2013	FENDL3 / JEFF3.2
$^{58}\text{Ni}(n, p)$ -35cm	5.2	13.7	22.9	1,03 / 0,98
-57cm	9.9	27.2	41.9	1,03 / 0,91
$^{115}\text{In}(n, n)$ -35cm	5.1	9.4	12.1	0,78 / 0,68
-57cm	8.9	18.7	23.5	0,69 / 0,54
$^{27}\text{Al}(n, \alpha)$ -57cm	13.1	33.2	51.9	0,88 / 0,77
$^{93}\text{Nb}(n, 2n)$ -57cm	13.8	34.7	53.4	0,92 / 0,79
$^{197}\text{Au}(n, \gamma)$ -57cm	Error	19.9	18.6	0,58 / 0,63
$^{186}\text{W}(n, \gamma)$ -57cm	Error	28.6	27.3	0,41 / 0,37

Table 3. ASPIS IRON-88 benchmark: computational vs. experimental uncertainties

Reaction & position	ΔC SAD (%)				ΔC Total ENDFB7.1 /JENDL4 /TENDL2015	ΔE (%)	
	EFF-2.4	ENDF/B7.1	JENDL4	TENDL2015			
$^{32}\text{S}(n, p)$	A7	1.3	1.3	2.9	12 / 17	6.5	
	A12	2.2	2.1	6.0	51	21 / 35 / 33	6.5
	A14	2.5	2.3	7.2	60	25 / 43 / 40	8.6
$^{115}\text{In}(n, n')$	A7	0.6	0.6	2.3		11 / 15	4.5
	A11	0.9	1.0	3.2	11	16 / 18 / 20	4.7
$^{103}\text{Rh}(n, n')$	A7		0.3	1.0		8 / 9	5.1
	A14		0.3	1.1		20 / 16 / 26	5.1
$^{27}\text{Al}(n, \alpha)$	A7	3.4	3.4	1.4	37	32 / 31 / (27)	4.7
$^{197}\text{Au}(n, \gamma)$	A7	0.1	0.1	0.3		10 / 9	4.2
	A11	0.1	0.1	0.3		9 / 9	4.2
	A14	0.1	0.1	0.3	1.1	8 / 8 / 4	4.2

An example of the SAD uncertainties for the ASPIS-IRON88 benchmark calculated using the SUS3D code and the above ^{56}Fe covariance matrices is given in Table 3. Considerable spread of results can be observed, however all suggesting that SAD uncertainties cannot be neglected for high-energy reactions.

3.4 SED uncertainties (MF35)

Uncertainties in the Secondary Energy Distributions are at present only available for the prompt neutron fission spectra (PFNS) and relatively complete data are included in recent evaluations such as JENDL-4.0, ENDF/B-VII.1 and JEFF-3.3. However, the correlations among the covariances for different incident neutron energies are missing. The conservative assumption of total correlation is in this conditions probably the most appropriate.

Several sensitivity methods were studied in the scope of the WPEC-26, concluding with recommending the constrained sensitivity method [26].

However, covariance information for other reactions is still missing. A simple method for evaluating covariances for delayed fission spectra, which are important for the calculation of β_{eff} uncertainty, was proposed in [9]. An approximate "two-block" covariance matrices were constructed based on a simple common sense assumption of

an energy-uniform standard deviation of 15% and a complete anti-correlation between the energies above and below the mean delayed neutron energy for each of the 6 delayed groups. Conservative assumption of the complete correlation between the 6 individual groups was adopted.

To test the validity of this method a similar procedure, except assuming a uniform 4% standard deviation instead of 15%, was applied to the prompt fission neutron spectra (PFNS), where comparison with detailed covariance matrices available in some nuclear data evaluation (JENDL-4.0, SCALE-6, etc.) was possible. Table 4 compares the uncertainties in k_{eff} and β_{eff} calculated using the above "two-block" PFNS covariances with those based on the PFNS covariances from JENDL-4.0 and SCALE-6.0. In spite of its simplicity the procedure is shown to predict similar uncertainties, both for k_{eff} and β_{eff} uncertainties, as the more sophisticated methods used in the JENDL-4.0 and SCALE-6.0 covariance data evaluations. This good agreement can be explained by the relatively narrow-energy sensitivity of the k_{eff} and β_{eff} to the fission spectra.

A similar procedure could be temporary applied to evaluate the SED uncertainties for other reactions such as (in)elastic scattering, until more sophisticated evaluations become available.

Benchmark	Isotope	k_{eff} uncertainty (pcm)			β_{eff} uncertainty (pcm)		
		Two-block	JENDL-4.0	SCALE-6.0	Two-block	JENDL-4.0	SCALE-6.0
SNEAK 7A	^{235}U	22	27	20	53	50	36
	^{238}U	71	99	78	49	25	17
	^{239}Pu	261	288	264	572	523	414
	Total	271	305	276	577	526	416
SNEAK 7B	^{235}U	41	49	37	78	71	51
	^{238}U	109	150	119	36	46	18
	^{239}Pu	335	377	343	551	489	377
	Total	354	409	364	557	496	381
Jezebel	^{239}Pu	292	367	343	637	820	774
Skidoo Jez-23	^{233}U	106	121	97	212	106	91
Popsy Flat-Pu	^{235}U	6	8	6	28	30	22
	^{238}U	47	68	54	105	94	79
	^{239}Pu	302	371	348	100	172	45
	Total	306	377	352	147	199	93
Topsy Flat-25	^{235}U	220	290	229	195	374	289
	^{238}U	44	64	50	47	92	70
	Total	224	279	234	201	385	297
Flattop 23	^{233}U	167	180	156	218	304	227
	^{235}U	5	7	5	16	17	13
	^{238}U	41	58	46	53	45	36
	Total	171	189	163	225	308	231
Big-ten	^{235}U	456	575	441	43	200	132
	^{238}U	189	273	217	218	400	307
	Total	493	637	491	218	448	334
ZPPR-9	^{235}U	6	7	5	14	13	9
	^{238}U	76	103	81	45	16	11
	^{239}Pu	331	371	332	706	639	520
	Total	340	385	342	708	639	521

Table 4. Fission spectra uncertainties in k_{eff} and β_{eff} calculated using the approximate "two-block" prompt fission spectra covariances (i.e. assuming flat anti-correlated 4% standard deviation) compared to those based on covariances from JENDL-4.0 and SCALE-6.0.

4 Conclusions

The availability of the covariance data improved over the last decades. Experience in using covariance matrices of different origin (such as JEFF, JENDL, ENDF, TENDL, SCALE, etc.) any types (MF31, MF33, MF34 and MF35) in sensitivity and uncertainty analysis of vast list of cases ranging from fission to fusion and from criticality, kinetics and shielding to adjustment applications is presented. The status of the available covariance and future needs in the areas including secondary angular and energy distributions is addressed. Of particular concern is the lack of correlation among different isotopes and reactions, the differences among the recent covariance matrices although the cross section evaluations are mostly based on similar experimental data, and the lack of covariance information for some more specific reactions and reaction types (such as for example SAD/SED).

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