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**Few group collapsing of covariance matrix data based on
a conservation principle**

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A new algorithm for a rigorous collapsing of covariance data is proposed, derived, implemented, and tested. The method is based on a conservation principle that allows preserving at a broad energy group structure the uncertainty calculated in a fine group energy structure for a specific integral parameter, using as weights the associated sensitivity coefficients.

I. Introduction

The standard procedure to derive few group covariance data to be used in applications is based on the use of a flat or standard flux weighting function. This procedure does not insure “a priori” that the uncertainty on any integral parameter obtained using different group structures stays constant, and in particular equal to the ideal reference case evaluated at the finest (continuous) energy structure. As for the classical case of cross section weighting, it has been proposed to use a collapsing algorithm, based on a conservation principle. This paper presents results of the use of the new algorithm and the comparison with results obtained with the standard collapsing procedure. The investigated parameters are the multiplication factors in different fast neutron systems with different fuels and coolants and some reactivity coefficients. The possibility to use only one set of collapsed covariance data to calculate uncertainties on integral parameters in different systems has also been explored.

The results also give some hints on the possible impact of the few group energy structures on the energy correlation effects.

II. Theoretical Background

The uncertainty on an integral parameter R_k is given by:

$$\Delta R_k^2 = S_{k,I} D_I S_{k,I}^+$$

D_I is defined as:

$$D_I = \left(d_{i,I}^k \right)_{i \in I},$$

where I corresponds to the number of fine group grids, and the sensitivity vectors $S_{k,I}$ have I components $S_{k,i}$ ($i=1, \dots, I$).

One can define a broad group grid ($j=1, \dots, J$, $J \ll I$) such that the fine group uncertainty is conserved:

$$S_{k,J} D_J^k S_{k,J}^+ \equiv \Delta R_k^2$$

That implies that:

$$S_{k,J} D_J^k S_{k,J}^+ = S_{k,I} D_I S_{k,I}^+$$

One can write for each element $d_{j,j}^k$ of the matrix D_J^k :

$$d_{j,j}^k = \frac{\sum_{i \in j} S_{k,i} \sum_{i' \in j'} d_{i,i'}^k S_{k,i'}^+}{S_{k,j} S_{k,j}^+} \quad (1)$$

where $S_{k,j} = \sum_{i \in j} S_{k,i}$ and $S_{k,j}^+ = \sum_{i \in j} S_{k,i}^+$. The

broad group matrix element $d_{j,j}^k$ in equation (1) corresponds to the value obtained by dividing the weighted sum of fine-group matrix element by the sum of exact weights (i.e., $S_{k,i}$). Thus, $d_{j,j}^k$ is the equivalent representation of fine group matrix elements within broad group grids j and j' .

D_J^k is the appropriate broad group covariance matrix, since its use allows the conservation of the uncertainty on the parameter k calculated at the fine (reference grid) level. We will call this method “ConsUnce”.

In principle, for each integral parameter p one should calculate the corresponding “broad” group covariance matrix D_J^p , according to the previous algorithm. However if the k parameter is the criticality coefficient k_{eff} , the D_J^k broad group covariance matrix can be also used to calculate the uncertainty of any reactivity coefficient, with a very modest approximation. In fact, the reactivity coefficient sensitivities that enter into the broad group covariance matrix definition given above are obtained via the Equivalent Generalized Perturbation Theory (EGPT) method [1] as differences of k_{eff} related quantities. In practice, the

uncertainty on a reactivity coefficient RC is given by:

$$\begin{aligned}\Delta R_{RC}^2 &= S_{RC,J} D_J^{RC} S_{RC,J}^+ \\ &\cong S_{k,J} D_J^k S_{k,J}^+ - S_{kp,J} D_J^{kp} S_{kp,J}^+ \cong S_{k,J} D_J^k S_{k,J}^+ - S_{kp,J} D_J^{kp} S_{kp,J}^+\end{aligned}$$

i.e., the following approximation is made:

$$D_J^k \cong D_J^{kp}$$

The approximation that has been made implies the similarity of the vectors $S_{k,i}$ and $S_{kp,i}$ which should be used for the weighting procedure and which have (e.g., in the case of a capture cross section) respectively the following components:

$S_{k,i} = \Phi_i \Phi_i^+$ where Φ_i and Φ_i^+ are calculated in the reference case (e.g., flooded, at reference temperature T, etc) and:

$S_{kp,i} = \Phi_i^P \Phi_i^{+P}$ where Φ_i^P and Φ_i^{+P} are calculated in the system ‘‘P’’ (e.g., in the core at higher temperature $T' > T$ in the case of the Doppler reactivity coefficient, or in the voided configuration in the case of the coolant void reactivity coefficient, etc).

Despite the obvious differences among the different systems (i.e., among the different real and adjoint flux distributions in energy), it will be explored if, for the purpose of the collapsing algorithm, it is possible to demonstrate that the sensitivity coefficients of the reference reactivity case are representative of the sensitivity coefficients of most ‘‘P’’ systems.

III. Application to fast reactor k_{eff}

A reference 230 energy group structure [2] has been adopted to serve as reference. Real and adjoint neutron fluxes have been calculated in this energy group structure for the Advanced Burner Reactor (ABR) fast reactor system, as defined in [3]. These fluxes have been used to calculate the perturbation sensitivity coefficients at the fine group level.

The following covariance matrices, based on JENDL 3.3 data files, were produced:

- ‘‘fine’’ energy group structure (230 groups, reference)
- 33-group structure, both with flat flux weighting function collapsing and with ConsUnce;
- 15-group structure, as for b);

for the following isotopes: U-235; U-238; Pu-239; Fe-56; Na-23.

These matrices have been used to calculate the uncertainty on the k_{eff} of different fast reactor systems previously investigated in Reference 4. The calculations performed allow evaluating the k_{eff} uncertainty values due to the uncertainty of the different cross sections of each isotope taken separately and also the global effect (see TABLES I and II).

For all the fast reactor systems that have been considered, the agreement on the total effect on the k_{eff} using the different collapsed matrices (i.e., with different number of energy groups and different collapsing algorithms) is relatively good, and discrepancies are between 0 and 10% (except for 24% discrepancies in ADMAB (Accelerator Driven Minor Actinide Burner) using the 15-group covariance matrix collapsed with flat flux weighting). This is a preliminary indication of the possibility to use only one set of collapsed covariance matrices for the different isotopes of interest, and to apply them to a wide range of systems, even if they have, for example, different core neutron spectra. Also, the use of few energy groups (e.g., 15) does not introduce large errors on the calculated uncertainty of the integral parameter (here the k_{eff}).

However, the investigation of the individual cross section uncertainty effects indicates that specific effects can be badly reproduced at few energy groups, if the flat flux weighting method is used. This is the case, for example, of the inelastic scattering cross section uncertainty effects for most isotopes. Since, in practically all systems considered, the inelastic scattering effects are not predominant, the global effect (i.e., the one that includes all cross sections of all isotopes) is not affected too severely.

However, this cannot always be the case, and it seems worthwhile to consider the more rigorous ConsUnce method to avoid unexpected effects. Moreover, the use of erroneous collapsed matrices for particular reactions and isotopes can have an impact in a statistical adjustment procedure [4].

The energy breakdown of the uncertainty values on k_{eff} allows pointing out the energy domains where the discrepancies are more significant (see TABLE III). Apart from the expected discrepancies in the inelastic cross sections, some discrepancies are found also, e.g., in the capture cross section of U-238 at relatively high energy.

Finally, it should be noted that to obtain the results relative to the ConsUnce method, the uncertainty values calculated at few groups as:

$$S_{k,J} D_J^k S_{k,J}^+ \quad (2)$$

did use as $S_{k,j}$ sensitivity coefficients those obtained from the fine energy sensitivity coefficients as:

$$S_{k,j} = \sum_{i \in j} S_{k,i} \quad \text{and} \quad S_{k,j}^+ = \sum_{i \in j} S_{k,i}^+$$

This is an approximation, since, for consistency, one should use the sensitivity coefficients directly calculated in the collapsed energy group structure. To test this approximation, the appropriate sensitivity coefficients have been used in the

equation (2), and the results are given in TABLE IV. These tables show that the use of the “collapsed” sensitivity coefficient or of the one calculated explicitly in the collapsed energy group structure, produce substantially the same results.

TABLE I. k_{eff} uncertainties [pcm] for Advanced Burner Reactors (ABRs) (Metal and Oxide cores) and Accelerator Driven Minor Actinide Burner (ADMAB) calculated with 230-group covariance matrices and matrices collapsed by, C33: ConsUnce 33-group ; C15: ConsUnce 15 group; F33 : flat flux weighting 33-group ; and F15 : flat flux weighting 15-group

Reactor Matrix Type	ABR Metal					ABR Oxide					ADMAB				
	230g	C33	F33	C15	F15	230g	C33	F33	C15	F15	230g	C33	F33	C15	F15
Total	744	744	739	744	709	882	875	872	872	834	796	748	738	746	604
U-238	457	457	458	457	452	441	442	442	440	437	0	0	0	0	0
σ_f	27.6	27.6	27.6	27.6	28.0	21.4	21.3	21.3	21.3	21.6	0	0	0	0	0
σ_{cap}	315	315	318	315	315	343	343	344	340	339	0	0	0	0	0
$\sigma_{elastic}$	37.3	37.3	37.6	37.3	37.6	23.7	23.5	23.5	23.2	23.3	0	0	0	0	0
σ_{inel}	317	317	315	317	309	269	270	269	270	265	0	0	0	0	0
ν_f	82.4	82.4	83.2	82.4	84.4	64.0	63.9	64.5	64.0	65.8	0	0	0	0	0
Pu-239	501	501	498	501	493	674	670	671	670	658	356	351	353	359	353
σ_f	472	472	468	472	462	647	643	643	644	630	344	339	341	347	340
σ_{cap}	118	118	120	118	116	137	137	140	136	136	56.0	55.0	56.4	55.4	55.2
σ_{el}	6.80	6.80	6.80	6.80	7.01	3.06	3.14	3.12	3.13	3.15	1.20	1.22	1.20	1.20	1.21
σ_{inel}	40.2	40.2	48.1	40.2	60.3	33.9	34.0	41.2	35.0	54.7	27.5	28.2	30.8	29.1	38.8
ν_f	113	113	112	113	112	124	124	123	123	122	65.7	65.8	65.5	65.8	65.1
Fe-56	306	306	296	306	234	356	347	336	341	266	712	660	648	654	491
σ_{cap}	94.8	94.8	95.1	94.8	97.5	158	156	158	155	156	72.1	71.9	72.2	71.9	73.8
σ_{el}	63.0	63.0	61.5	63.3	58.1	37.3	36.3	33.2	35.2	31.8	16.9	16.6	13.9	11.9	10.7
σ_{inel}	284	284	274	284	204	317	308	294	301	212	708	656	643	650	485

TABLE II. k_{eff} uncertainties [pcm] for Gas-cooled fast reactor (GFR), Lead-cooled Fast Reactor (LFR), and Sodium-cooled Fast Reactor (SFR) calculated with 230-group covariance matrices and matrices collapsed by, C33: ConsUnce 33-group ; C15: ConsUnce 15 group; F33 : flat flux weighting 33-group ; and F15 : flat flux weighting 15-group

Reactor Matrix Type	GFR					LFR					SFR				
	230g	C33	F33	C15	F15	230g	C33	F33	C15	F15	230g	C33	F33	C15	F15
Total	885	872	882	887	876	542	546	544	548	529	480	474	461	462	430
U-238	632	632	630	630	623	308	310	311	309	306	71.9	72.4	73.6	72.3	72.4
σ_f	27.4	27.4	27.4	27.4	27.7	20.0	20.0	20.0	20.0	20.3	6.97	6.96	6.97	6.96	7.05
σ_{cap}	291	293	296	289	290	232	232	235	231	232	57.5	57.5	58.8	57.5	58.0
$\sigma_{elastic}$	21.3	21.2	21.2	20.7	20.6	17.4	17.6	18.0	17.5	17.9	19.7	19.7	20.0	19.7	20.0
σ_{inel}	554	553	548	552	544	192	195	194	195	188	32.1	33.0	33.1	32.9	31.8
ν_f	84.1	84.1	84.9	84.0	86.2	59.0	59.0	59.5	59.1	60.6	20.2	20.2	20.3	20.2	20.6
Pu-239	620	600	618	624	616	403	408	406	412	405	269	268	267	268	264
σ_f	597	578	594	602	590	373	378	376	384	375	245	244	243	245	240
σ_{cap}	115	109	116	114	115	110	109	111	109	108	79.6	79.7	80.9	79.9	79.1
σ_{el}	2.32	2.32	2.42	2.36	2.56	3.93	3.95	3.89	3.97	3.91	12.7	12.8	12.7	12.8	13.1
σ_{inel}	63.2	61.3	74.0	56.6	91.0	26.9	27.2	31.0	28.7	38.7	14.8	14.8	16.7	15.4	22.6
ν_f	104	104	104	103	102	102	102	102	102	101	72.7	72.7	72.3	72.8	71.9
Fe-56	0	0	0	0	0	192	189	185	186	146	363	351	337	334	296
σ_{cap}	0	0	0	0	0	57.8	57.7	57.9	57.8	58.8	92.2	92.2	92.6	92.3	95.7
σ_{el}	0	0	0	0	0	32.5	30.8	31.6	33.8	30.2	241	248	232	229	221
σ_{inel}	0	0	0	0	0	180	178	173	174	130	255	231	226	225	172

IV. Application to reactivity coefficients

As indicated previously, a full application of the ConsUnce method implies the use of the appropriate weighting function for each integral parameter. It was also indicated that the use of the

few group matrices, collapsed using the k_{eff} weighting functions, is expected to be a reasonable approximation for the case of the reactivity coefficients. We have tested this assumption in the case of the Na-void reactivity coefficient.

TABLE V compares the following calculations for the Na-void reactivity coefficient in both ABR-Metal and ABR-Oxide:

- a) Use of the collapsed matrices with flat flux weighting
- b) Use of the ConsUnce derived matrices with the exact weighting functions
- c) Use of the ConsUnce derived matrices with the k_{eff} weighting function

The results show that the methods b) and c) agree very well. As for method a), the agreement with b) is in general good, with the exception of some cases, mostly related to inelastic scattering effects, in a very similar manner as for the k_{eff} cases discussed previously. This effect is also not unexpected, due to similarity of the phenomena involved in the k_{eff} and in the reactivity coefficients.

V. Energy correlation and multigroup features

An investigation of the correlation matrices features at the fine group level, can provide, when compared to the different few group energy structures, some

indications of the potential problems (e.g., loss of information, introduction of artificial correlations etc) when using few group energy structures in uncertainty analysis or, even more important, in statistical nuclear data adjustment procedures.

In order to provide an immediate evaluation of the possible effects previously mentioned, a visual comparison of the different correlations, as well of diagonal standard deviations, has been carried out for the three different energy group structures. Typical results are shown in Figures 1 and 2. In Figure 1 the correlations for the Pu-239 fission cross sections at 230 groups and 15 groups (flat and ConsUnce weighting) are plotted. One can observe that a very consistent agreement exists for both standard deviations and collapsed correlations. In Figure 2 the same plotting is shown for the Fe-56 inelastic cross sections. Notable differences are now present; in particular the standard deviation difference in the last non-zero group of the inelastic, and in the energy range of highest neutron flux values, is responsible for the observed discrepancy between flat and ConsUnce weighting.

TABLE III. The energy breakdown of the k_{eff} uncertainty for selected nuclides in 15-group energy structure calculated using covariance matrices by (A) ConsUnce; and (B) flat flux weighting.

Reactor	ABR-Metal								ADMAB					
	U-238 σ_{cap}		Pu-239 σ_f		Pu-239 σ_{inelas}		Fe-56 σ_{inelas}		Pu-239 σ_f		Pu-239 σ_{inelas}		Fe-56 σ_{inelas}	
	(A)	(B)	(A)	(B)	(A)	(B)	(A)	(B)	(A)	(B)	(A)	(B)	(A)	(B)
1.96E+07	0	0	12.6	12.3	10.6	16.8	12.8	25.9	6.61	6.43	0	0	4.32	12.1
6.07E+06	40.6	30.4	43	42.6	34.5	56.4	101	27.6*	23.2	22.9	22.4	36.3	132	60.0*
2.23E+06	49.2	71.1	48.7	48.8	3.58*	14.0*	197	168	30.1	30.2	12.3	3.7	413	363
1.35E+06	37.5	36.1	98.4	97	7.74	3.99	177	117	59.0	58.2	11.7	10.2	484	327
4.98E+05	53	59.4	126	126	11.6	13.4	0	0	70.1	69.6	5.92	6.56	0	0
1.83E+05	164	159	121	121	10.3	12	0	0	67.5	67.2	4.69	5.34	0	0
6.74E+04	178	175	188	179	6.11	6.76	0	0	127	120	0	0	0	0
2.48E+04	179	180	347	341	3.12*	3.58*	0	0	251	247	0	0	0	0
9.12E+03	2.48	2.55	149	146	0	0	0	0	165	162	0	0	0	0
2.04E+03	5.17	3.82	3.62	3.4	0	0	0	0	2.10	1.97	0	0	0	0
4.54E+02 ^(a)	0.104	0.197	0.426	0.437	0	0	0	0	0.246	0.252	0	0	0	0
Total	315	315	472	462	40.2	60.3	284	204	347	340	29.1	38.8	650	485

^(a) Only values above ~100 eV are shown

*The number is the imaginary value.^{§§}

^{§§} An imaginary value appears in uncertainties of some energy groups because of strong negative correlations among energy groups. For instance, in case of a two-group problem, the k_{eff} variance of each energy group, $\text{Var}(j)$, $j=1,2$, is calculated by: $\text{Var}(1) = s_1^k d_{1,1}^k s_1^k + s_2^k d_{2,1}^k s_1^k$ and $\text{Var}(2) = s_1^k d_{1,2}^k s_2^k + s_2^k d_{2,2}^k s_2^k$. Here, terms $s_2^k d_{2,1}^k s_1^k$ and $s_1^k d_{1,2}^k s_2^k$ can be negative when their correlations, $d_{i,j}^k$'s, are negative, or when signs of two-group sensitivity coefficients are different even if their correlations are positive. If magnitudes of these two negative terms are larger than other terms, then $\text{Var}(j)$ will be negative. This will lead to the imaginary value of the uncertainty after taking the square root of $\text{Var}(j)$.

TABLE IV. k_{eff} uncertainties [pcm] calculated with ConsUnc derived matrices using collapsed sensitivity coefficients and directly calculated sensitivity coefficients in collapsed group structures.

Energy group structure	33-group				15-group			
	ABR-Metal		ABR-Oxide		ABR-Metal		ABR-Oxide	
Type of sensitivity coefs	Collapsed	Direct	Collapsed	Direct	Collapsed	Direct	Collapsed	Direct
Total	744	736	875	867	744	730	872	855
Pu-239	501	495	670	668	501	495	670	668
σ_f	472	465	643	642	472	464	644	640
σ_{cap}	118	119	137	138	118	122	136	139
σ_{elas}	6.80	6.70	3.14	3.29	6.80	6.59	3.13	3.14
σ_{inelas}	40.2	41.4	34.0	34.8	40.2	39.1	35.0	35.0
ν_f	113	113	124	124	113	113	123	123
Fe-56	306	298	347	333	306	281	341	306
σ_{cap}	94.8	95.7	156	158	94.8	97.4	155	159
σ_{elas}	63.0	73.2	36.3	38.0	63.3	68.1	35.2	27.4
σ_{inelas}	284	272	308	291	284	255	301	260

TABLE V. The uncertainty [pcm] in Na-void reactivity using 230-group and 15-group collapsed covariance matrices generated by (a) the flat flux weighting; (b) ConsUnc with the exact weighting function; and (c) ConsUnc with the k_{eff} weighting function.

Reactor	ABR-Metal				ABR-Oxide			
	230 g	(a)	(b)	(c)	230 g	(a)	(b)	(c)
Total	180	170	180	173	83.9	74.8	84.4	82.1
U-238	90.4	84.0	90.4	84.5	43.2	41.4	48.5	42.9
σ_f	2.10	2.14	2.10	2.09	1.57	1.58	1.55	1.55
σ_{cap}	81.5	76.3	81.5	76.0	30.6	28.7	32.0	30.2
σ_{elas}	7.05	6.65	7.05	6.55	1.44	1.37	1.46	1.42
σ_{inelas}	37.9	33.8	37.9	35.7	30.0	29.3	36.0	29.9
ν_f	6.60	6.85	6.60	6.60	4.87	5.16	4.91	4.91
Pu-239	150	142	150	144	28.7	26.0	25.6	25.8
σ_f	146	138	146	141	22.9	18.9	18.6	19.3
σ_{cap}	23.1	22.8	23.1	22.7	5.31	5.27	5.78	5.75
σ_{elas}	0.519	0.556	0.519	0.523	0.161	0.138	0.142	0.136
σ_{inelas}	5.19	6.10	5.19	4.13	3.55	7.56	6.21	4.89
ν_f	21.4	19.5	21.4	19.5	16.0	15.3	15.4	15.4
Fe-56	35.2	32.2	35.2	37.0	52.5	44.5	48.7	50.0
σ_{cap}	20.9	20.1	20.9	20.2	37.8	37.9	36.0	36.1
σ_{elas}	10.9	10.1	10.9	9.60	12.3	9.56	12.1	10.3
σ_{inelas}	26.2	23.0	26.2	29.5	34.3	21.3	30.6	33.0
Na-23	25.5	28.1	25.5	25.5	39.8	35.1	41.6	41.6
σ_{cap}	8.25	6.42	8.25	8.25	31.6	23.9	32.2	32.2
σ_{elas}	10.1	9.39	10.1	10.1	7.53	6.93	10.7	10.7
σ_{inelas}	22.0	25.7	22.0	22.0	23.0	24.8	24.1	24.1

Moreover, visual disparities appear in the correlation matrix with negative values for the flat weighting that are not present in those obtained with the ConsUnc methodology.

VI. Conclusions

A new algorithm for a rigorous collapsing of covariance data has been proposed, derived, implemented, and tested. The method is based on a conservation principle that allows preserving at a broad energy group structure the uncertainty calculated in a fine group energy structure for a specific integral parameter, using as weights the associated sensitivity coefficients.

Comparisons against uncertainties calculated with the most commonly used flat weighting collapsed covariance data have shown that:

- No significant effects have been observed on very important cross sections of major actinides (e. g., Pu-239 fission, U-238 capture) that can be attributed to the collapsing technique used.
- Significant effects on uncertainties, standard deviations, and correlation data have been found on values associated to inelastic cross sections for a very broad energy group structure (15 groups).
- If an enough fine energy group structure is used (e. g., 33 groups), the flat flux collapsed data can perhaps be used, even if there is the need of preliminary verifications, looking for specific effects, e.g., on scattering data.

Therefore, a preliminary recommendation for future work on the production of reliable multigroup covariance data is to use a sufficient number of groups (30 to 50) and in the case of data adjustment, particular caution has to be applied for the inelastic cross section values.

Some more tests will be performed to investigate other integral parameters, in order to consolidate the recommendation for a standard collapsing procedure.

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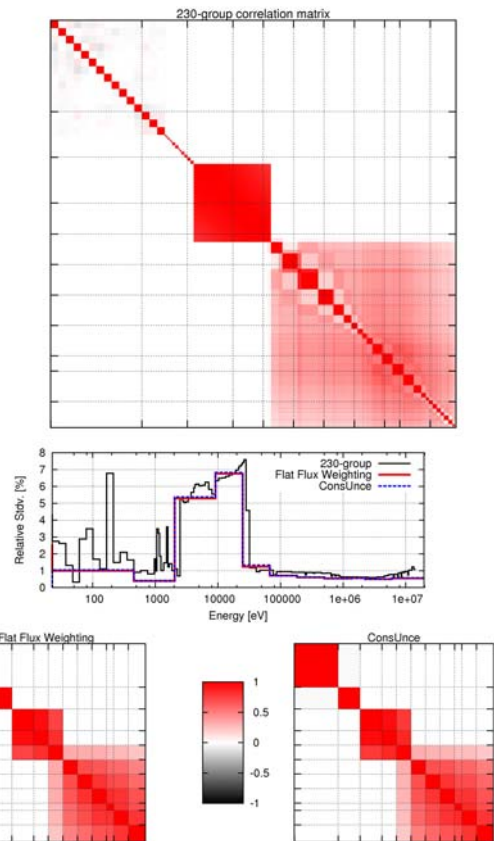


Figure 1. Pu-239 fission cross section covariance 230 and 15 group data.

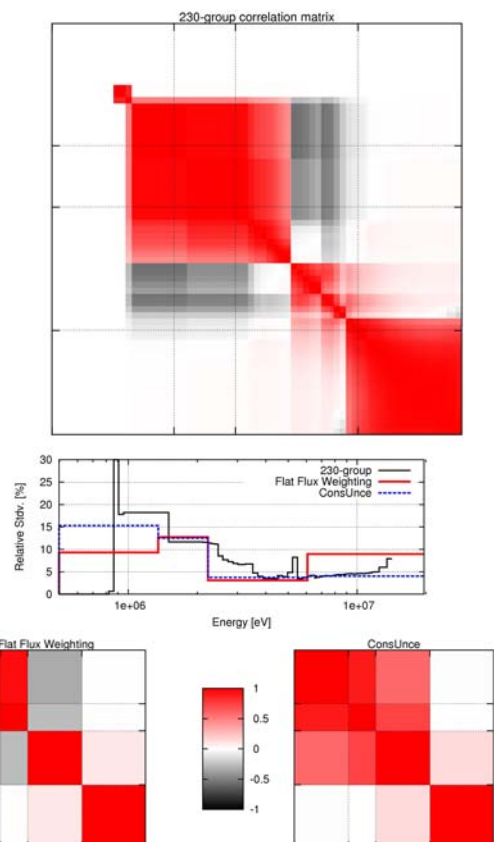


Figure 2. Fe-56 inelastic scattering cross section covariance 230 and 15 group data.