INL Activities with Covariance Data Multigroup Adjustment with COMMARA 2.0 and ENDF/B-VII.0

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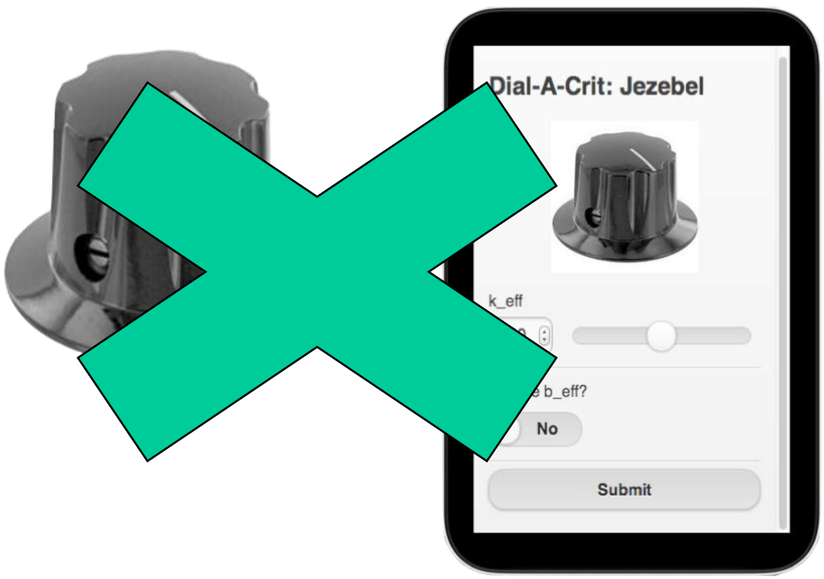
Introduction

- **Why this presentation belongs to the Validation Session:**
  - **It is not a knob job!**
  - **It is intended to provide feedback to both nuclear data evaluators and differential measurement experts on which cross section needs improvements**
  - **It is a validation of the covariance matrix used in the adjustment**
  - **It is intended for reducing uncertainties on target advanced reactor systems (in particular fast reactors)**



← YES

Adjustment

- **The methodology for the cross section adjustment (aka assimilation, tuning, calibration, knob) makes use of the following input quantities:**
  - **C/E for the measured integral parameters**
  - **Associated experimental and calculational uncertainties on integral parameters, and, if available, correlations among them**
  - **“A priori” covariance data on cross sections**
  - **Sensitivities of cross sections to integral parameters**

Adjustment

- A comprehensive multigroup neutron cross section adjustment has been carried out using ENDF/B-VII.0 data files and COMMARA 2.0 covariance matrix.
- An initial set of 148 integral experimental quantities has been analyzed (using the best calculational tool available) in order to provide C/E and associated calculational and experimental uncertainties and correlations.
- The initial set was reduced to 87 experimental values based on several considerations (duplications, some covariance data not available, experiments reserved for Fe adjustment, etc.).
- A 33 energy group structure was adopted and sensitivity coefficients were calculated. Generalized Perturbation Theory (by ERANOS system) was used for static integral parameters and Depletion Perturbation Theory for time dependent parameters (done at ANL).

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Type of experiments used in adjustment

	keff	Other	Spectral index	Irradiation	total # cases
Jezebel	2		3		5
Flattop	1		2		3
ZPPR-6/7,9	3	2	6		11
JOYO	1				1
Godiva	1		3		4
BigTen	1		3		4
Np Sphere	1				1
ZPPR-10,15	3	5			8
COSMO			9		9
PROFIL				26	26
TRAPU				15	15

Experimental Covariance Matrix PROFIL-1

*** *indicates uncertainty derived from sample dispersion***

No.	Sample	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	σ_{capt} ^{235}U	0.2*																	
2	σ_{capt} ^{238}U	0	0.7*																
3	σ_{capt} ^{238}Pu	0	0	0.6*															
4	σ_{capt} ^{239}Pu	0	0	0	6														
5	$\sigma_{n,2n}$ ^{239}Pu	0	0	0	0	0.4*													
6	σ_{capt} ^{240}Pu	0	0	0	0	0	0.2												
7	$\sigma_{n,2n}$ ^{240}Pu	0	0	0	0	0	0	11											
8	σ_{capt} ^{241}Pu	0	0	0	0	0	0	0	0.3*										
9	σ_{capt} ^{242}Pu	0	0	0	0	0	0	0	0	2.5									
10	σ_{capt} ^{241}Am	0	0	0	0	0	0	0	0	0	2.2								
11	σ_{capt} ^{243}Am	0	0	0	0	0	0	0	0	0	0	5.6							
12	σ_{capt} ^{95}Mo	0	0	0	0	0	0	0	0	0	0	0	3.7*						
13	σ_{capt} ^{97}Mo	0	0	0	0	0	0	0	0	0	0	0	0	3.3*					
14	σ_{capt} ^{101}Ru	0	0	0	0	0	0	0	0	0	0	0	0	0	0.6*				
15	σ_{capt} ^{105}Pd	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.3			
16	σ_{capt} ^{133}Cs	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.3*		
17	σ_{capt} ^{145}Nd	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.0*	
18	σ_{capt} ^{149}Sm	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5*

Calculational Covariance Matrix PROFIL-1

No.	Sample	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	σ_{capt} ^{235}U	2.3																	
2	σ_{capt} ^{238}U	0.72	2.4																
3	σ_{capt} ^{238}Pu	0.72	0.69	2.4															
4	σ_{capt} ^{239}Pu	0.72	0.69	0.69	2.4														
5	$\sigma_{n,2n}$ ^{239}Pu	0.27	0.26	0.26	0.26	6.4													
6	σ_{capt} ^{240}Pu	0.72	0.69	0.69	0.69	0.26	2.4												
7	$\sigma_{n,2n}$ ^{240}Pu	0.19	0.18	0.18	0.18	0.07	0.18	9.3											
8	σ_{capt} ^{241}Pu	0.76	0.72	0.72	0.72	0.27	0.72	0.19	2.3										
9	σ_{capt} ^{242}Pu	0.72	0.69	0.69	0.69	0.26	0.69	0.18	0.72	2.4									
10	σ_{capt} ^{241}Am	0.64	0.62	0.62	0.62	0.23	0.62	0.16	0.64	0.62	2.7								
11	σ_{capt} ^{243}Am	0.76	0.72	0.72	0.72	0.27	0.72	0.19	0.76	0.72	0.64	2.3							
12	σ_{capt} ^{95}Mo	0.67	0.64	0.64	0.64	0.24	0.64	0.17	0.67	0.64	0.57	0.67	2.6						
13	σ_{capt} ^{97}Mo	0.64	0.62	0.62	0.62	0.23	0.62	0.16	0.64	0.62	0.55	0.64	0.57	2.7					
14	σ_{capt} ^{101}Ru	0.72	0.69	0.69	0.69	0.26	0.69	0.18	0.72	0.69	0.62	0.72	0.64	0.62	2.4				
15	σ_{capt} ^{105}Pd	0.72	0.69	0.69	0.69	0.26	0.69	0.18	0.72	0.69	0.62	0.72	0.64	0.62	0.69	2.4			
16	σ_{capt} ^{133}Cs	0.64	0.62	0.62	0.62	0.23	0.62	0.16	0.64	0.62	0.55	0.64	0.57	0.55	0.62	0.62	2.7		
17	σ_{capt} ^{145}Nd	0.64	0.62	0.62	0.62	0.23	0.62	0.16	0.64	0.62	0.55	0.64	0.57	0.55	0.62	0.62	0.55	2.7	
18	σ_{capt} ^{149}Sm	0.72	0.69	0.69	0.69	0.26	0.69	0.18	0.72	0.69	0.62	0.72	0.64	0.62	0.69	0.69	0.62	0.62	2.4

Symmetric

34 COMMARA-2.0 nuclei with covariances used in adjustment

- **Light Nuclei:**

  ^{10}B, ^{16}O

- **Structural materials and fission fragments:**

  ^{23}Na, ^{52}Cr, ^{56}Fe, ^{58}Ni, ^{95}Mo, ^{97}Mo, ^{101}Ru, ^{105}Pd, ^{106}Pd, ^{133}Cs, ^{143}Nd, ^{145}Nd, ^{149}Sm, ^{151}Sm, ^{153}Eu

- **Major actinides:**

  ^{235}U, ^{238}U, ^{239}Pu

- **Minor actinides:**

  ^{234}U, ^{236}U, ^{237}Np, ^{238}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu

  ^{241}Am, ^{242m}Am, ^{243}Am, ^{242}Cm, ^{243}Cm, ^{244}Cm, ^{245}Cm

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Only five major reactions included in adjustment

- **(n,f)**:
  - cross section
  - nubar
  - PFNS (3 cases)
- **(n,el)**:
  - cross section
  - P1 (2 cases)
- **(n,inel)**: cross section
- **(n,g)**: cross section
- **(n,2n)**: cross section

In all, 8976 points could have been adjusted, but only 1126 most important kept:

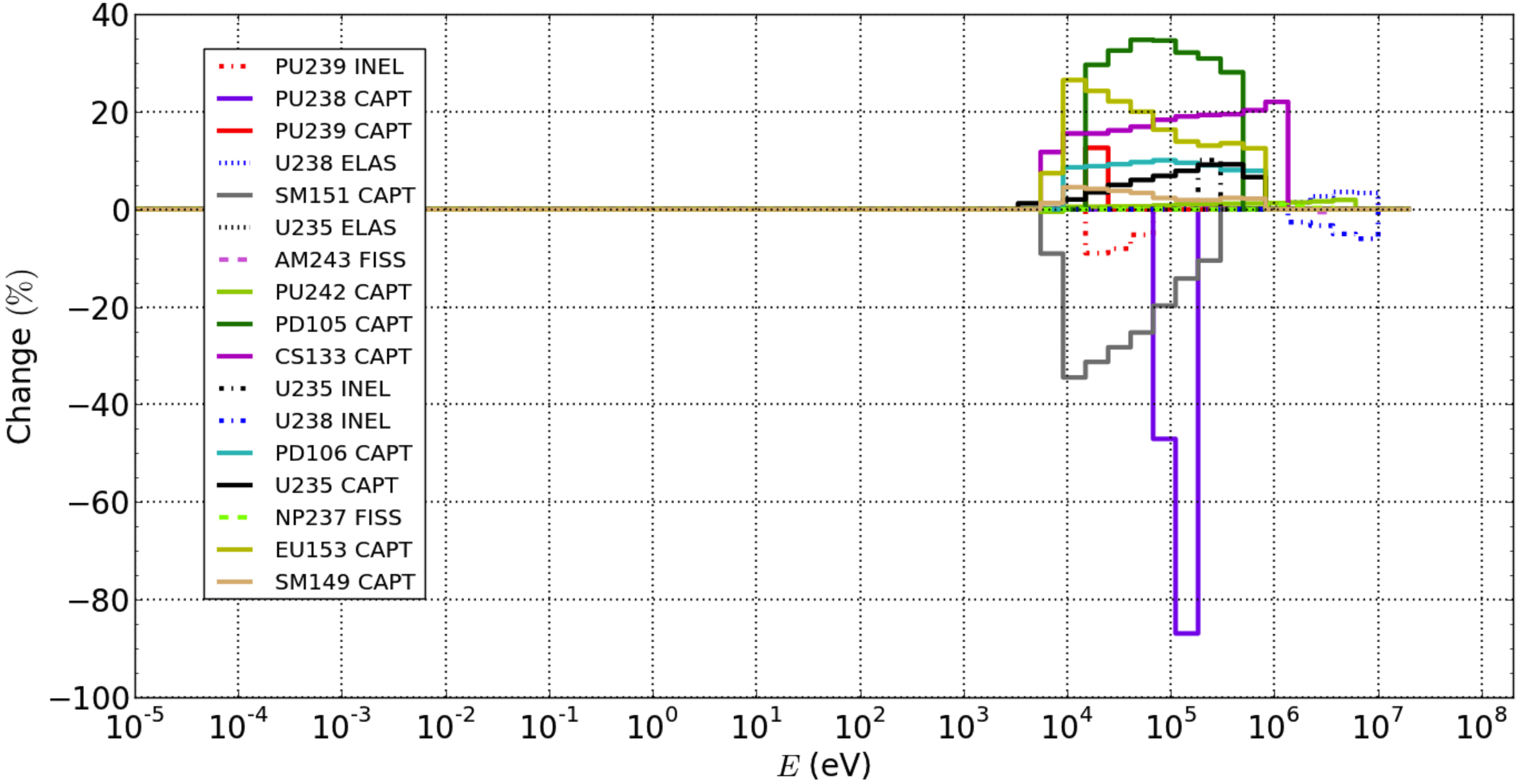
$$\left|\Delta R_{ip}^{2}\right| = \left|S_R^{t} D S_R\right| \geq \varepsilon^{2}$$

$$\mathbf{S}_{\mathbf{R}pj} = \frac{\Delta R_p}{\Delta \sigma_j}$$

These are the benchmarks whose uncertainty changed the most as a result of the evaluation adjustment

#	Experiment	(E-C)/C Change (%)	Old Stan. Dev. (%)	New Stan. Dev. (%)	Rel. Change (%)
1	TRAPU2 PU239 BUILD UP	-0.92	2.72	0.21	92.09
2	TRAPU2 U235 BUILD UP	0.12	2.41	0.19	91.93
3	TRAPU2 AM241 BUILD UP	0.43	4.33	0.43	90.17
4	ZPR6/7 F9/F5	0.36	2.52	0.33	86.89
5	TRAPU2 PU241 BUILD UP	0.86	3.01	0.46	84.58
6	TRAPU2 PU240 BUILD UP	1.93	2.62	0.41	84.33
7	ZPPR9 F9/F5	0.43	2.12	0.33	84.25
8	GODIVA F49/F25	0.99	1.84	0.35	81.27
9	COSMO F41/F25	0.10	2.03	0.39	80.64
10	ZPPR-10 STEP2	-1.53	9.69	2.11	78.25
11	TRAPU2 PU242 BUILD UP	0.97	2.43	0.54	77.76
12	ZPR6/7 C8/F5	-0.03	2.68	0.60	77.55
13	PROFIL1 PU239 IN U238 SAMPLE	-1.15	2.50	0.59	76.60
14	COSMO F49/F25	0.42	1.30	0.33	74.75
15	TRAPU2 PU238 BUILD UP	7.97	2.43	0.67	72.36
16	ZPPR9 STEP3	-2.07	7.74	2.28	70.59
17	ZPPR9 C8/F5	-0.12	1.99	0.60	69.74
18	ZPR6/7 F8/F5	1.39	3.50	1.07	69.36
19	ZPR6/7 KEFF	0.05	0.23	0.08	67.31
20	ZPPR-10 CENTER ROD	-2.24	2.20	0.73	66.53

These data changed the most during adjustment (relative to pre-adjustment value)



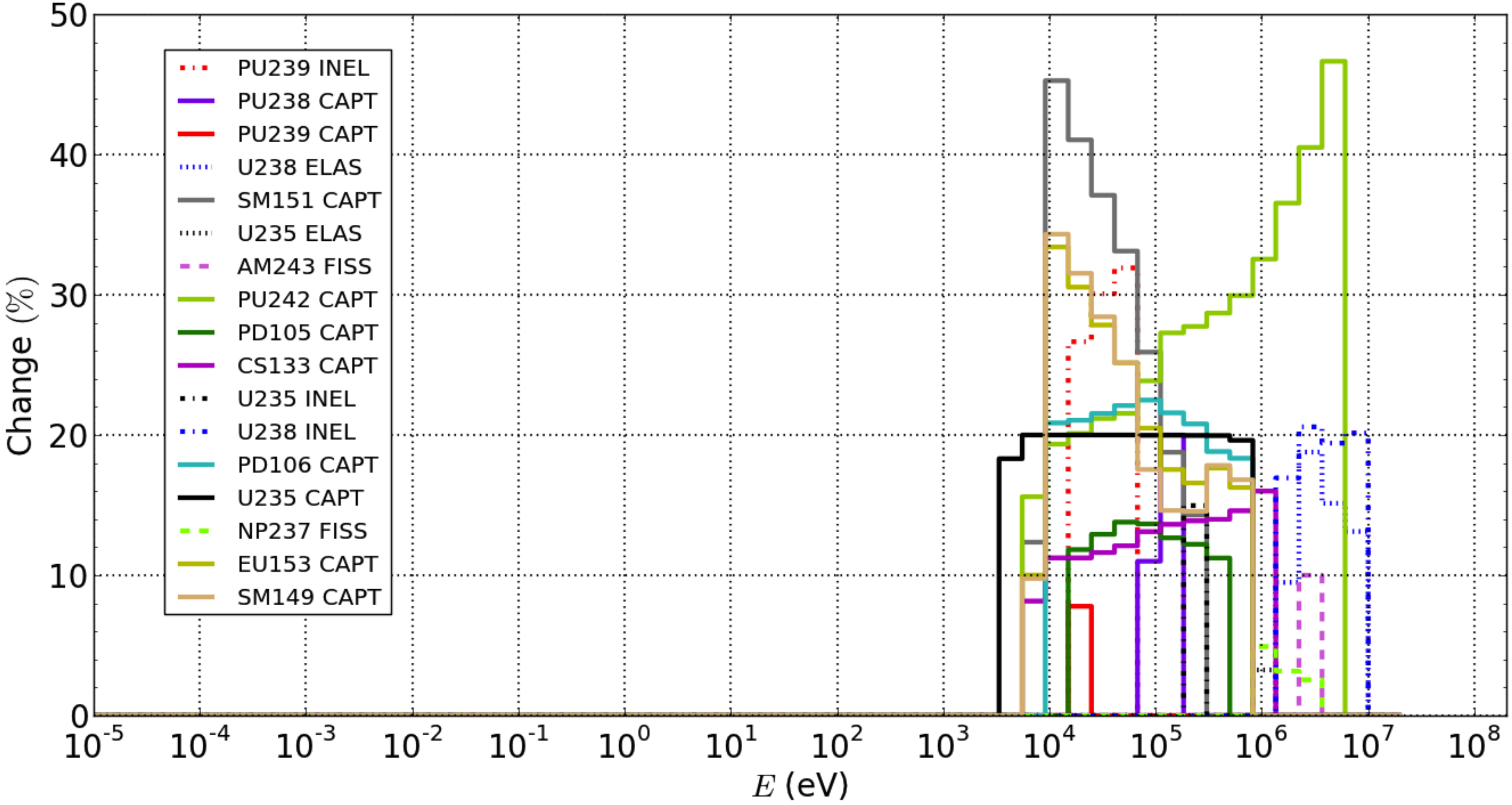
These isotopes had the largest standard deviation relative change

#	σ	σ change (%)	Old Stand. Dev. (%)	New Stan. Dev. (%)	Rel. Change (%)
1	PU239 INEL GR.15	-9.00	26.65	3.17	88.09
2	U235 CAPT GR.17	1.28	20.00	2.42	87.91
3	U235 CAPT GR.16	2.00	20.00	2.64	86.81
4	U235 CAPT GR.10	9.13	19.97	2.85	85.75
5	U235 CAPT GR.15	3.49	20.00	2.95	85.25
6	U235 CAPT GR.11	7.88	19.99	3.09	84.54
7	U235 CAPT GR.14	4.99	20.00	3.11	84.46
8	U235 CAPT GR.13	6.01	20.00	3.14	84.30
9	U235 CAPT GR. 9	9.21	19.96	3.19	84.04
10	U235 CAPT GR.12	6.85	19.98	3.23	83.84
11	U238 INEL GR. 4	-5.05	19.42	3.33	82.85
12	SM151 CAPT GR.13	-25.25	33.11	6.35	80.82
13	SM151 CAPT GR.12	-19.76	25.91	4.98	80.80
14	PU242 CAPT GR.12	0.79	23.86	4.59	80.77
15	SM151 CAPT GR.14	-28.28	37.09	7.15	80.72
16	PU242 CAPT GR.17	-0.50	15.60	3.03	80.56
17	SM151 CAPT GR.15	-31.28	41.04	8.04	80.40
18	SM151 CAPT GR.16	-34.46	45.26	9.05	80.00
19	PU242 CAPT GR.13	0.61	21.54	4.87	77.37
20	PD106 CAPT GR.12	10.04	22.49	5.20	76.90
21	PU242 CAPT GR.16	0.51	19.35	4.48	76.83
22	SM151 CAPT GR.11	-14.19	18.77	4.35	76.81
23	PU242 CAPT GR.14	0.58	21.17	4.92	76.75
24	PU242 CAPT GR.15	0.52	20.11	4.81	76.06
25	U238 ELAS GR. 4	3.54	15.13	3.63	75.98
26	PU242 CAPT GR.11	1.05	27.28	6.56	75.95
27	PU242 CAPT GR. 8	1.18	29.94	7.31	75.60
28	EU153 CAPT GR.12	16.31	20.49	5.00	75.59
29	EU153 CAPT GR.13	20.00	25.14	6.17	75.45
30	EU153 CAPT GR.14	22.12	27.84	6.96	75.00

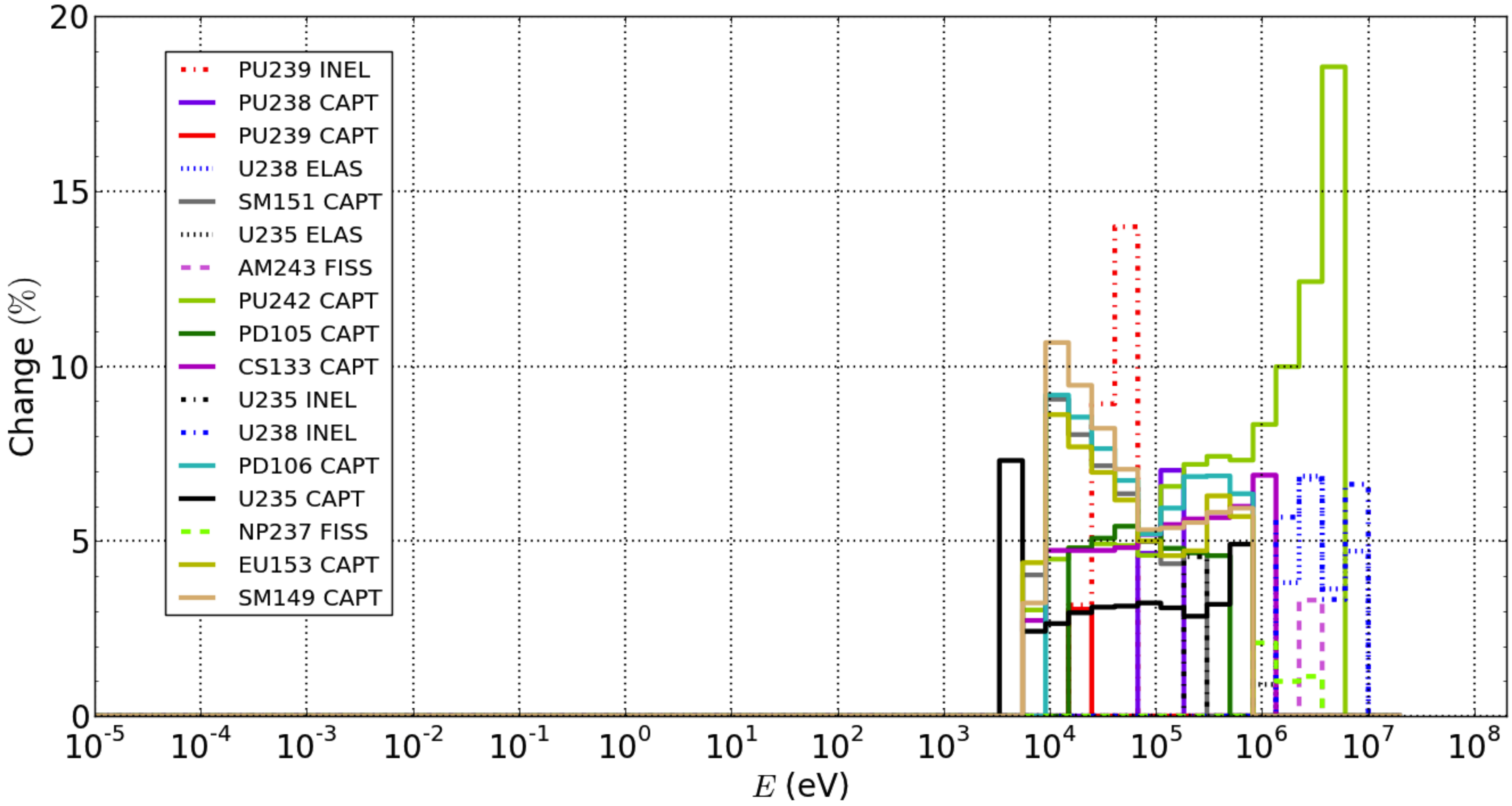
Major isotopes and reactions where standard deviation is likely underestimated

- **Pu-238 capture**
- **Am-241 fission**
- **Pd-105 capture**
- **U-238 fission**
- **Pu-238 fission**
- **Pu-239 fission**
- **Cm-242 capture**
- **Pu-239 (n,2n)**
- **U-238 capture**
- **Pu-239 capture**
- **U-238 inelastic**
- **Na-23 elastic**
- **Na-23 inelastic**
- **Fe-56 elastic**
- **O-16 elastic**
- **Pu-239 fission spectrum**

Pre-adjustment standard deviations



Post-adjustment standard deviations



Conclusions

- A comprehensive adjustment was carried out using 87 integral experimental values, ENDF/B-VII.0 libraries, and COMMARA 2.0 covariance matrix.
- Overall the adjustment is quite satisfactory, but some standard deviations are underestimated:
  - ^{238}Pu, ^{241}Am, and ^{242}Cm,
  - ^{238}U (fission, capture, and inelastic),
  - ^{239}Pu (fission, capture, and (n,2n),
  - ^{56}Fe and ^{23}Na
- Central values of (n,γ) for ^{238}Pu, ^{242}Cm and ^{244}Cm, and for ^{105}Pd, ^{133}Cs, ^{151}Sm, and ^{153}Eu needed most adjustment.
- ^{235}U capture, ^{238}U and ^{239}Pu inelastic, ^{237}Np fission, and captures of some fission products are the most promising for having some impact in future studies for reducing uncertainties of neutronic design parameters of advanced nuclear systems.