

DE LA RECHERCHE À L'INDUSTRIE

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**STATUS AND REQUIREMENTS OF NUCLEAR DATA  
VARIANCE-COVARIANCE MATRICES  
FOR THE NEUTRONIC ASSESSMENT  
OF FAST REACTOR CORES.**

**G. Rimpault, G. Noguère, L. Buiron**

**CEA, DEN, DER, CADARACHE, FRANCE**

**WPEC 44 :**

**“Investigation of Covariance Data in General  
Purpose Nuclear Data Libraries”**

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- During the design of different SFR cores, the main neutronic variables of interest are evaluated in order to analysis the core behavior in transient.
- To ensure a good knowledge of design safety performance, associated margins on safety parameters (sodium and fuel temperatures, reactivity, effective delayed neutron fraction ( $\beta_{eff}$ ), neutron generation lifetime ( $\lambda$ ) ...) must thus be evaluated taking account uncertainties on the neutronic parameters.
- Kinetic parameters are estimated at the neutronic level from nuclear data evaluation and in particular from cross section of nuclear reactions. These nuclear data are affected by uncertainties which should be propagated through the code system to determine the available safety margins in transient.

## Transient behavior: point kinetic model

- > Flux shape preserved.
- > Amplitude updated with the reactivity variation

$$\rho = \rho^o + \Delta\rho_{ext} + \Delta\rho_{CR}$$

### Neutronic parameters used :

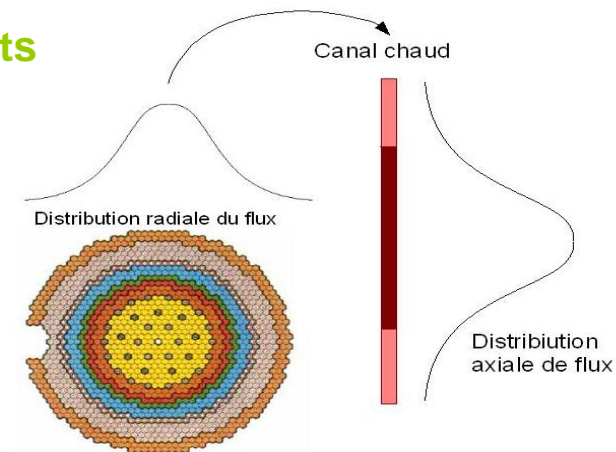
Power Distribution in Nominal Conditions

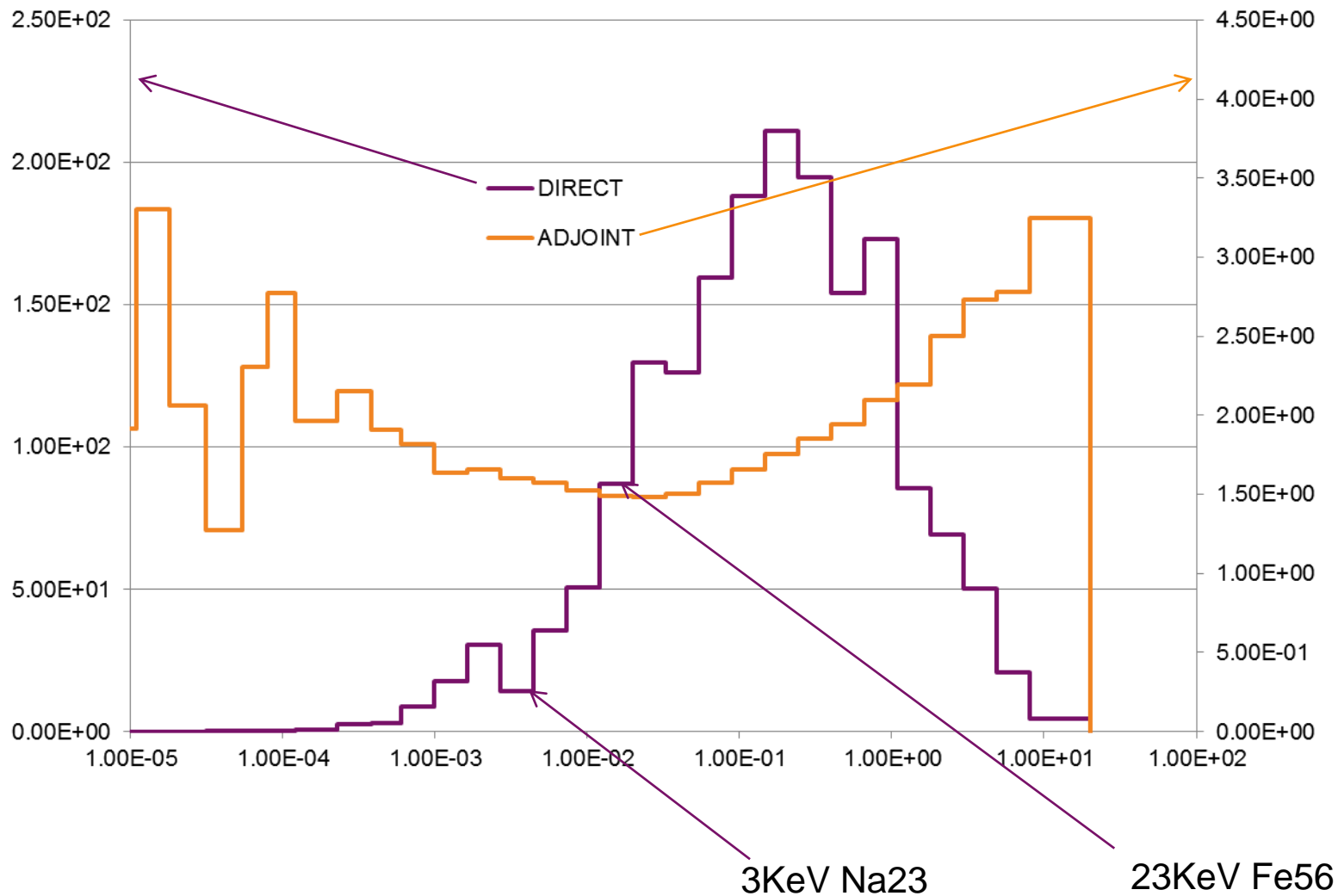
Spatial Distribution of reactivity feedback coefficients

$$\Rightarrow \Delta\rho_{CR} = \sum_i k_i (T_i - T_{i\_NOM})$$

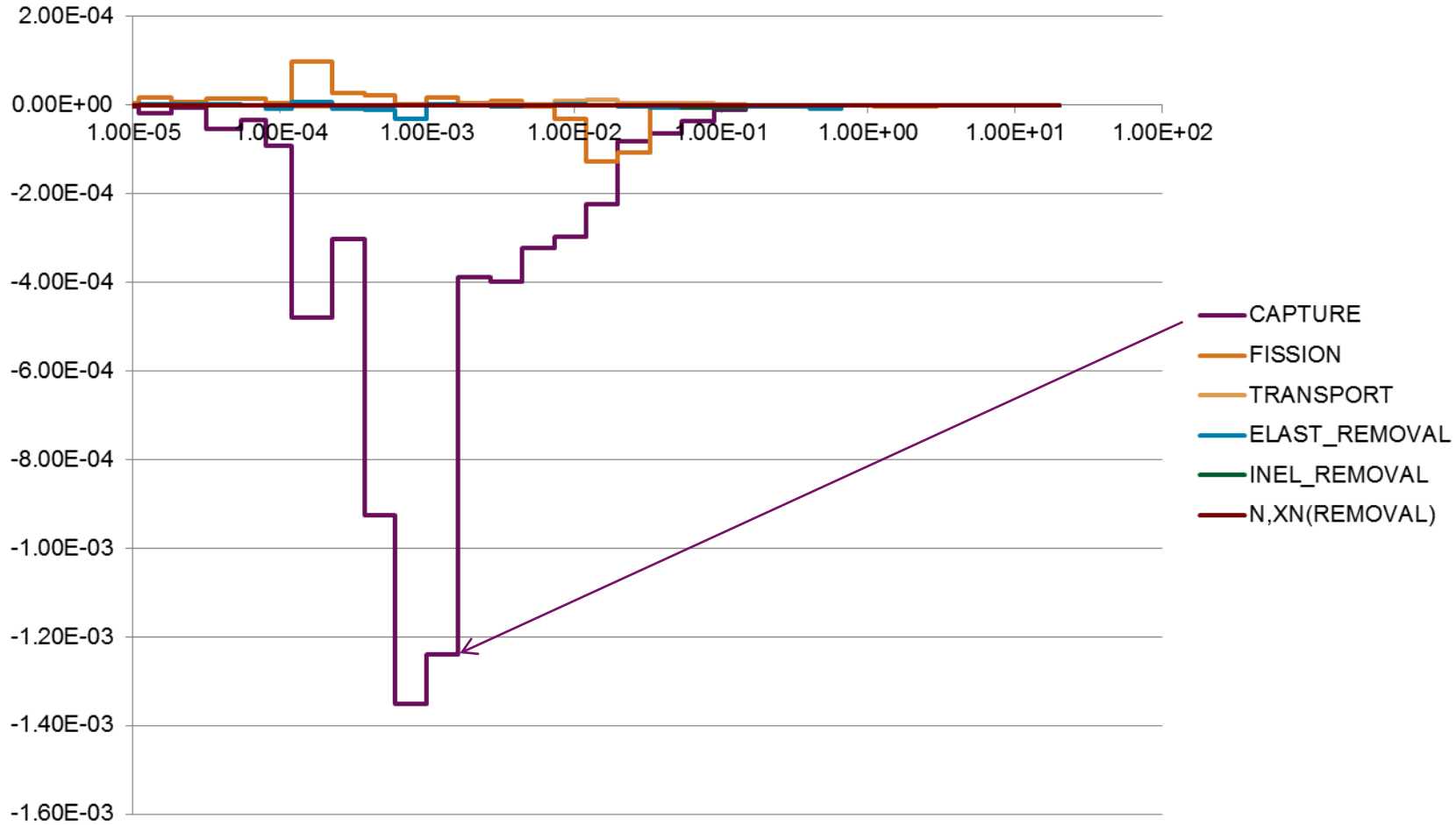
Kinetic Parameters

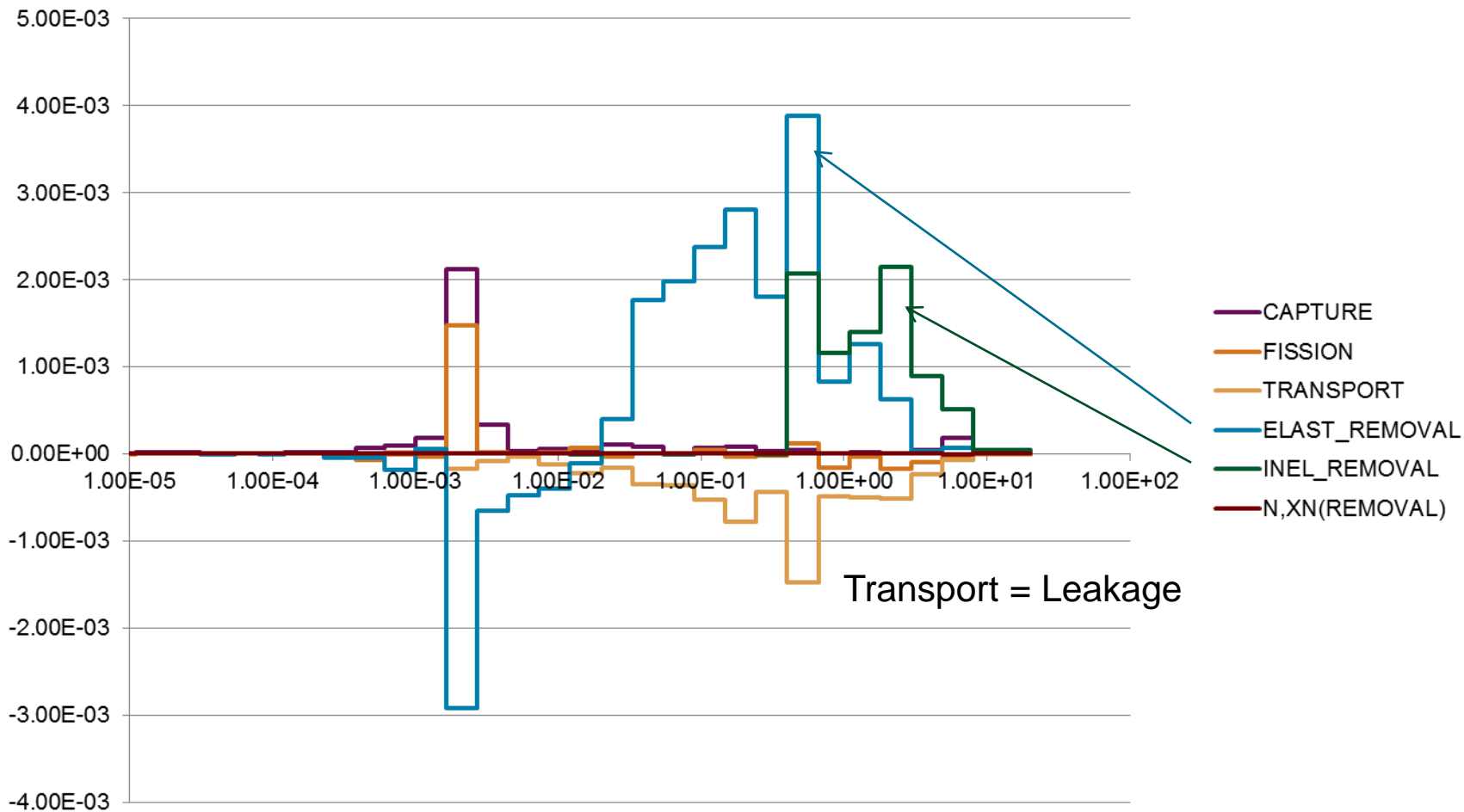
$$\Lambda(t), \quad \beta(t) = \sum_i \beta_i(t)$$





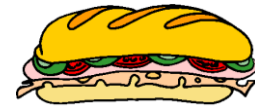
# DOPPLER EFFECT COMPONENTS AT BOL





## Uncertainty Expression : (« sandwich formula»)

$$\sigma = \sqrt{SDS^T}$$



with S: sensitivity vector  
and D: dispersion matrix on nuclear data

## Sensitivities

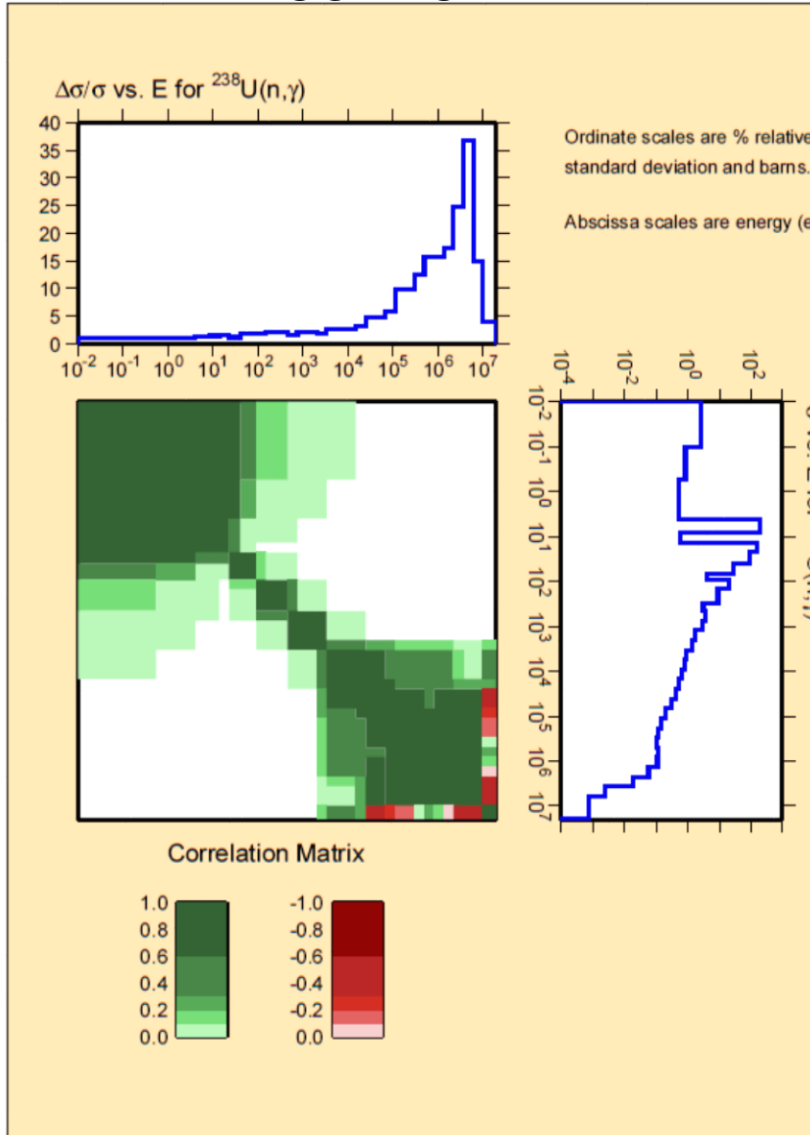
$$S(R, \sigma) = \frac{\frac{dR}{R}}{\frac{d\sigma}{\sigma}}$$

- The sensitivities were calculated for the effective delayed neutron fraction ( $\beta_{\text{eff}}$ ), and the neutron generation lifetime ( $\lambda$ )
- Calculations have also been performed for reactivity, for  $\rho_{\text{Doppler}}$  and  $\rho_{\text{Na Void}}$
- The uncertainties due to nuclear data are being calculated with different covariances (COMAC, ENDF BVII.1, JENDL4.0)
- COMAC anticipates covariances for JEFF3.3 but was complemented for what concerns delayed neutron constants by those of JENDL4.0

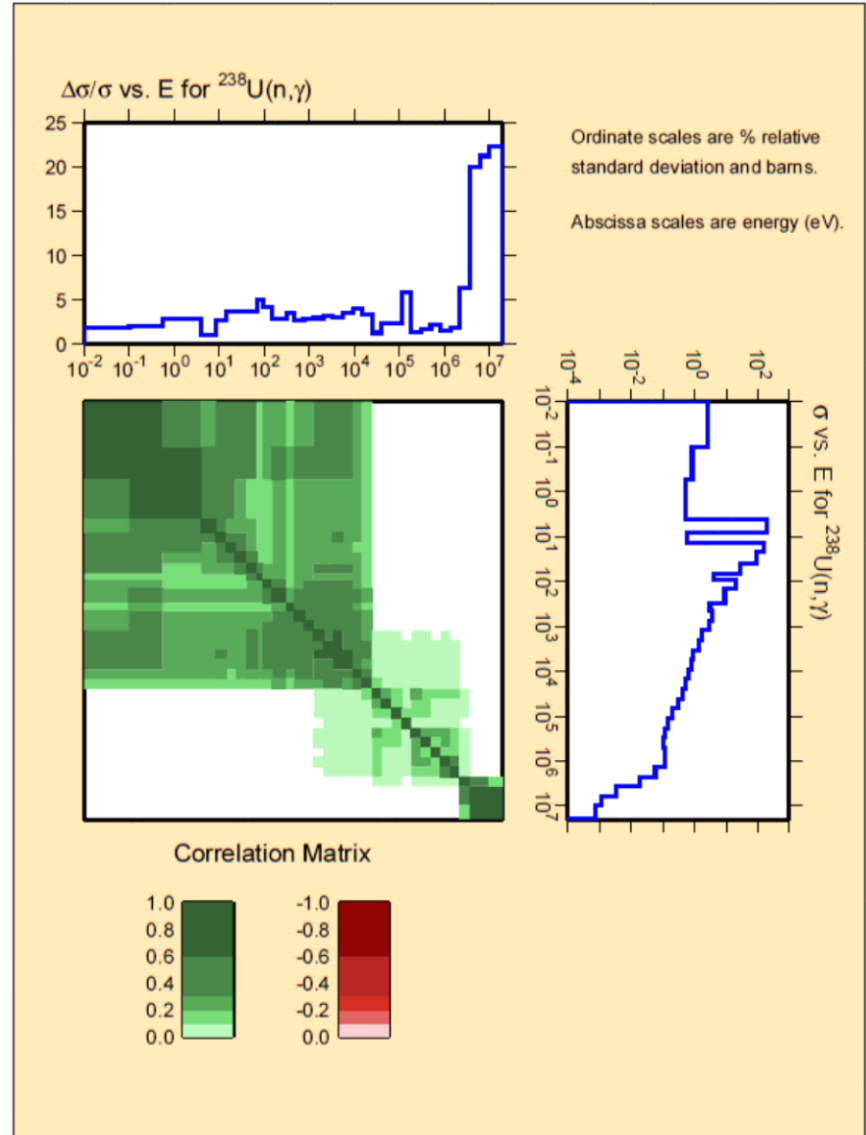
- The different covariances (COMAC, ENDF BVII.1, JENDL4.0) should, in principle reflect the way the nuclear data evaluation has been made.
- This means that differential measurement uncertainties should have been propagated towards the evaluation itself. Since, there is a rationale in the choice of these differential measurements which depends on the evaluator, the final induced uncertainty might differ.
- The nuclear model being used links together the different differential measurements and might add some more correlations (some exists already since differential measurements are conducted in a limited range of energy) in energy and between different cross section types.
- Assimilation of integral experiments might have been done (JEZABEL is often used) which might add more correlations and a reduction of the variances

# U238 CAPTURE COVARIANCES

## COMAC

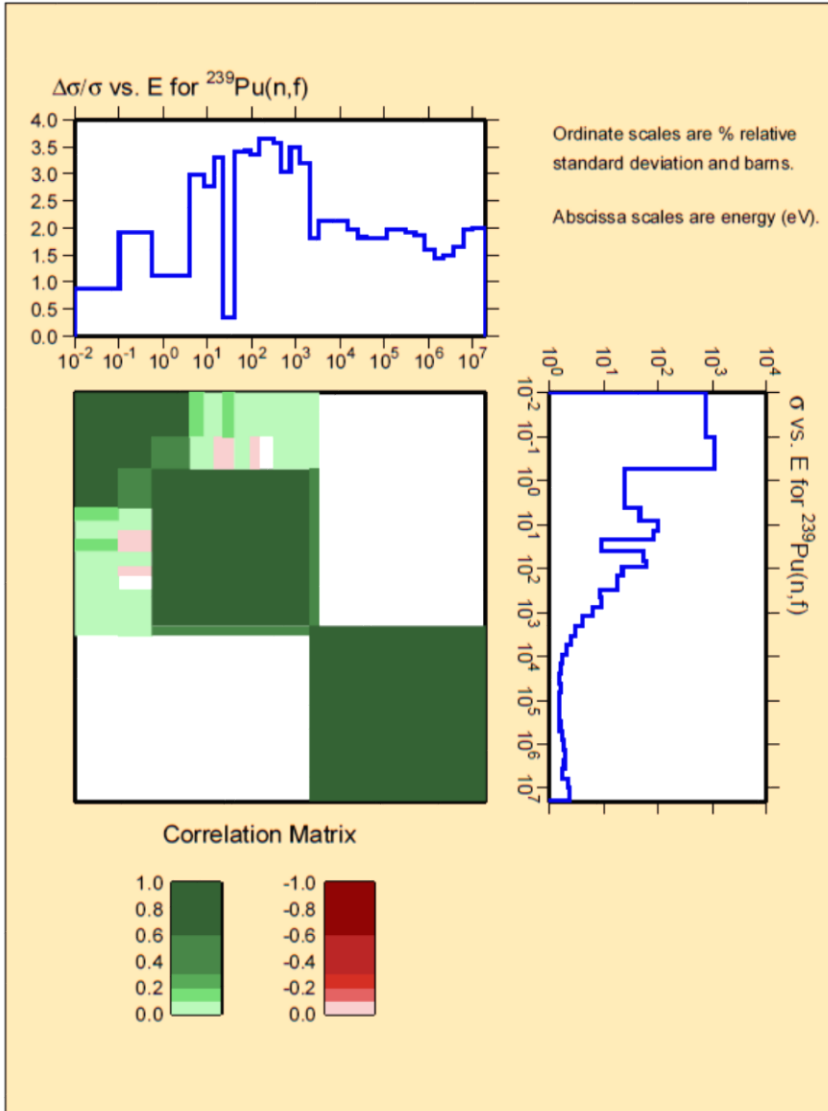


## ENDF B VII

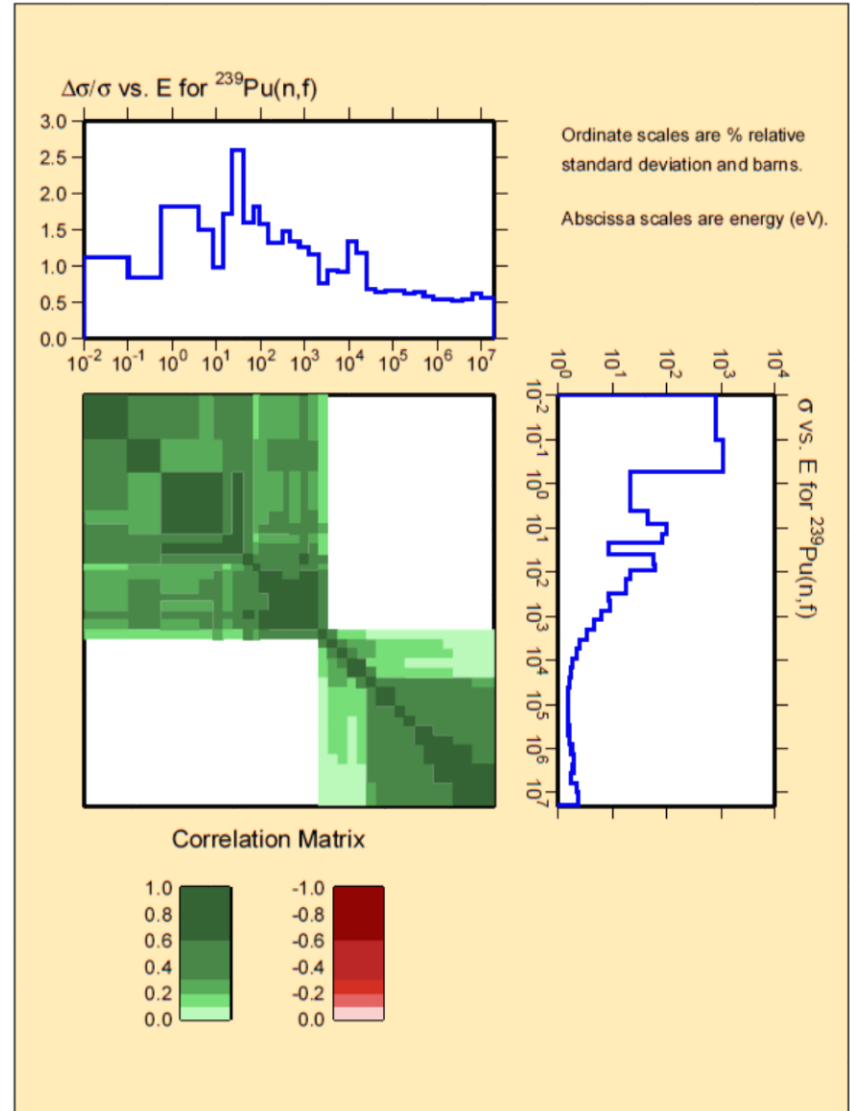


# PU239 FISSION COVARIANCES

## COMAC

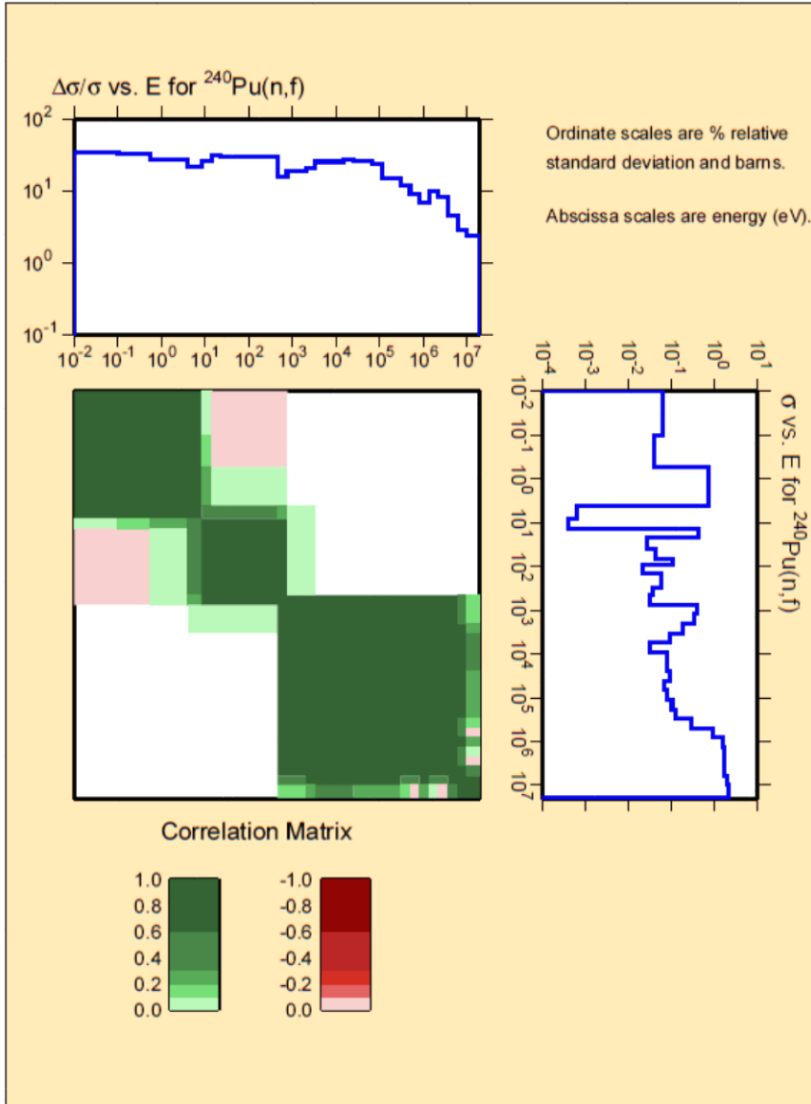


## ENDF B VII

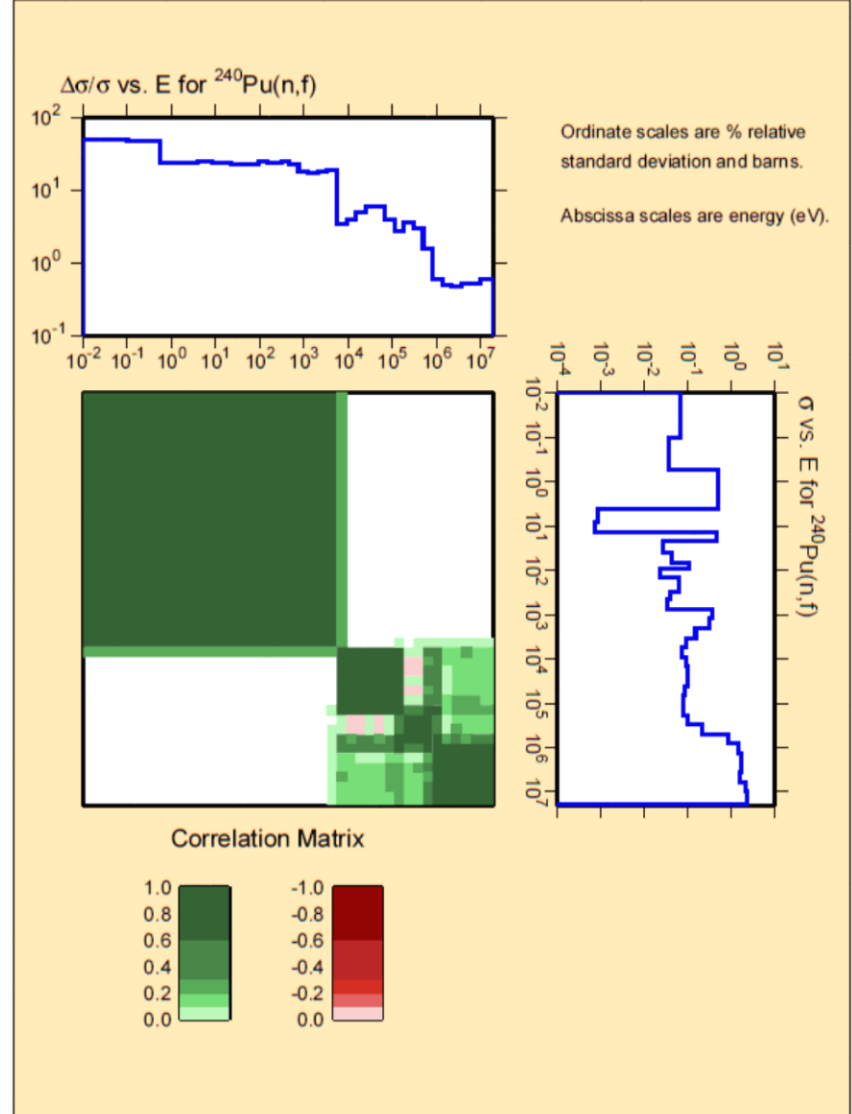


# PU240 FISSION COVARIANCES

## COMAC



## ENDF B VII



Uncertainties (indirect term +direct terms) on  $\beta_{\text{eff}}$  in %.

Isotope	Fis.	Cap.	Elas.	Ine.	n,xn	$\nu$	$\nu d$	X	Total
U235	0.00	0.02	0.00	0.00	0.00	-0.00	0.04	0.01	0.04
U238	1.82	1.25	-0.14	-0.82	-0.05	0.19	1.49	0.14	2.55
Pu239	1.65	0.27	-0.01	0.06	0.02	0.08	1.32	0.20	2.14
Pu241	0.23	0.09	0.00	0.00	0.00	0.11	0.71	0.11	0.76
Pu242	0.01	0.03	0.00	0.00	0.00	-0.01	0.20	0.02	0.21
Am241	0.01	0.01	0.00	0.00	0.00	0.01	0.01	0.00	0.01
Na23	0.00	0.02	0.03	0.01	-0.00	0.00	0.00	0.00	0.04
Pu238	0.02	0.02	0.00	0.00	0.00	0.12	0.00	0.00	0.12
O16	0.00	0.10	0.03	0.01	0.00	0.00	0.00	0.00	0.11
Fe56	0.00	0.10	0.06	0.03	0.00	0.00	0.00	0.00	0.12
TOTAL	2.47	1.29	-0.12	-0.82	-0.05	0.26	2.12	0.26	<b>3.42</b>

The total uncertainty in  $\beta_{\text{eff}}$  is 3.5 %. With COMAC covariance data, the main sources of uncertainty to  $\beta_{\text{eff}}$  are delayed neutron yields and fission of  $U^{238}$  and  $Pu^{239}$ , also the capture and inelastic scattering on  $U^{238}$  and with a lower contribution the delayed neutron yield of  $Pu^{241}$ .

Non-negligible contribution of inelastic of  $U^{238}$  is also noticed. Some dedicated measurements (such as JEZABEL) might be used to improve its nuclear data evaluation and to reduce the uncertainty contribution of this cross section.

- ✓ Sensitivity coefficients of the effective delayed neutron fraction were obtained with generalized perturbation theory.
- ✓ The perturbation tools were developed inside the ERANOS code and allow to estimate uncertainties on these parameters. Results were obtained for the SFR core at the beginning of life.  $\beta_{\text{eff}}$  uncertainty was found to be 3.5%.
- ✓ The  $\beta_{\text{eff}}$  uncertainty is predominantly due to the uncertainties in delayed neutron yields, the fission of  $\text{Pu}_{239}$  and U238 and inelastic scattering of U238.
- ✓ This statement is only valid for COMAC since there are significant differences in covariances between COMAC, ENDF BVII.1 and JENDL4.0

ENDF-BVII	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
Na23	0.00000	0.00059	0.00058	0.00091	0.00000	0.00000	0.00123
Fe56	0.00000	0.00095	0.00025	0.00140	0.00000	0.00000	0.00171
U238	0.00041	0.00294	0.00051	0.01117	0.00007	0.00153	0.01167
Pu238	0.00007	0.00019	0.00000	0.00002	0.00000	0.00015	0.00025
Pu239	0.00201	0.00224	0.00005	0.00096	0.00000	0.00059	0.00321
Pu240	0.00058	0.00078	0.00000	0.00075	0.00000	0.00053	0.00134
Pu241	0.00049	0.00048	0.00000	0.00014	0.00000	0.00022	0.00074
Pu242	0.00021	0.00029	0.00000	0.00009	0.00000	0.00012	0.00039
TOTAL	0.00220	0.00418	0.00150	0.01137	0.00007	0.00175	0.01253

Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	0.00565	0.00252	0.00068	0.00403	0.00023	0.00156	0.00758
ENDF-BVII	0.00220	0.00418	0.00150	0.01137	0.00007	0.00175	0.01253
JENDL-4	0.00281	0.00451	0.00076	0.00601	0.00009	0.00156	0.00821

- ✓ By comparing Uncertainties on Keff using different covariances: COMAC, ENDF BVII.1 and JENDL4.0, one can notice significant differences

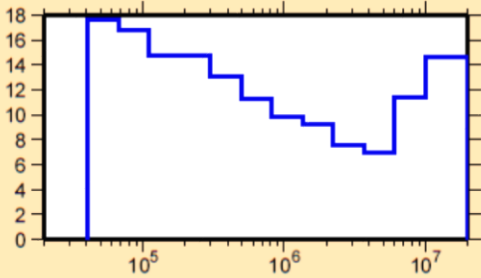
U238 Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	0.00022	0.00235	0.00035	0.00393	0.00023	0.00078	0.00464
ENDF-BVII	0.00041	0.00294	0.00051	0.01117	0.00007	0.00153	0.01167
JENDL-4	0.00046	0.00376	0.00005	0.00556	0.00009	0.00078	0.00678

- ✓ ENDF BVII.1 U238 inelastic and JENDL4.0 U238 capture are much larger.

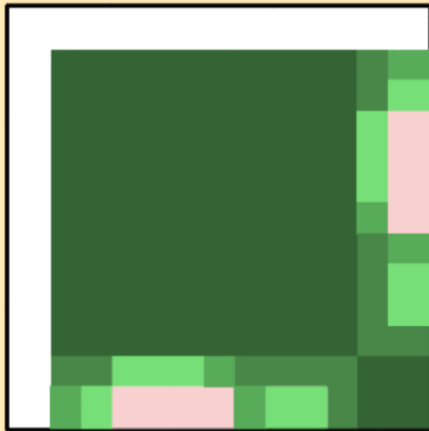
# U238 INELASTIC COVARIANCES

## COMAC

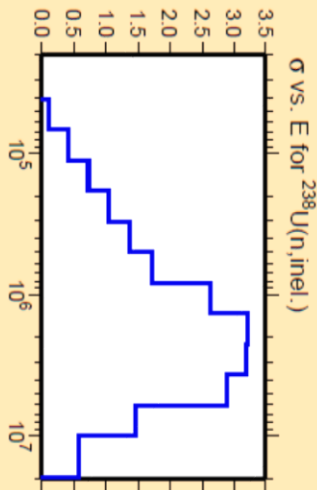
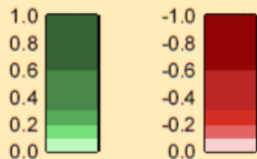
$\Delta\sigma/\sigma$  vs. E for  $^{238}\text{U}(n,\text{inel.})$



Ordinate scales are % relative standard deviation and bars.  
Abscissa scales are energy (eV).



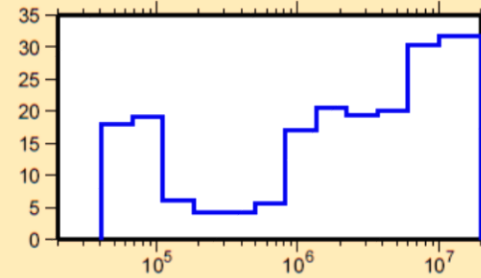
Correlation Matrix



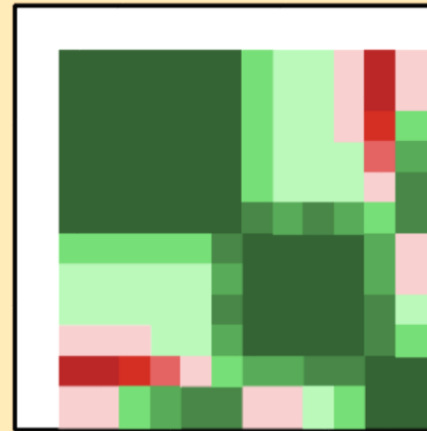
$\sigma$  vs. E for  $^{238}\text{U}(n,\text{inel.})$

## ENDF B VII

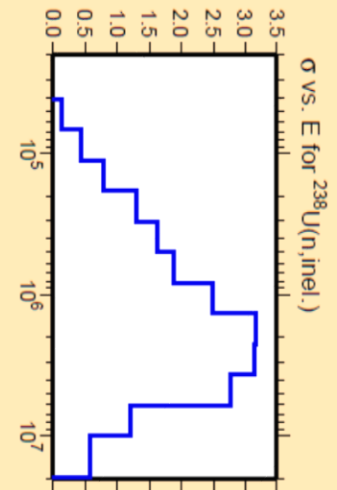
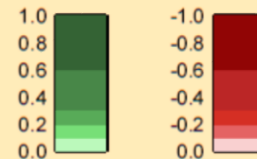
$\Delta\sigma/\sigma$  vs. E for  $^{238}\text{U}(n,\text{inel.})$



Ordinate scales are % relative standard deviation and bars.  
Abscissa scales are energy (eV).



Correlation Matrix



$\sigma$  vs. E for  $^{238}\text{U}(n,\text{inel.})$

Pu239 Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	0.00347	0.00152	0.00001	0.00065	0.00001	0.00115	0.00401
ENDF-BVII	0.00201	0.00224	0.00005	0.00096	0.00000	0.00059	0.00321
JENDL-4	0.00257	0.00167	0.00001	0.00032	0.00000	0.00115	0.00329

- ✓ COMAC Pu239 is significantly larger than the one of ENDF BVII and JENDL4.

Pu240 Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	0.00441	0.00226	0.00006	0.00044	0.00000	0.00015	0.00376
ENDF-BVII	0.00058	0.00078	0.00000	0.00075	0.00000	0.00053	0.00134
JENDL-4	0.00035	0.00100	0.00000	0.00022	0.00000	0.00015	0.00109

✓ COMAC Pu240 fission is much larger.

ENDF-BVII	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
Na23	0.00%	0.44%	1.23%	0.22%	0.00%	0.00%	1.32%
Fe56	0.00%	0.53%	0.96%	0.29%	0.00%	0.00%	1.13%
U238	0.06%	0.31%	0.02%	2.35%	0.02%	0.16%	2.38%
Pu238	0.01%	0.12%	0.00%	0.01%	0.00%	0.01%	0.12%
Pu239	0.44%	0.99%	0.03%	0.47%	0.00%	0.12%	1.19%
Pu240	0.09%	0.20%	0.01%	0.20%	0.00%	0.05%	0.30%
Pu241	0.10%	0.19%	0.00%	0.08%	0.00%	0.04%	0.24%
Pu242	0.03%	0.31%	0.01%	0.03%	0.00%	0.01%	0.32%
TOTAL	0.46%	1.47%	2.07%	2.44%	0.02%	0.21%	3.56%

Resonances at 3keV for Na23 and at 23keV for Fe56 influences flux level at 1keV  
Also U238 inelastic and Pu239 capture

Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	1.47%	1.82%	1.23%	1.35%	0.05%	0.20%	2.97%
ENDF-BVII	0.46%	1.47%	2.07%	2.44%	0.02%	0.21%	3.56%
JENDL-4	0.56%	1.20%	1.76%	1.52%	0.03%	0.20%	2.68%

- ✓ By comparing Uncertainties on  $K_{\text{eff}}$  using different covariances: COMAC, ENDF BVII.1 and JENDL4.0, one can notice significant differences

U238 Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	0.09%	0.63%	0.12%	1.34%	0.05%	0.08%	1.49%
ENDF-BVII	0.06%	0.31%	0.02%	2.35%	0.02%	0.16%	2.38%
JENDL-4	0.07%	0.44%	0.17%	1.41%	0.03%	0.08%	1.49%

- ✓ ENDF BVII.1 U238 inelastic and JENDL4.0 U238 capture are much larger.

Pu239 Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	1.03%	1.17%	0.06%	0.12%	0.00%	0.17%	1.57%
ENDF-BVII	0.44%	0.99%	0.03%	0.47%	0.00%	0.12%	1.19%
JENDL-4	0.52%	0.57%	0.02%	0.28%	0.00%	0.17%	0.84%

- ✓ COMAC Pu239 fission and capture are significantly larger than the ones of ENDF BVII and JENDL4.

Pu240 Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	1.04%	0.82%	0.04%	0.17%	0.00%	0.01%	1.31%
ENDF-BVII	0.09%	0.20%	0.01%	0.20%	0.00%	0.05%	0.30%
JENDL-4	0.06%	0.44%	0.02%	0.10%	0.00%	0.01%	0.46%

✓ COMAC Pu240 fission and capture are much larger.

ENDF-BVII	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
Na23	0.00%	2.00%	2.54%	3.45%	0.00%	0.00%	4.72%
Fe56	0.00%	0.52%	0.29%	0.42%	0.00%	0.00%	0.73%
U238	0.04%	1.48%	0.46%	3.49%	0.01%	0.23%	3.83%
Pu238	0.02%	0.09%	0.00%	0.01%	0.00%	0.02%	0.09%
Pu239	1.13%	0.55%	0.07%	0.51%	0.00%	0.40%	1.42%
Pu240	0.24%	0.21%	0.01%	0.29%	0.00%	0.11%	0.45%
Pu241	0.32%	0.17%	0.00%	0.12%	0.00%	0.06%	0.39%
Pu242	0.05%	0.28%	0.00%	0.03%	0.00%	0.03%	0.29%
TOTAL	1.20%	2.73%	2.70%	4.96%	0.01%	0.48%	6.41%

Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	3.16%	2.10%	1.39%	1.90%	0.03%	0.50%	4.50%
ENDF-BVII	1.20%	2.73%	2.70%	4.96%	0.01%	0.48%	6.41%
JENDL-4	1.37%	1.87%	1.39%	3.63%	0.01%	0.50%	4.55%

- ✓ By comparing Uncertainties on  $\rho_{\text{Na void}}$  using different covariances: COMAC, ENDF BVII.1 and JENDL4.0, one can notice significant differences

U238 Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	0.07%	1.38%	0.06%	1.66%	0.03%	0.11%	2.16%
ENDF-BVII	0.04%	1.48%	0.46%	3.49%	0.01%	0.23%	3.83%
JENDL-4	0.04%	1.60%	0.06%	1.92%	0.01%	0.11%	2.50%

✓ ENDF BVII.1 U238 inelastic and JENDL4.0 U238 capture are much larger.

Pu239 Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	3.09%	0.91%	0.04%	0.15%	0.00%	0.48%	3.26%
ENDF-BVII	1.13%	0.55%	0.07%	0.51%	0.00%	0.40%	1.42%
JENDL-4	1.19%	0.32%	0.02%	0.13%	0.00%	0.48%	1.33%

- ✓ COMAC Pu239 fission is significantly larger than the one of ENDF BVII and JENDL4.

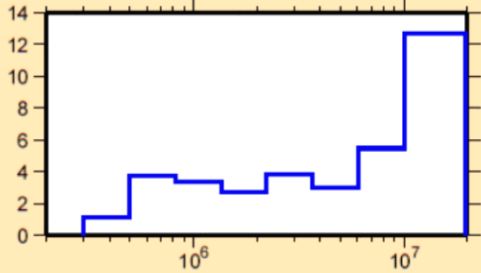
Na23	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	0.00%	0.74%	1.32%	0.87%	0.00%	0.00%	1.75%
ENDF-BVII	0.00%	2.00%	2.54%	3.45%	0.00%	0.00%	4.72%
JENDL-4	0.00%	0.29%	1.31%	3.00%	0.00%	0.00%	3.29%

✓ ENDF-B VII Na23 capture, elastic and inelastic are much larger.

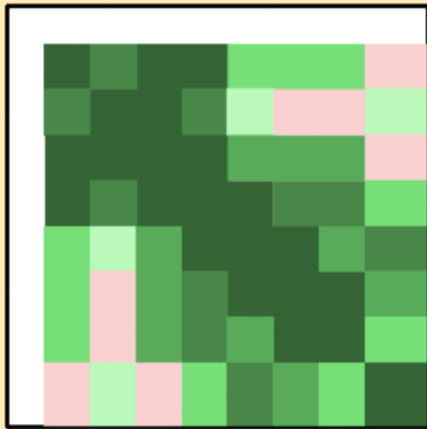
# NA23 INELASTIC COVARIANCES

## COMAC

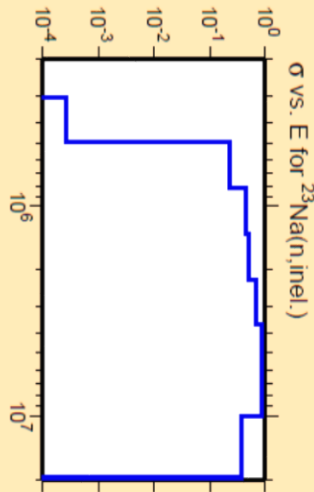
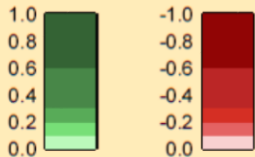
$\Delta\sigma/\sigma$  vs. E for  $^{23}\text{Na}(n,\text{inel.})$



Ordinate scales are % relative standard deviation and bars.  
Abscissa scales are energy (eV).

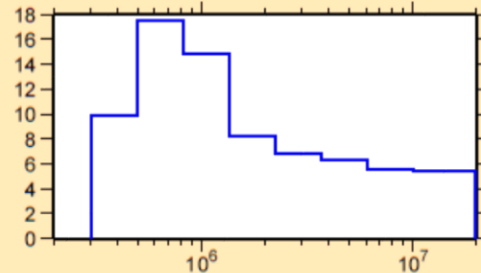


Correlation Matrix

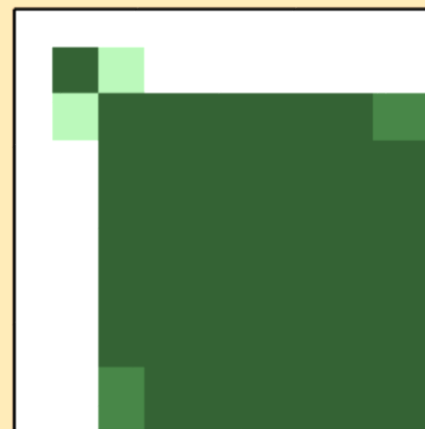


## ENDF B VII

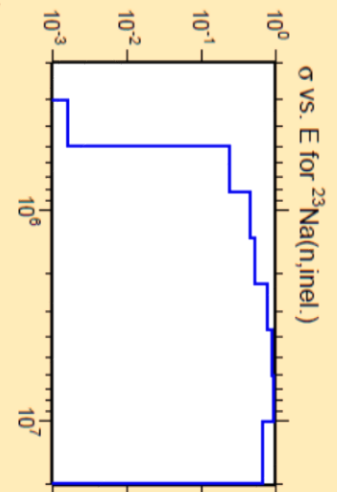
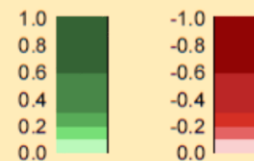
$\Delta\sigma/\sigma$  vs. E for  $^{23}\text{Na}(n,\text{inel.})$



Ordinate scales are % relative standard deviation and bars.  
Abscissa scales are energy (eV).



Correlation Matrix



- ✓ The  $k_{\text{eff}}$  uncertainty is predominantly due to the uncertainties in inelastic scattering of U238 and in the fissions of Pu239 and U238.
- ✓ The  $\rho_{\text{Doppler}}$  uncertainty is predominantly due to the uncertainties in inelastic scattering of U238 and in the capture of Pu239 and in the elastic removal of Na23 and Fe56.
- ✓ The  $\rho_{\text{Na void}}$  uncertainty is predominantly due to the uncertainties in inelastic scattering of U238 and Na23, in the capture of U238, in the fission of Pu239 and in the elastic and inelastic removal of Na23.
- ✓ There are significant differences between covariances coming from COMAC, ENDF BVII.1 and JENDL4.0.

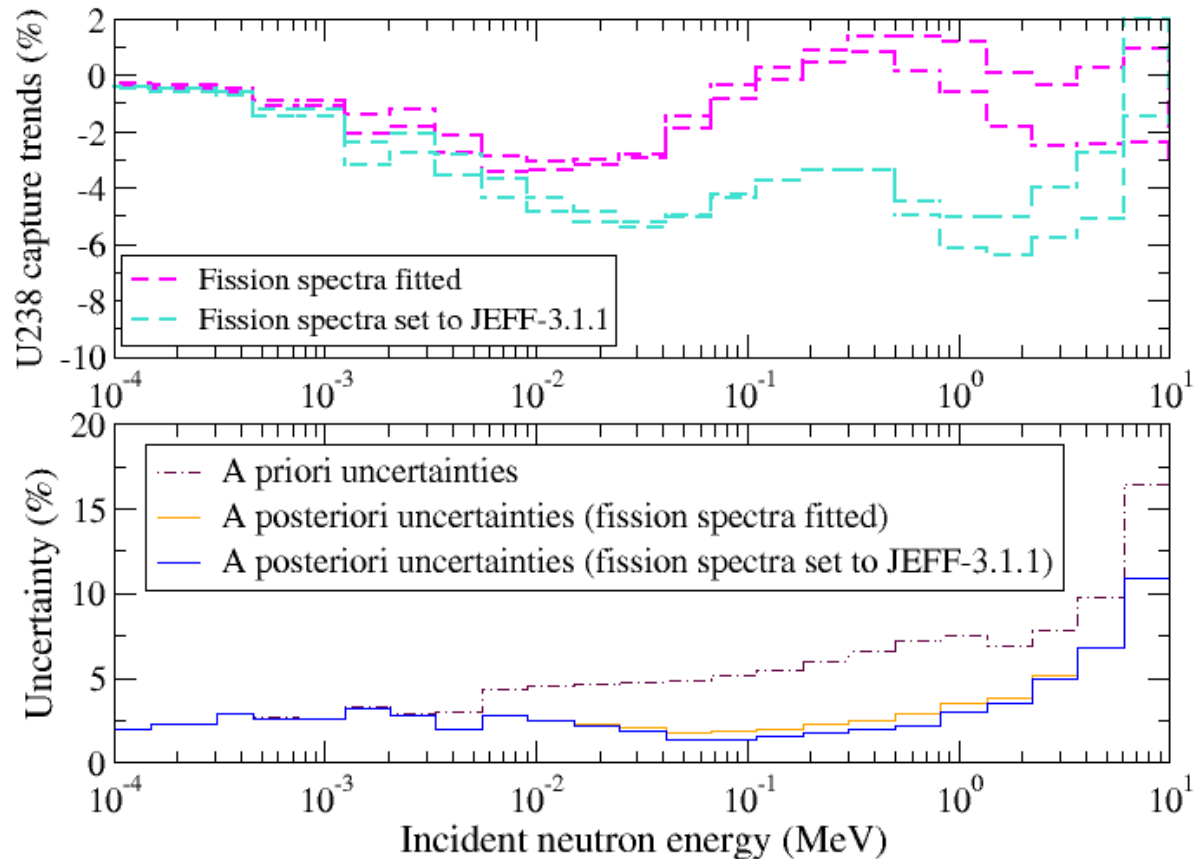
Results taken from OECD WPRS SFR-UAM group

Results in [%]	Medium Metallic SFR				Large Oxide SFR		
	ANL	CEA Cad	IPPE- GRS	IPPE- S/U	CEA Cad	IPPE- GRS	IPPE- S/U
<b>k-effective</b>	1.3	0.8	1.5	1.5	0.8	1.5	1.6
<b><math>\beta_{\text{eff}}</math></b>	1.1	3.4	1.1	-	3.5	1.2	-
<b>Control Rod Worth</b>	2.8	1.1	2.7	2.5	1.4	2.8	3.6
<b><math>K_{\text{Doppler}}</math></b>	5.8	3.9	7.5	6.2	3	5.9	5.3
<b>Na Void Worth</b>	19.2	-	26.3	28.2	4.5	14.5	13

- Uncertainty calculations from ANL (with COMMARA), CEA (COMAC) and IPPE (ABBN).
- Larger uncertainty is estimated by CEA on  $\beta_{\text{eff}}$  since they take into account uncertainties from delayed neutron constants
- Differences in covariance matrices should be further understood (see SG44 on Investigation of Covariance Data in General Purpose Nuclear Data Libraries)

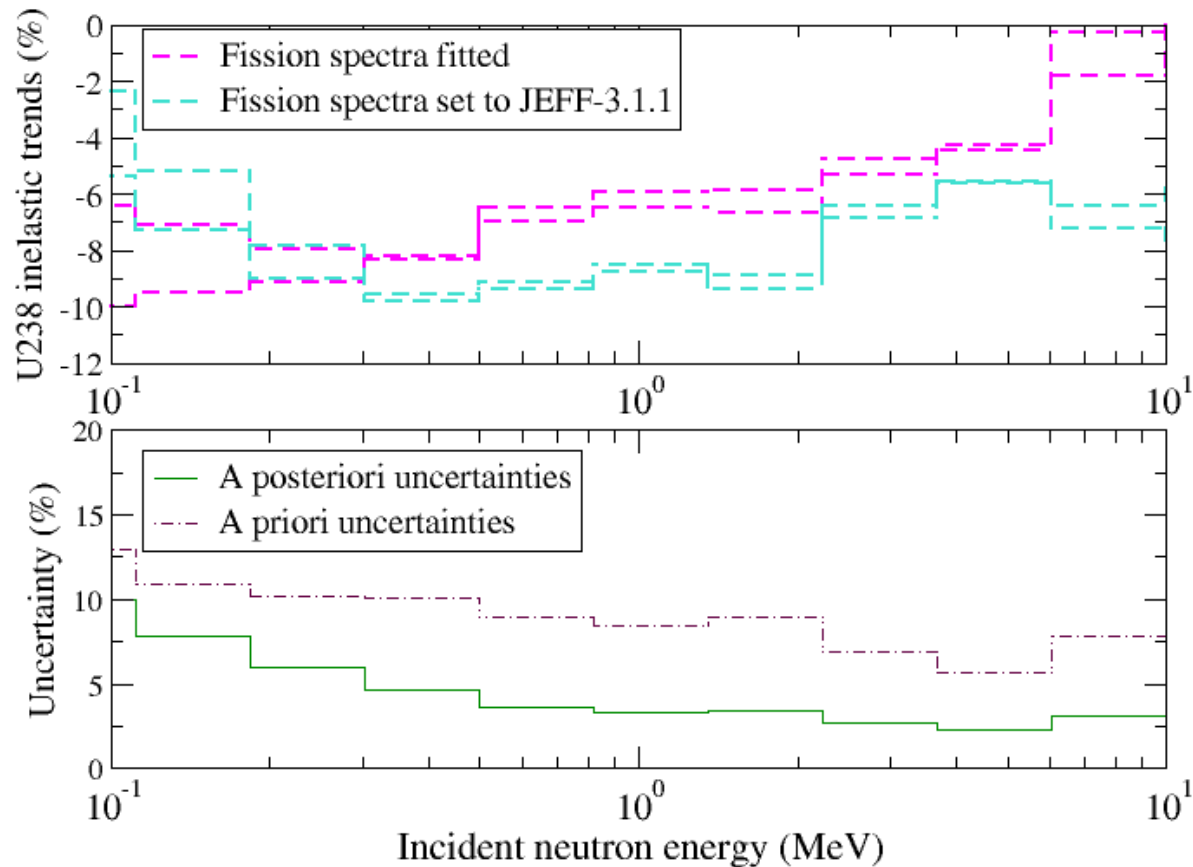
- Integral data assimilation can contribute to the nuclear data improvement
- **Parametric studies** have been done so as not be too dependent to the nuclear data **covariance data** that are **still perfectible** or even missing (COMAC V1 used).
- **Marginalization technique** has been **used for light and structural isotopes** for which approximations (anisotropy, secondary neutron energy distribution) in the integral data assimilation technique are rather high.
- **Attention is being given to ways that minimize compensating errors.**
- Compensating errors between U238 capture and Pu239 fission (such as in **CARNAVAL IV**) has been eliminated by using first only U-fueled experiments then adding Pu-fueled experiments.
- A test on whether PFNS needs to be fitted or not (such as in **ERALIB1**). It appears that PFNS is a major source of uncertainty and requires to be fitted

- Trends noticeably differ depending on whether fission spectrum is fitted or not.



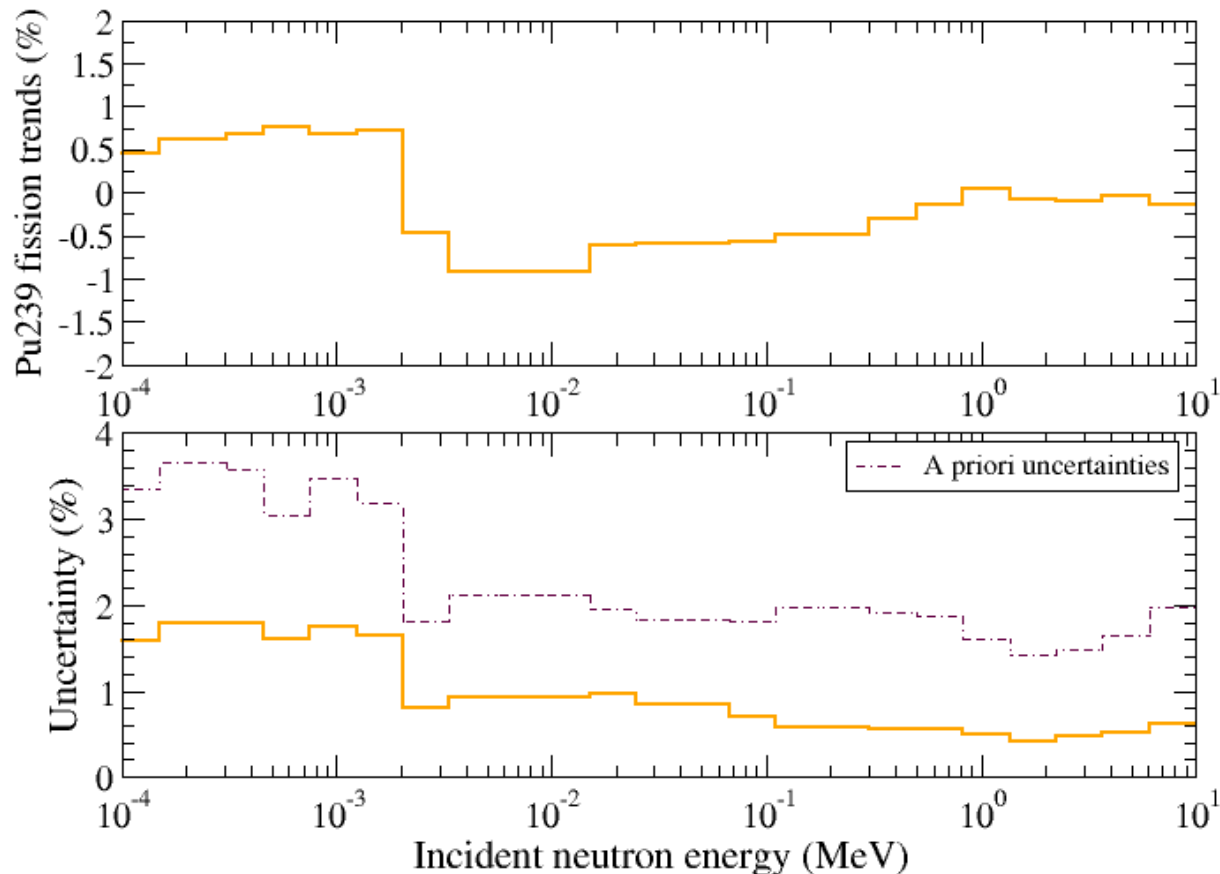
→ Fission spectra have been identified as the **main source of uncertainties** in our assimilation work.

Trends noticeably differ depending on whether fission spectrum is fitted or not.

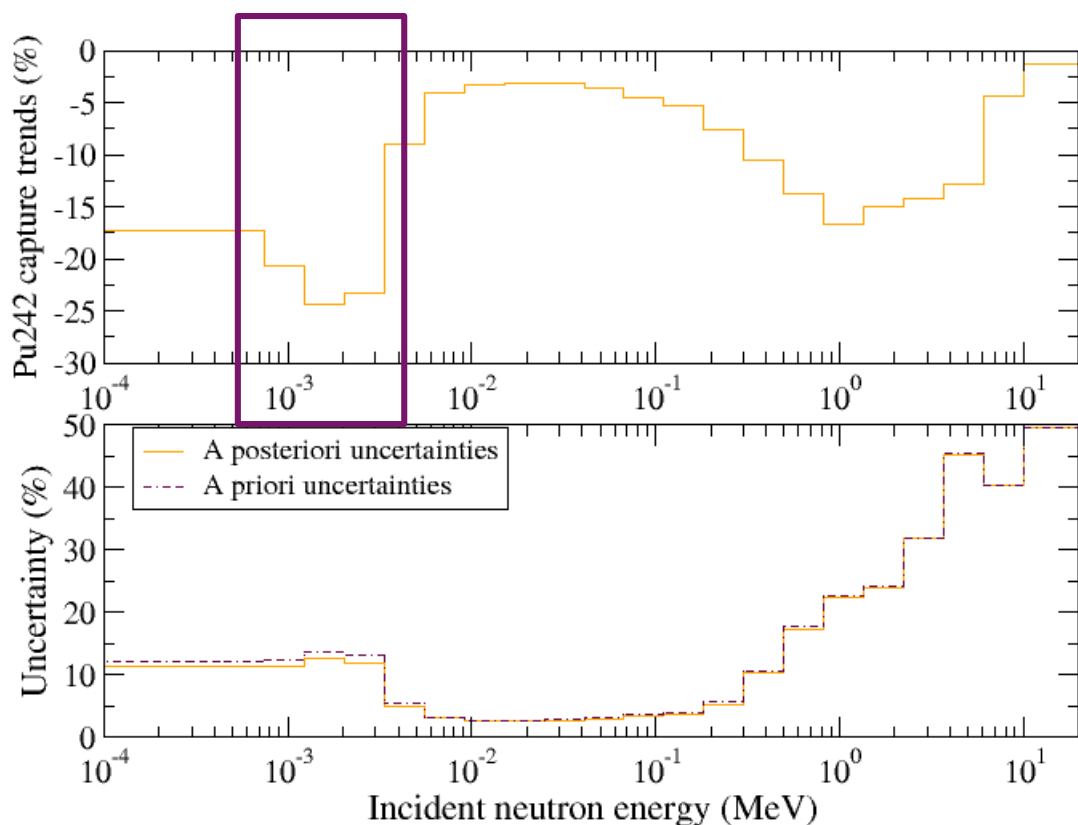


→ Fission spectra have been identified as the **main source of uncertainties** in our assimilation work.

Even though there is a variety of different experiments, changes in xs are mainly focused where uncertainties are estimated to be larger.



- Trends are driven by a single integral information: PROFIL (C/E~1.14 with JEFF-3.1.1) and follow prior uncertainties.
- IDA trends hence have an unreliable energy breakdown with prior uncertainty greatly **underestimated below 4keV (beginning of the URR)**.



- Integral data assimilation has identified the lack of differential measurements, in particular for prompt fission neutron spectrum or U238 inelastic.
- Parametric studies have shown that nuclear data covariance data with better reliability are required (for PFNS and some capture cross sections).
- The differences in the U238 inelastic cross section are presumably due to optical models being used, differential measurements being scarce.
- The differences in the Na23 cross sections are due to the use of more recent differential measurements performed at IRMM (inelastic) and Oak Ridge (total).
- Marginalization has been used for anisotropy of scattering and distribution of secondary energy neutrons since covariance data is missing. Hence, there is a request to have those covariance in particular for light and structural isotopes.
- Covariances on delayed neutron constants (including delayed neutron spectrum) are needed to estimate uncertainties on  $\beta_{\text{eff}}$  (only available in JENDL-4 and used in COMAC)

