Joint Meeting of CIELO and WPEC Subgroup 39 on
Methods and approaches to provide feedback from nuclear and covariance data adjustment for improvement of nuclear data files

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Revised Recommendations from ADJ2010 Adjustment

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Introduction

ADJ2010 is a 70-group adjusted library based on JENDL-4.0, where 488 integral experimental data from 8 facilities (ZPPR, ZEBRA, JOYO, MONJU, BFS, MASURCA, SEFOR and Los Alamos) were used for the adjustment.

Here, the major alteration of nuclear data by the adjustment is summarized for 5 nuclides (Pu-239, U-238, U-235, Fe-56 and Na-23), and compared with ENDF/B-VII.1 and JEFF-3.1.2.

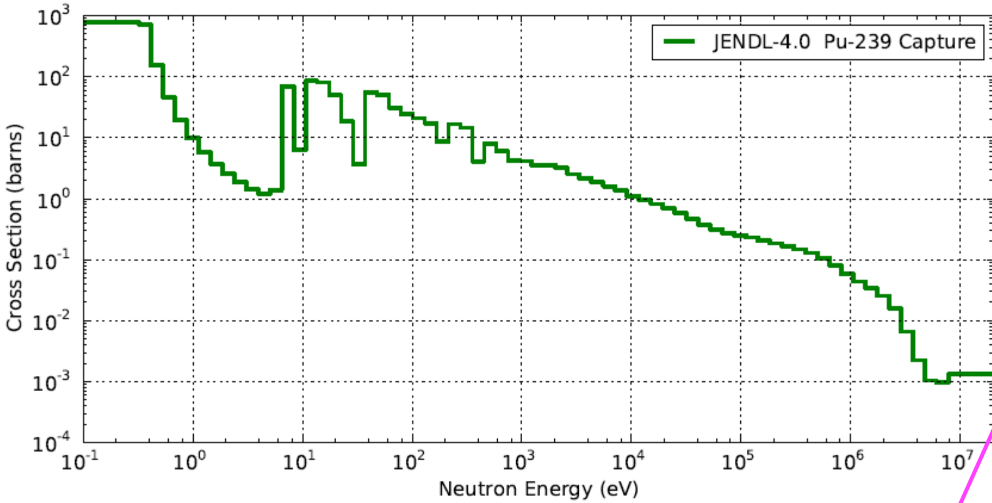
Finally, we try to make some recommendations to nuclear-data evaluators, though it is not mature.

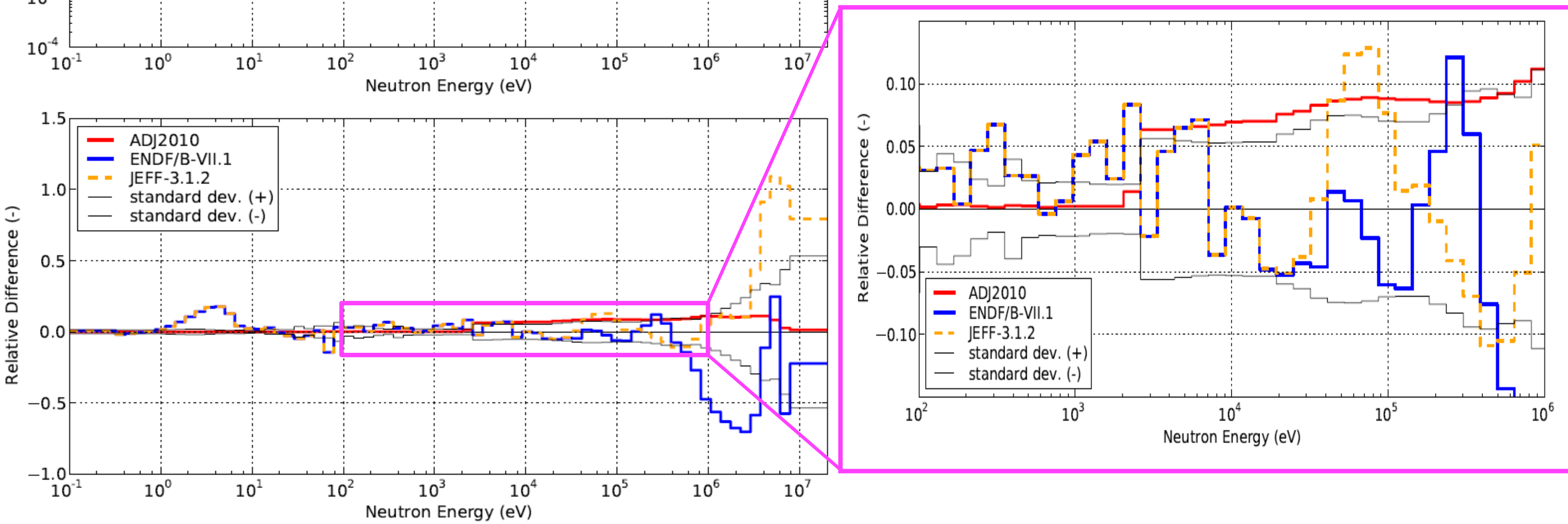
A thick report of ADJ2010 is available from the URL below with the huge numerical results in digital files.

http://jolissrch-inter.tokai-sc.jaea.go.jp/search/servlet/search?5035118&language=1

Pu-239

Pu-239 Capture





- ADJ2010 increases Pu-239 capture cross-section over 3keV by 7 to 9%. This large alteration is at the variance bound of JENDL-4, but agrees with NEITHER of the three major libraries. The increase is determined by a combination of integral experiments. -> next slides.
- Present measured data are quite old before 1976. New DANCE data will be published soon.

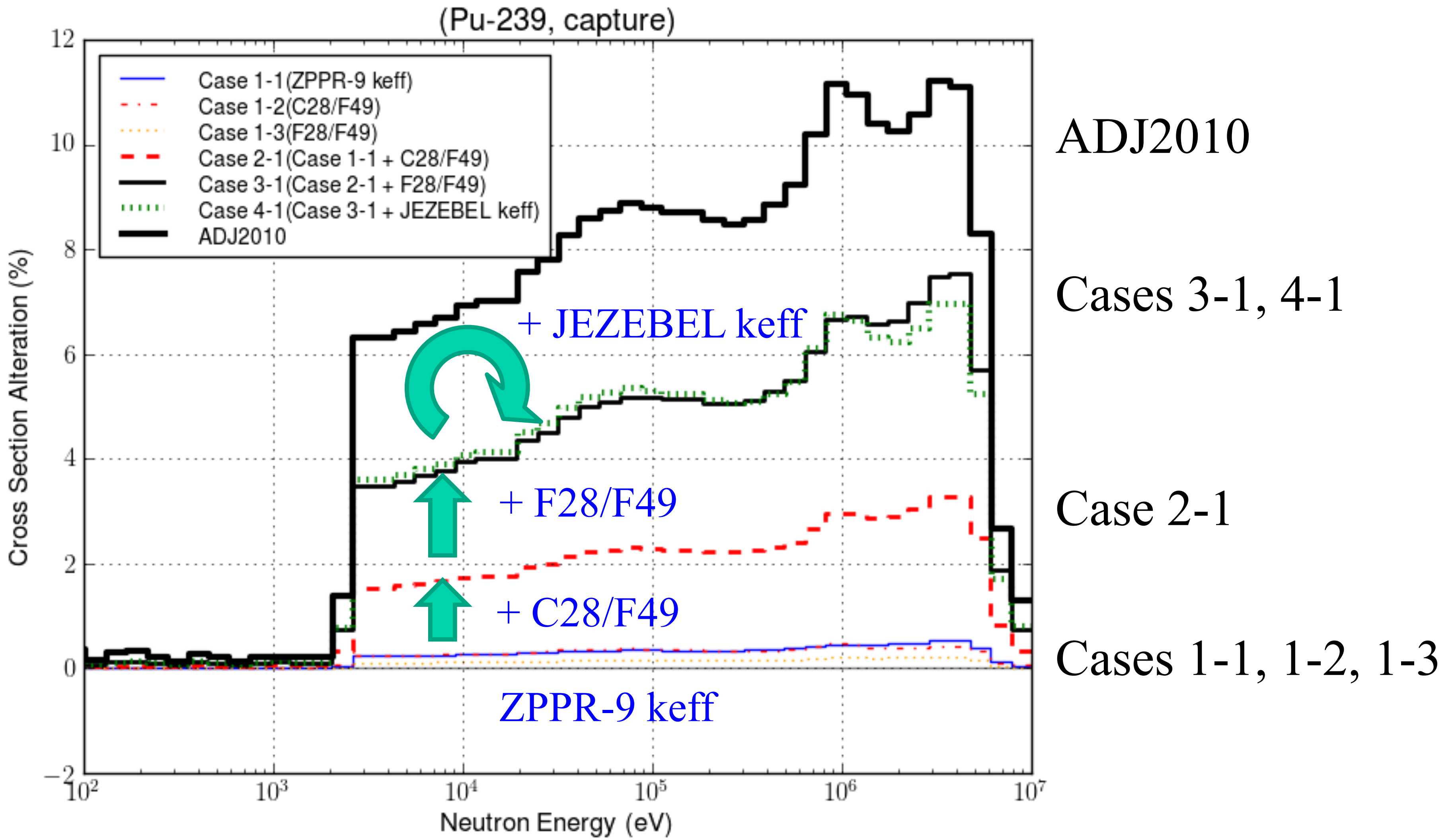
Small Test Cases to Investigate Mechanisms

Integral Experiments Used in Small Test Cases

	ZPPR-9			JEZEBEL
	keff	C28/F49	F28/F49	keff
Case 1-1	X			
Case 1-2		X		
Case 1-3			X	
Case 2-1	X	X		
Case 3-1	**X**	**X**	**X**	
Case 4-1	X	X	X	X

- It is heuristically found that Case 3-1 reproduces well the cross-section alteration of Pu-239 capture of ADJ2010
- In spite of using only 3 data, compared with 488 data of ADJ2010

Cross-section Alteration of Pu-239 capture

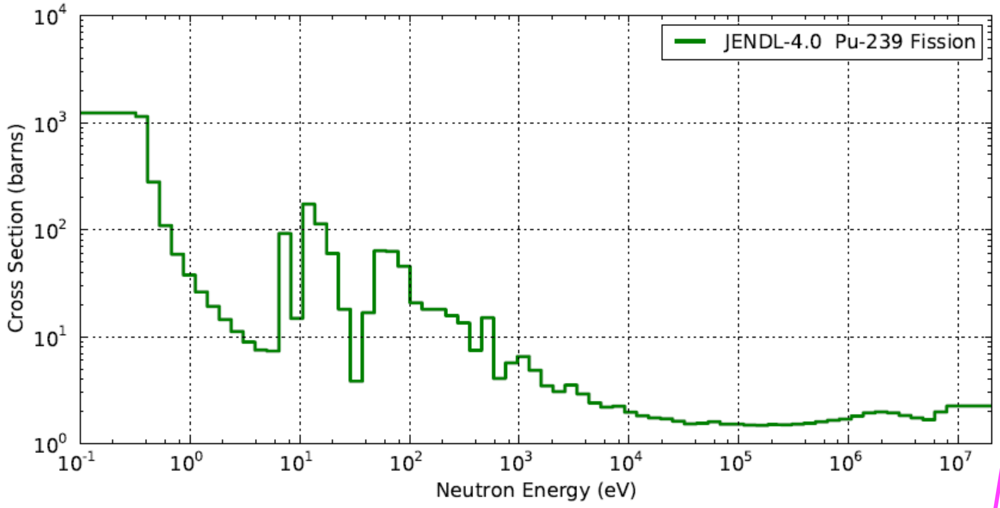


- Not moved by using only ZPPR-9 keff (*motive force* = +2.45)
- Begin to move by a combination of integral experiments

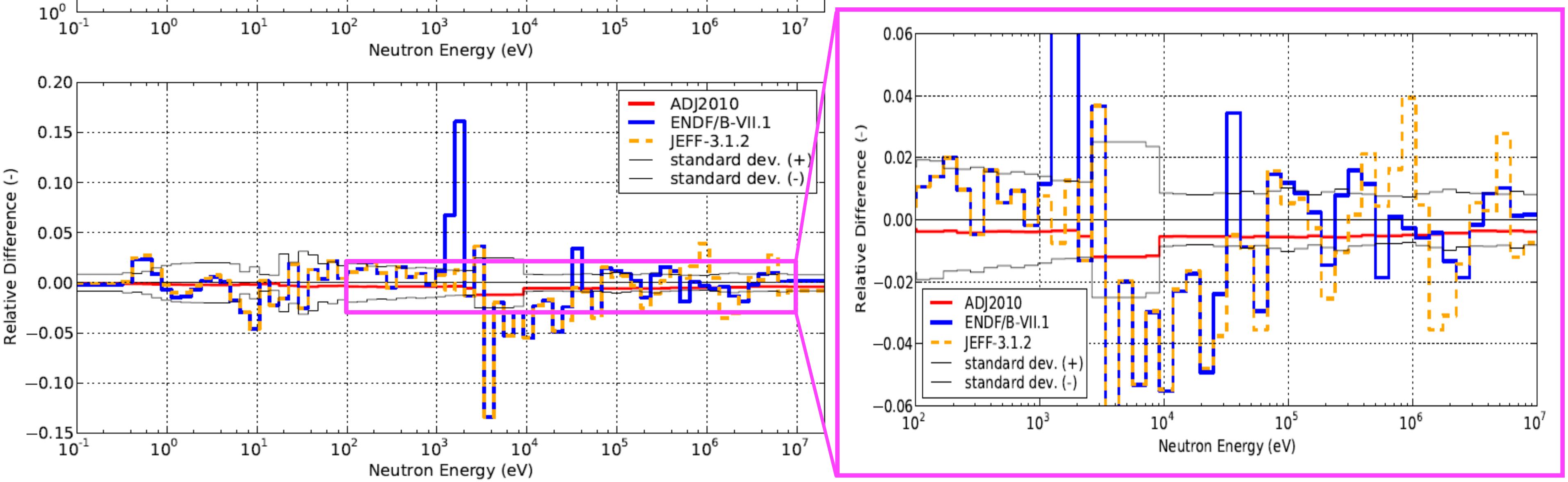
Summary of "Conflict" and "Freely Adjustable"

Case	1-1	1-2	1-3	2-1	3-1	4-1
Integral experiments used for adjustment	Z9-keff	C28/F49	F28/F49	Z9-keff C28/F49	Z9-keff C28/F49 F28/F49	Z9-keff C28/F49 F28/F49 JZ-keff
Pu-239 capture	F	F	F	F	F	C
Pu-238 fission	F	F	F	C	C	C
Pu-239 χ	F	F	F	C	C	C
Pu-239 (n, n)	-	-	-	-	-	F
U-238 capture	F	F	F	C	C	C
U-238 fission	F	F	F	F	C	C
U-238 (n, n')	F	F	F	C	C	C

- Case 2-1: Pu-239 capture begins to move
- Case 3-1: Pu-239 capture moves more
- Case 4-1: Conflict but Pu-239 (n, n) begins to move



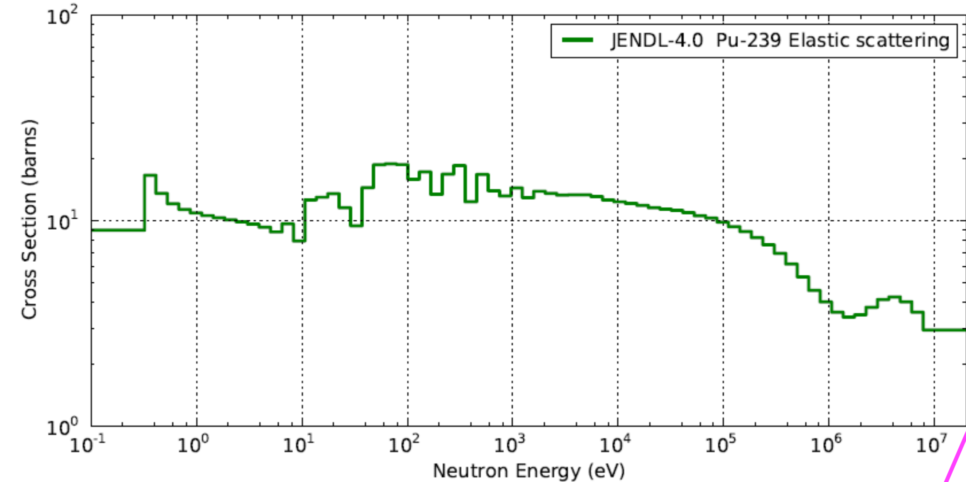
Pu-239 Fission

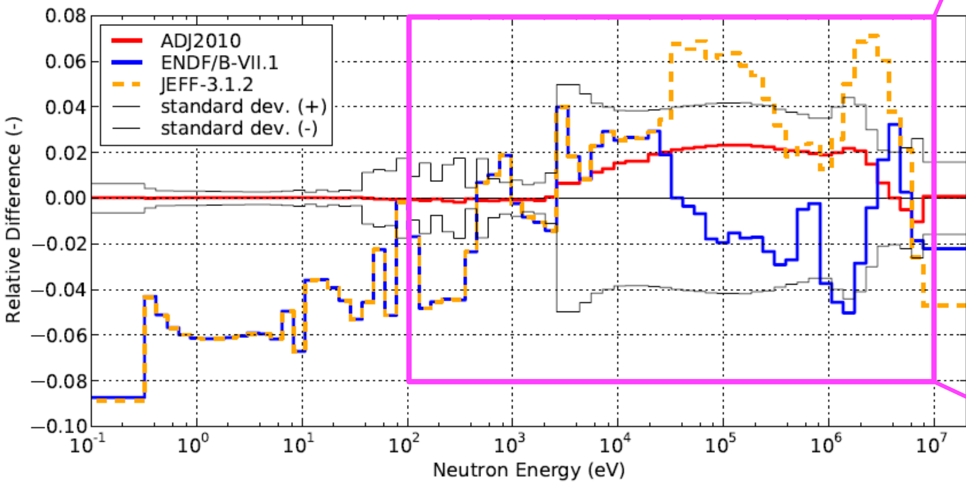


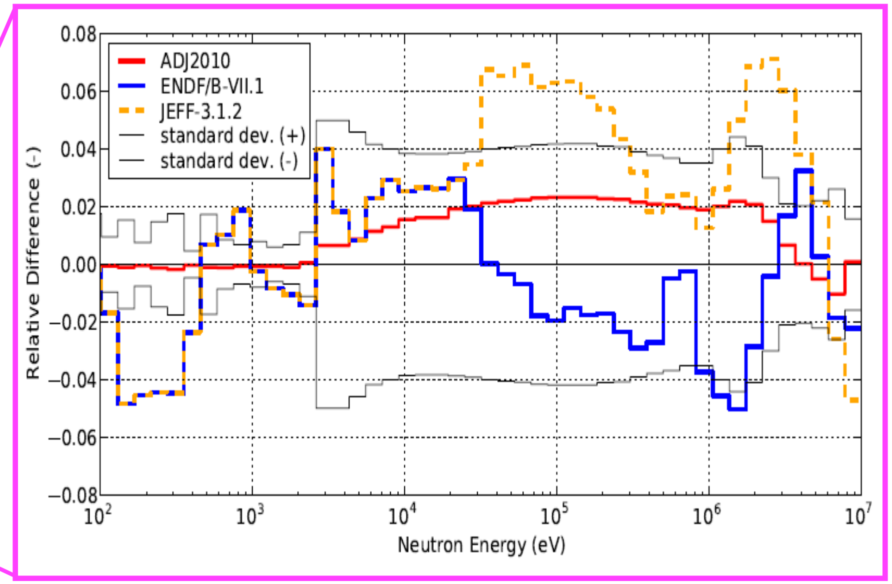
- ADJ2010 decreases Pu-239 fission cross-section by approximately 0.5%.
- ENDF and JEFF seem to be consistent with JENDL-4.0 or ADJ2010 in average, but there are large fluctuations exceeding the variance. It may be better to consult nuclear data people about the reason.

Pu-239

Elastic scattering

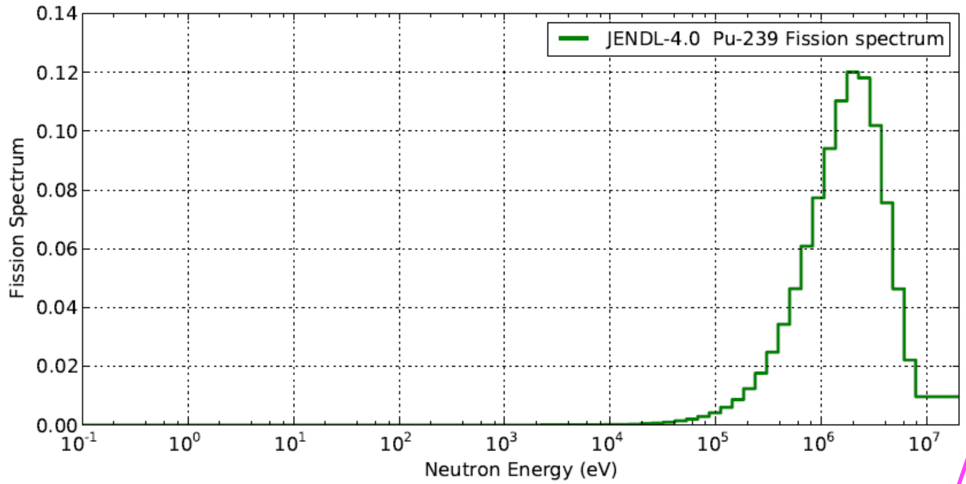


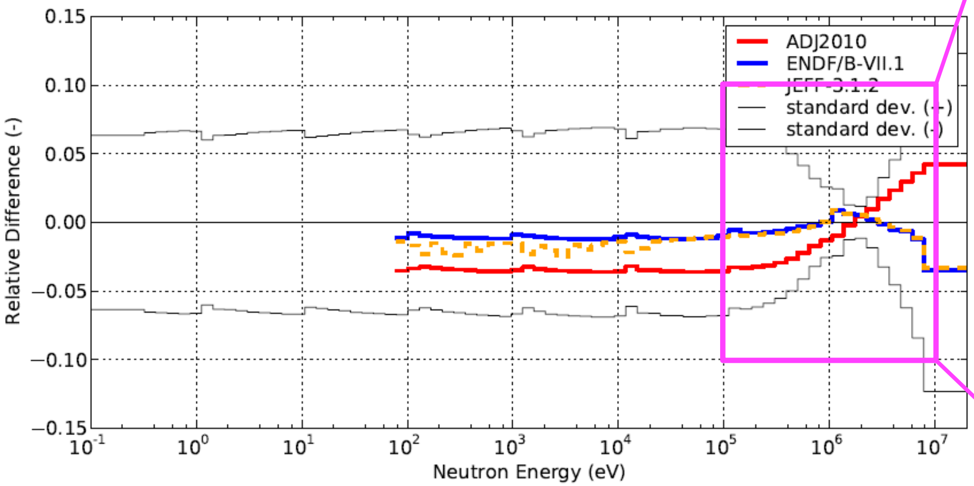


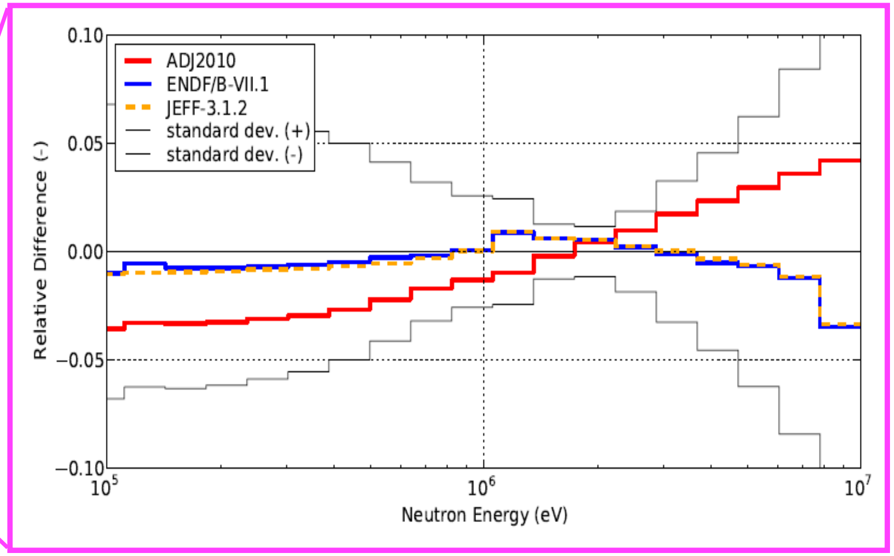


- ADJ2010 increases Pu-239 elastic-scattering cross-section by 2% at the maximum. This alteration is within the variance of JENDL-4.

Pu-239 Fission spectrum



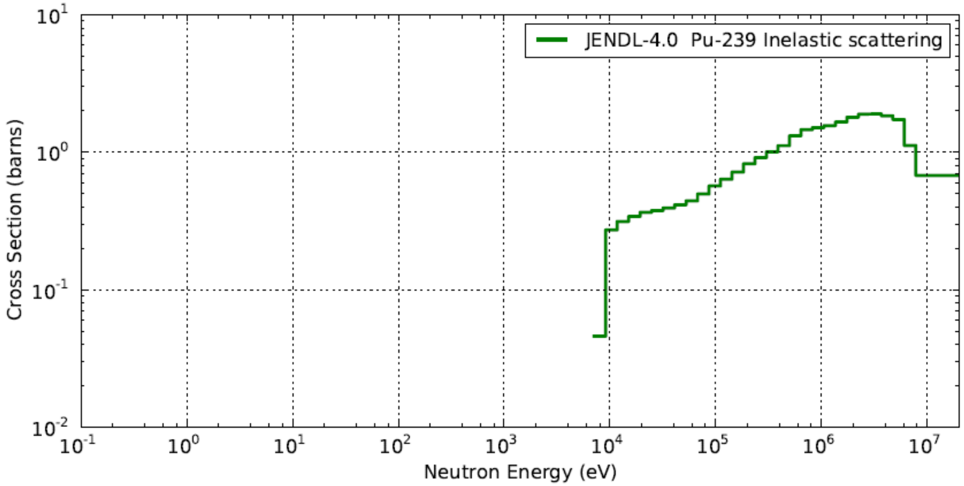


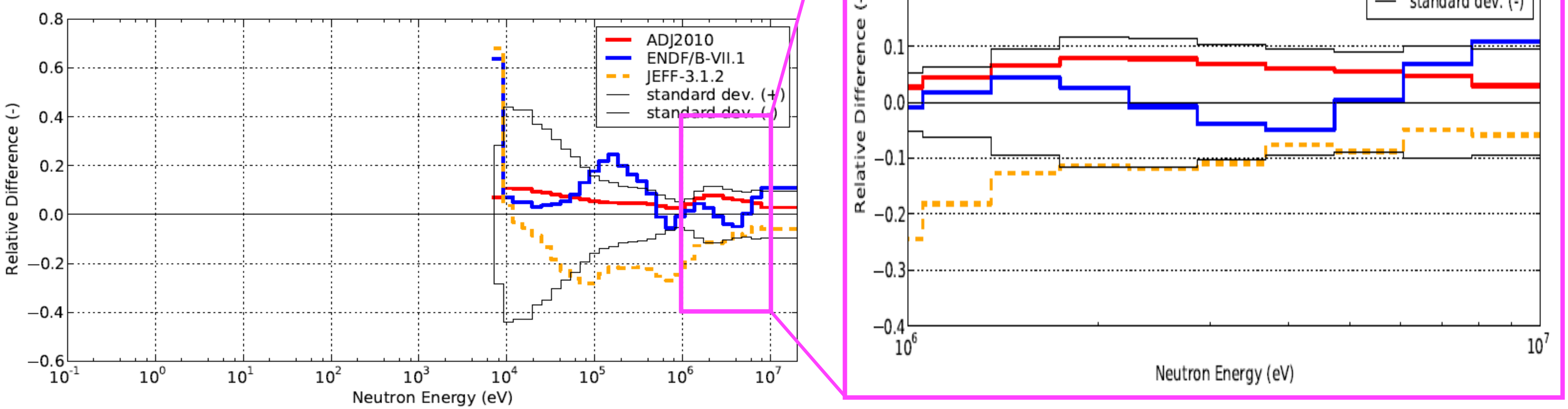


- ADJ2010 hardened Pu-239 fission spectrum by 4% at the maximum.
- This large alteration is within the variance of JENDL-4, but agrees with NEITHER of the three major libraries.
- Current covariance fixes the peak value of spectrum at 2MeV.

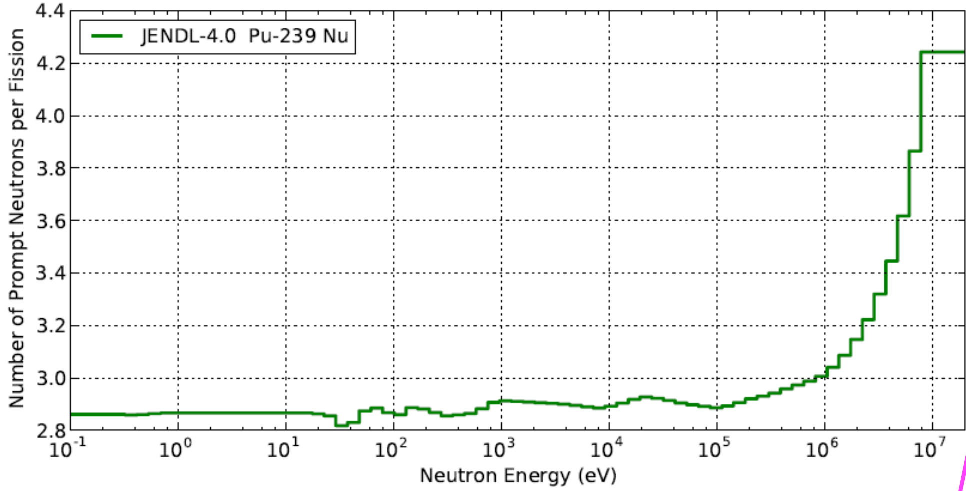
Pu-239

Inelastic scattering



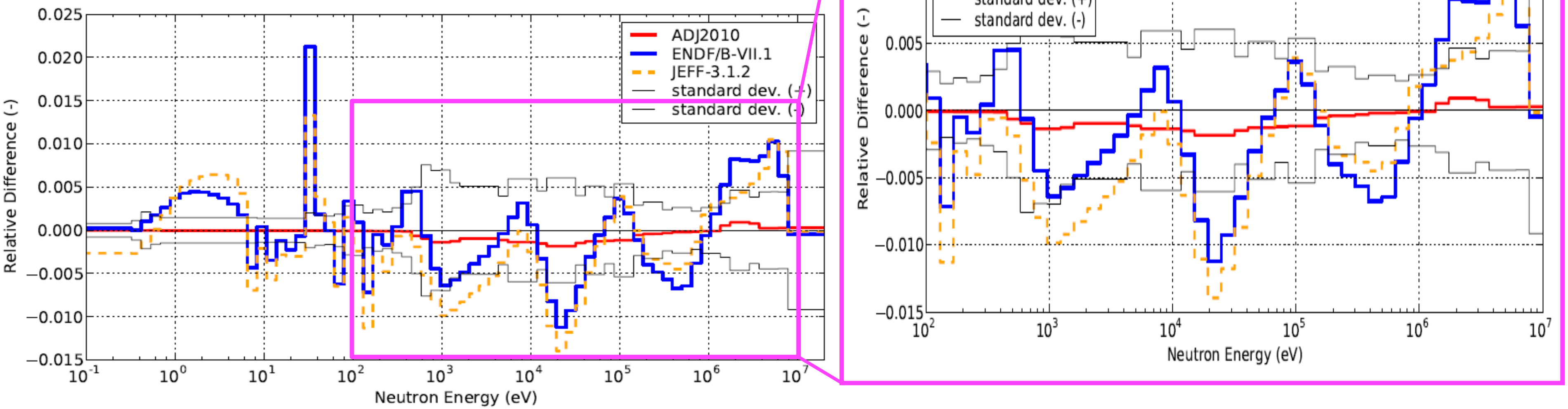


- ADJ2010 increases Pu-239 inelastic scattering cross-section by 10% at the maximum. This alteration is within the variance of JENDL-4.
- Increase of inelastic scattering compensates the effect of the Pu-239 fission spectrum hardening on Na void reactivity, but the mechanism of increase is NOT known.



Pu-239

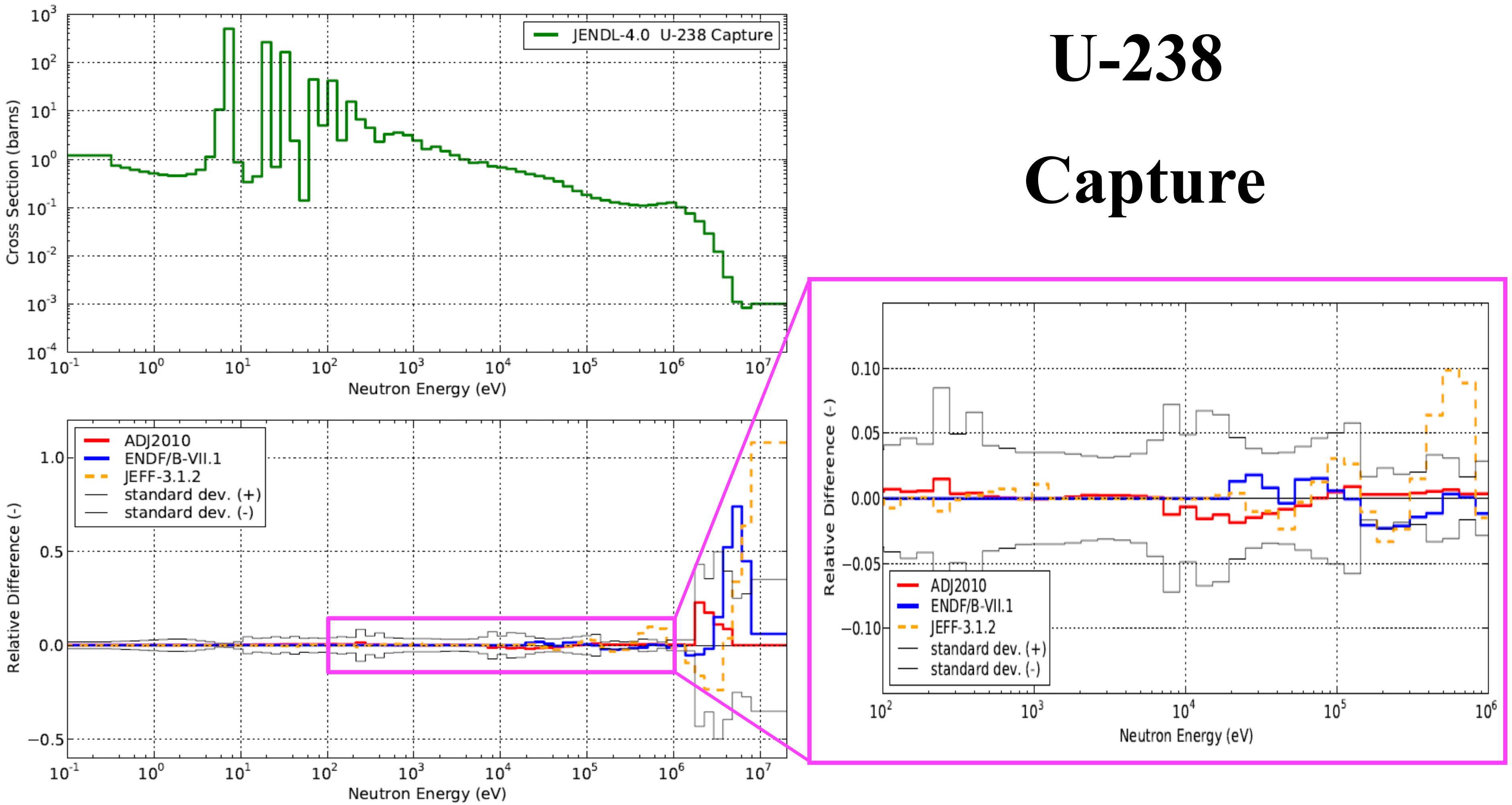
Nu



- ADJ2010 decreases prompt neutron number from Pu-239 fission by 0.2%. This small decrease is consistent with the 0.2%dk overestimation of JENDL-4 for large Pu-fueled cores.
- The difference between JENDL-4.0 and ENDF/JEFF shows strange wave-shape.

U-238

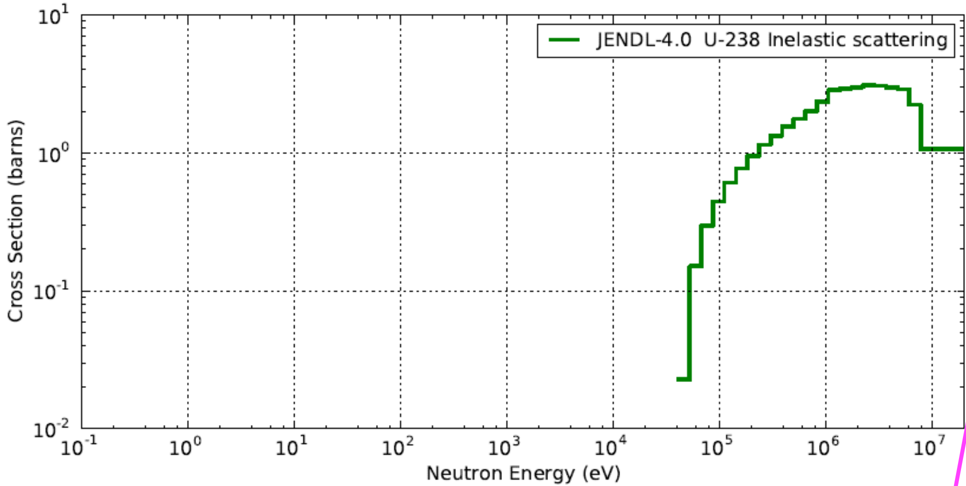
U-238 Capture

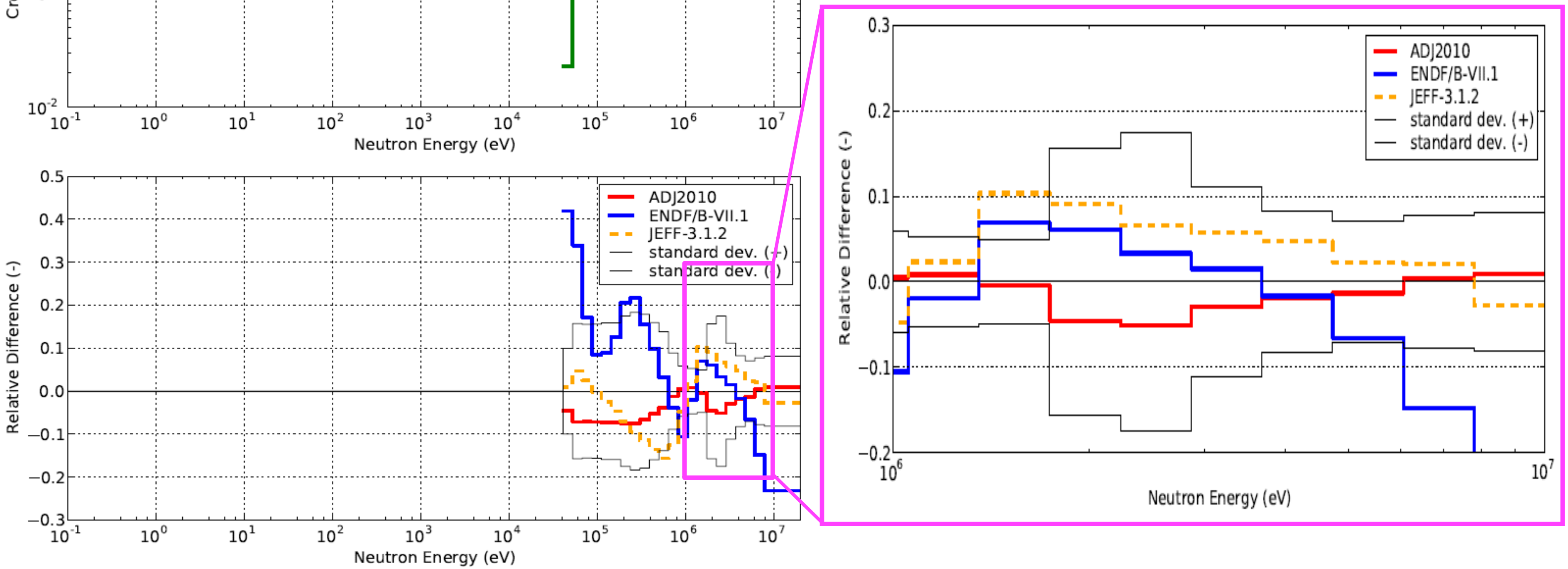


- ADJ2010 changes U-238 capture cross-section between +2 and -2%. This small alteration is within the variance of JENDL-4, and agrees with the three major libraries.

U-238

Inelastic scattering

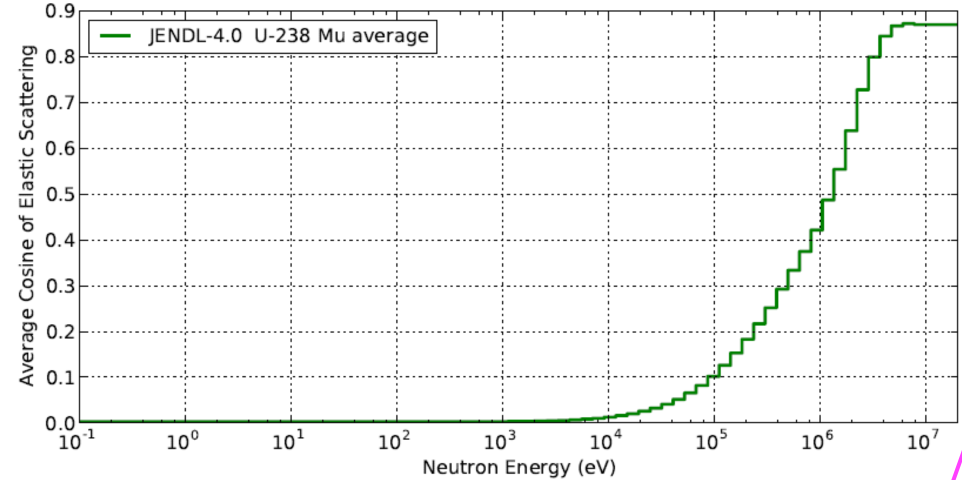


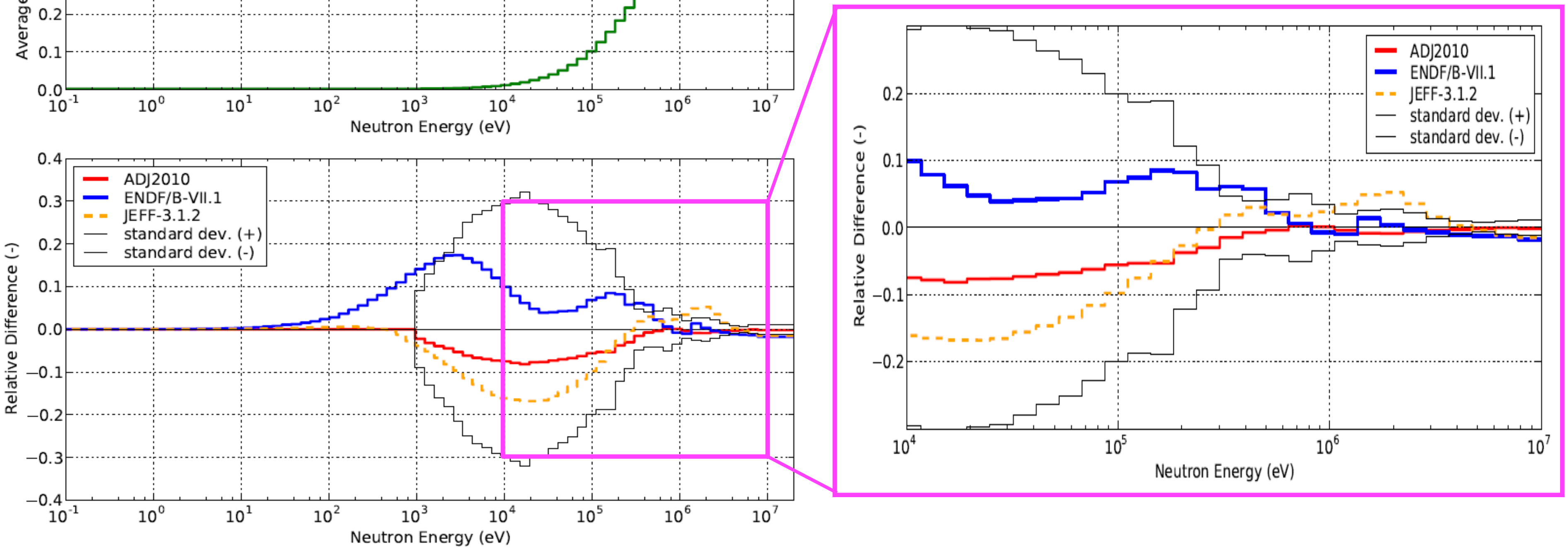


- ADJ2010 slightly decreases Pu-239 inelastic-scattering cross-section between 0 and 5% over 1MeV. This alteration is within the variance of JENDL-4.
- This decrease of inelastic-scattering is the opposite direction to correct the overestimation of Na void reactivity for Pu-fueled cores with JENDL-4.0.

U-238

Mu-ave.

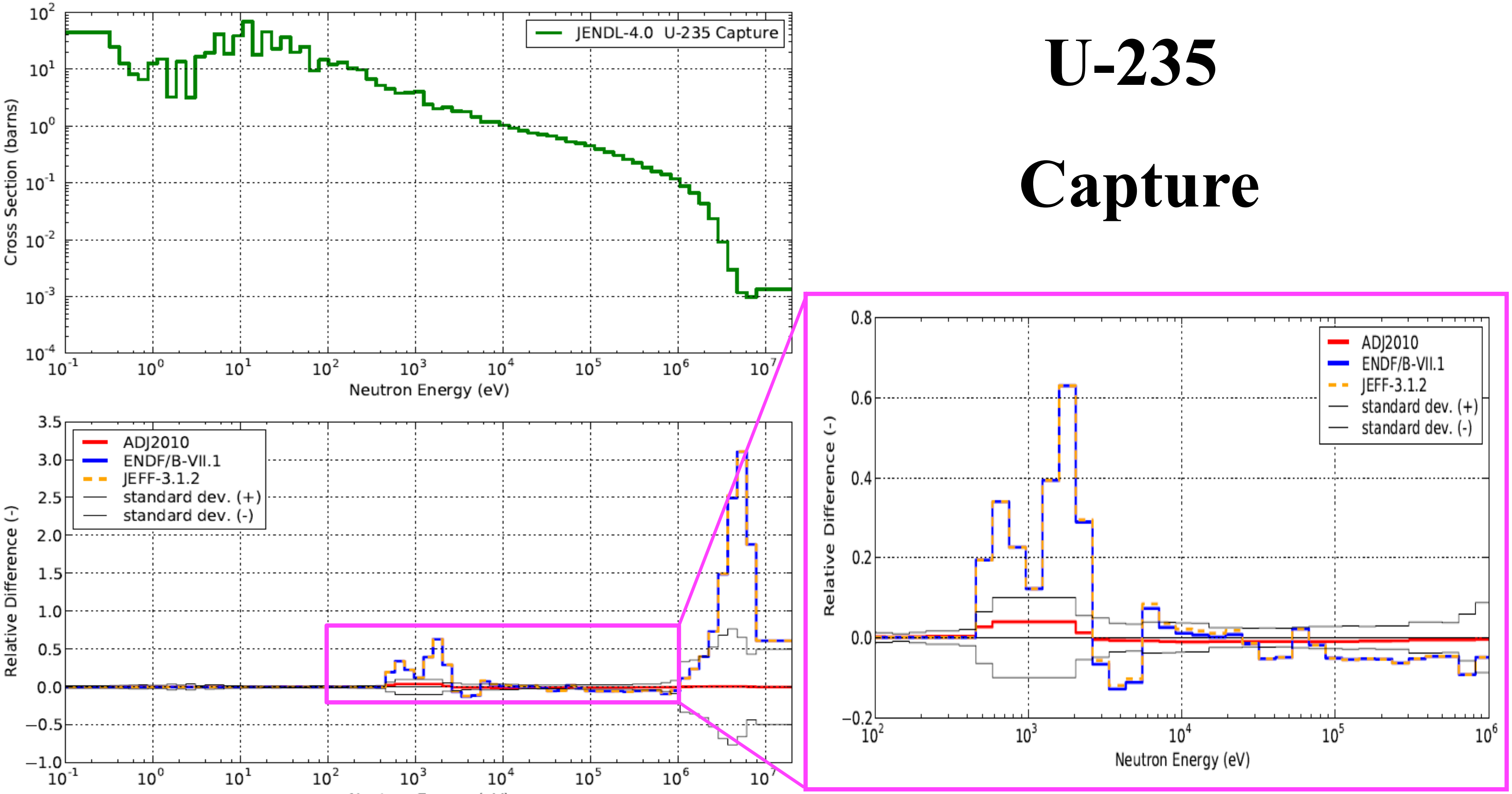




- ADJ2010 decreases U-238 mu-ave. by 8% at maximum. The effect of this alteration to adjusted C/Es are NOT clear.
- The evaluation of mu-ave. does NOT seem converged at all. Expect to be improved by SG35.

U-235

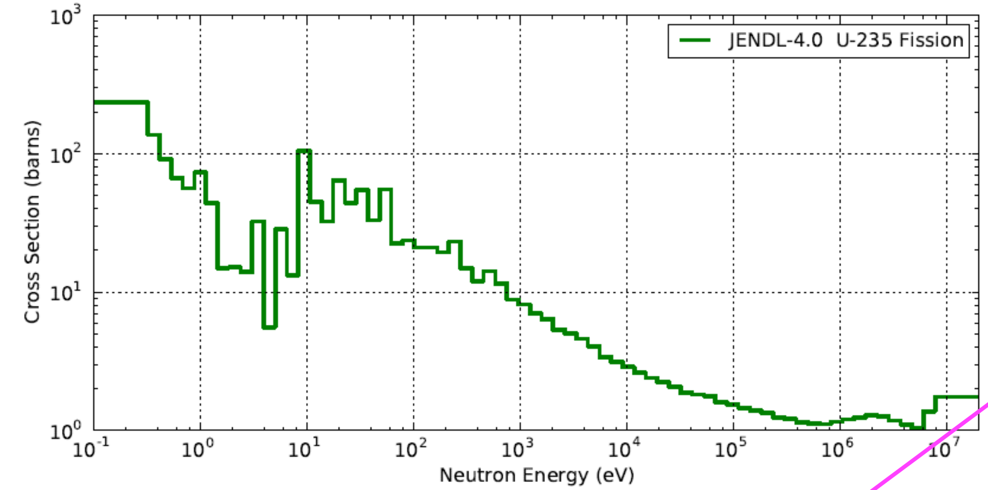
U-235 Capture

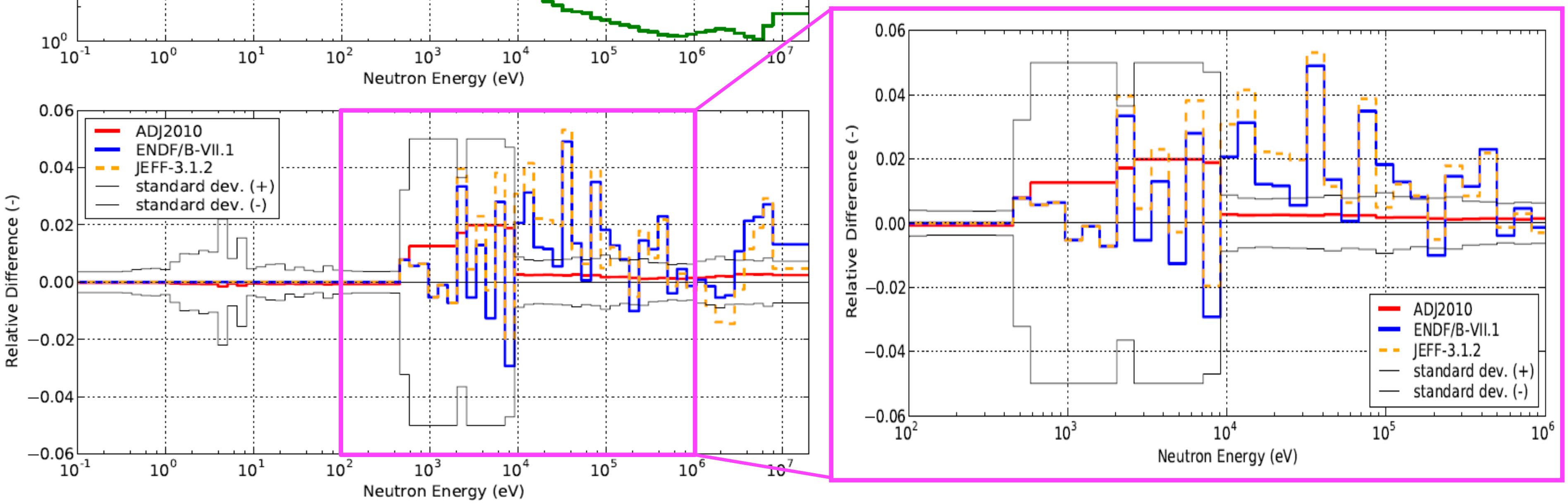


- ADJ2010 slightly changed U-235 capture cross-section only around 1 keV. This little alteration is consistent with CIELO evaluation, which is similar with JENDL-4.0.

U-235

Fission



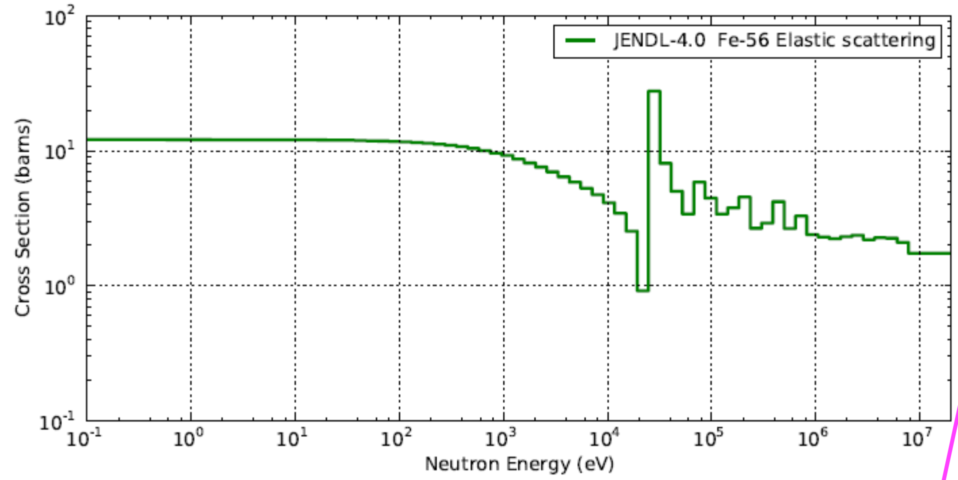


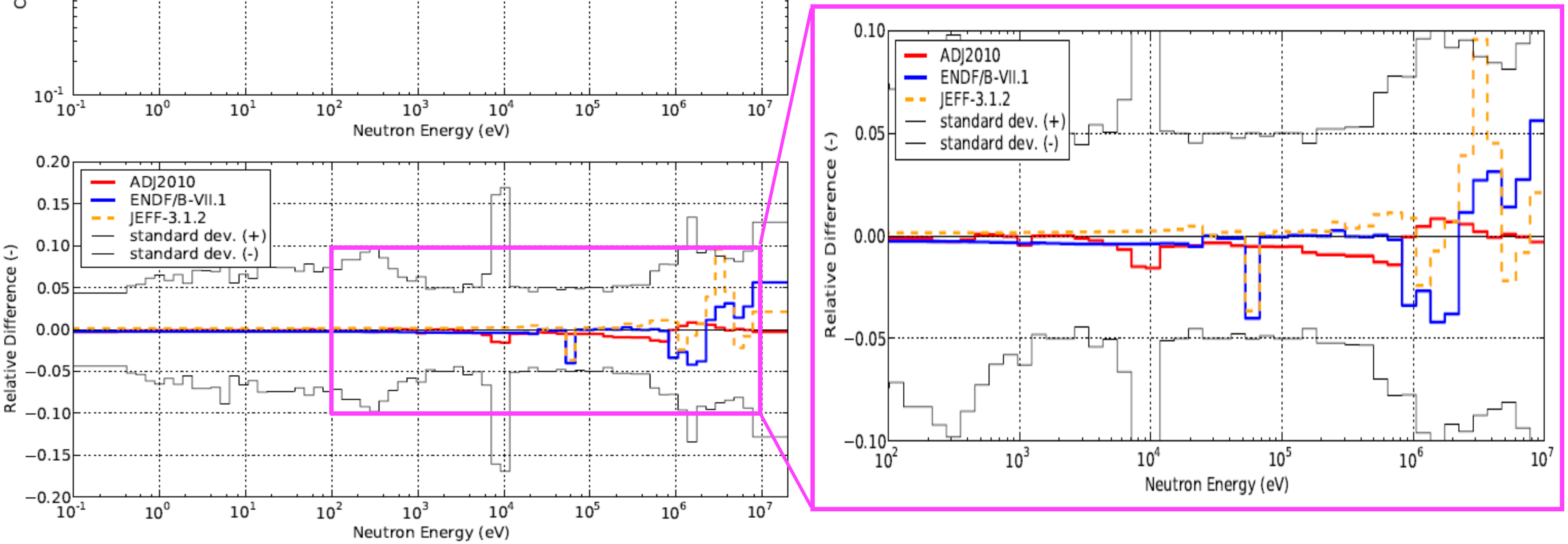
- No comments for ADJ2010.
- Even this major cross-section has quite large difference among libraries in high energy region, since it is not related to thermal reactors, maybe.

Fe-56

Fe-56

Elastic scattering

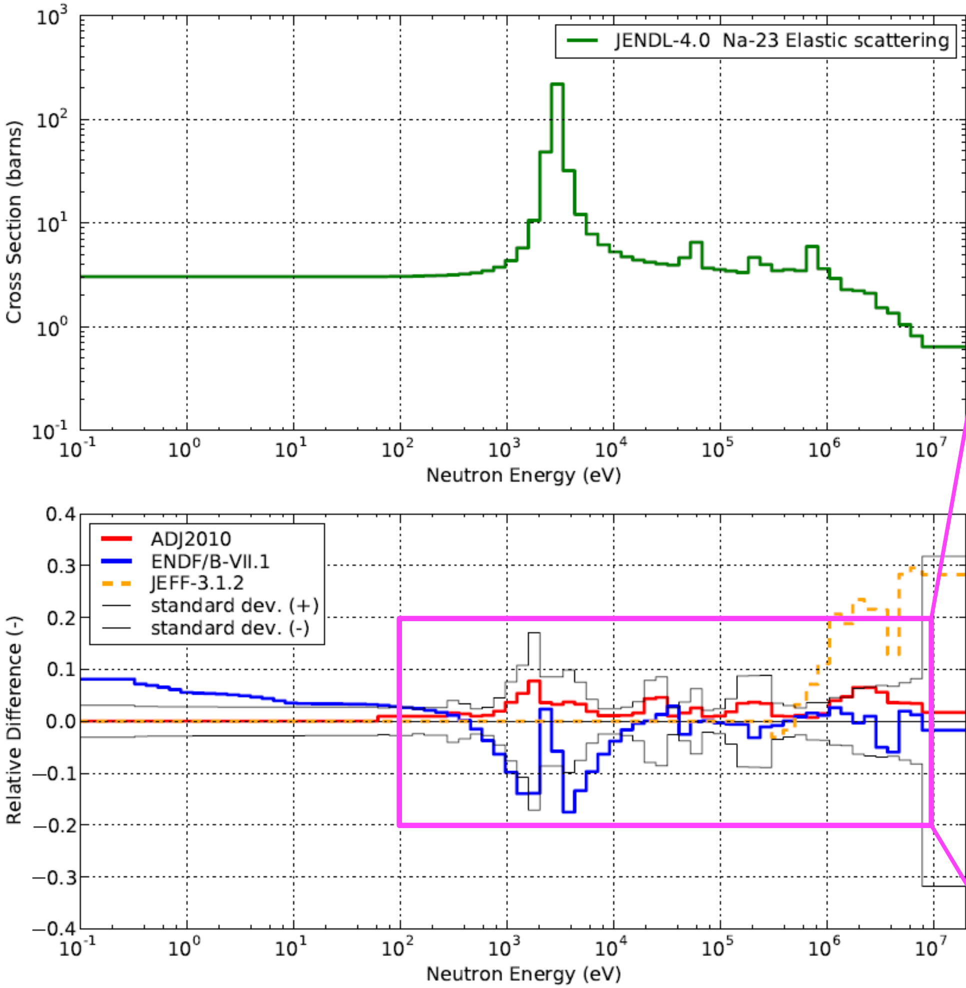


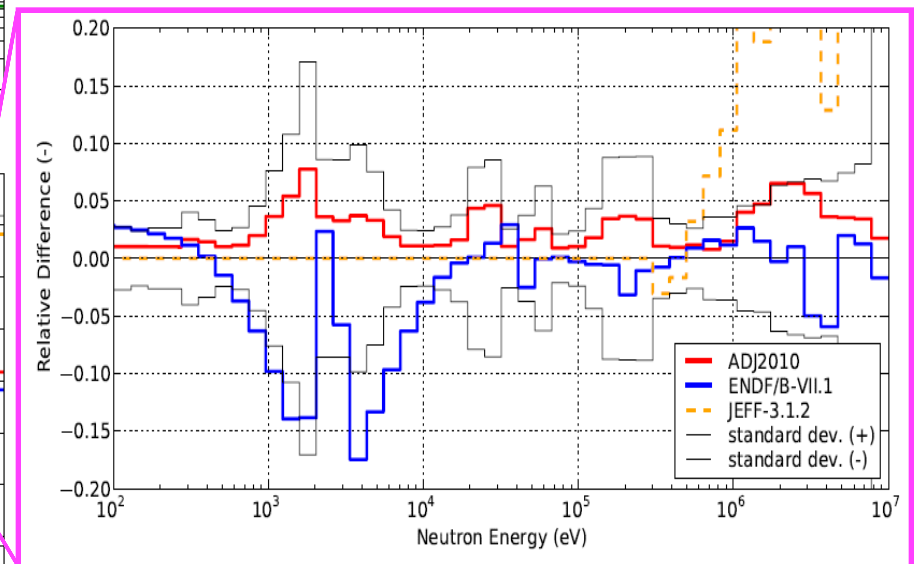


- No comments for ADJ2010.
- Three libraries are rather similar, but re-evaluation is underway in CIELO, using new measured data.

Na-23

Na-23
Elastic scattering





- ADJ2010 increases Na-23 elastic-scattering cross-section between 2 and 8%. This alteration is within the variance of JENDL-4.
- ENDF largely differs from JENDL and JEFF, since it is newer evaluation. The covariance of JENDL and COMMARA is consistent with this fact. -> next slide.

SG33 Final Report

Chap.3 Covariance

(Feb.20, 2013)

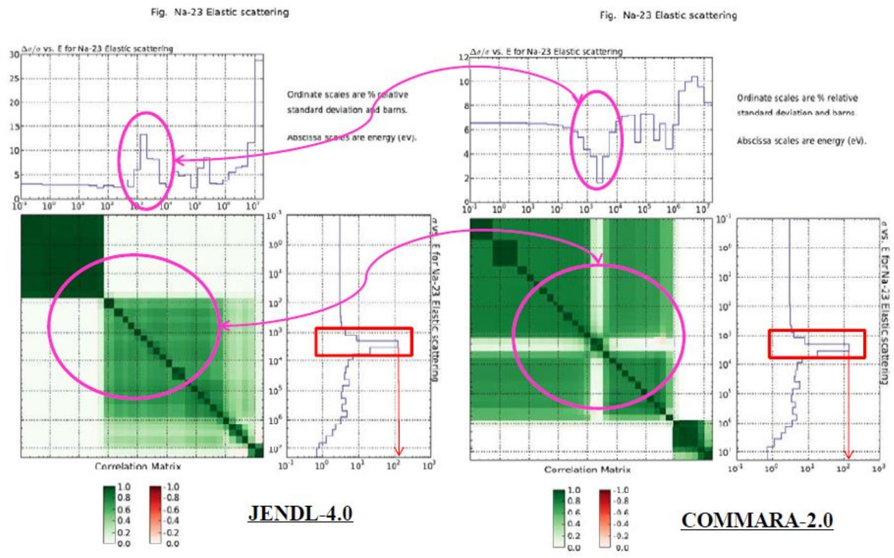


Figure 3.2 Comparison of JENDL-4.0 and COMMARA-2.0 Covariance (2/3) - Na-23 Elastic -

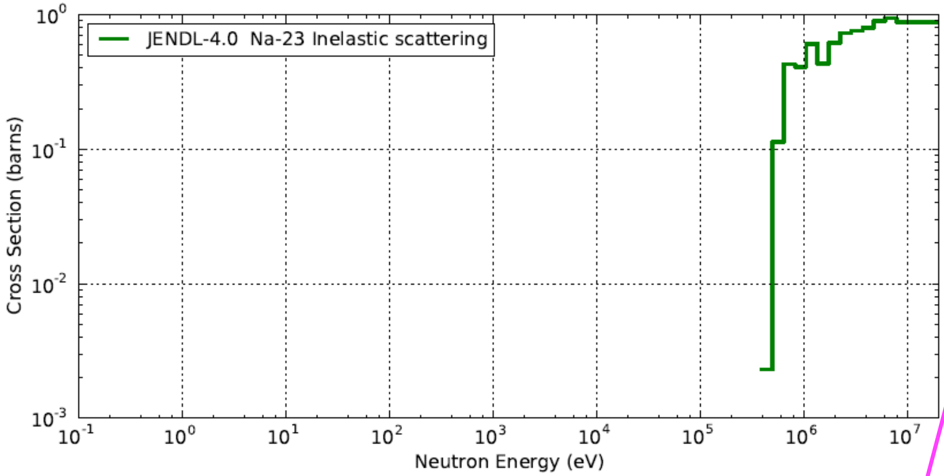
2) Na-23 elastic scattering data around 2 keV

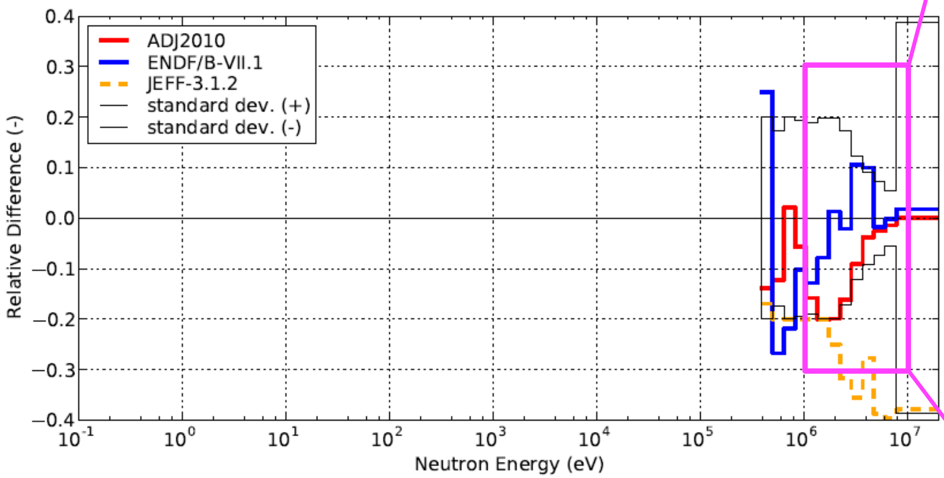
At this energy, there appears a giant resonance peak which affects significantly the sodium-voiding reactivity in sodium-cooled fast reactor cores. As found in Fig.3.2, the shape of Standard deviation (STD) is extremely different between two libraries, that is, the minimum STD value occurs at the cross-section peak energy in C-2.0, on the contrary, the maximum appears there in J-4.0. With a simple consideration, the trend of C-2.0 seems more natural, since the larger cross-sections would be more accurate due to the small statistical error in the measurement. The correlations are also quite different. In the C-2.0 covariance, the 2 keV peak has no correlations with other energy[3], while J-4.0 is partially positive everywhere above 100 eV. The covariance of C-2.0 is evaluated by the EMPIRE/KALMAN combination, where the prior resonance model parameter uncertainties are derived from Mughabghab (Ref.15), on the other hand, J-4.0 applies the GMA code with some corrections to meet the measured cross-sections with the evaluated ones of J-4.0 which is based on the multi-level Breit-Wigner formula with rather old resonance parameter values recommended by BNL in 1981. The cross-section difference between ENDF/B-VII.0 and J-4.0 is -17~+4% around 2keV, therefore, the difference of STDs might be reasonable if we take into account the corrections given to J-4.0 covariance.

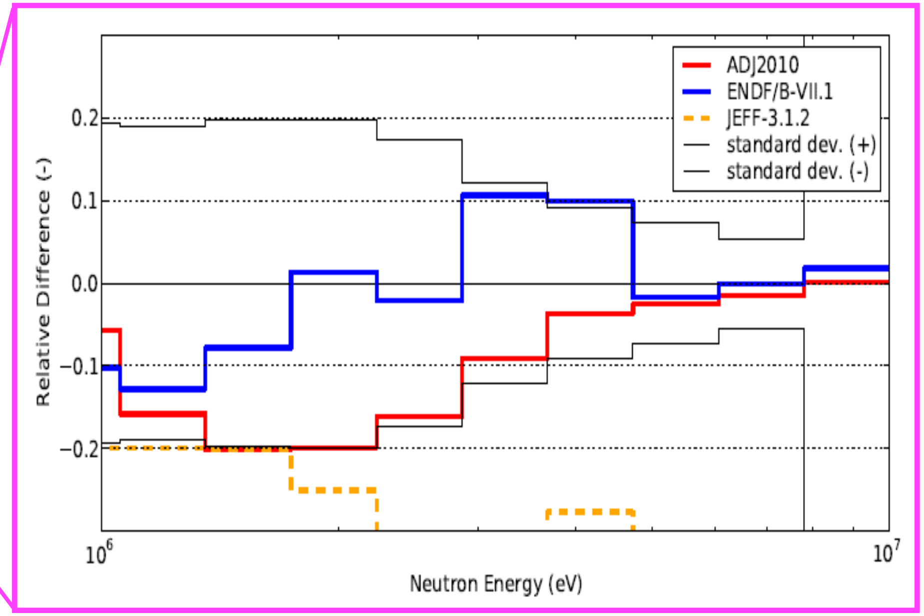
[3] This energy independency of 2 keV peak in the C-2.0 covariance is not well imagined from the general least-square analysis. There might have been some special treatments for the covariance evaluation in this resonance peak.

Na-23

Inelastic scattering

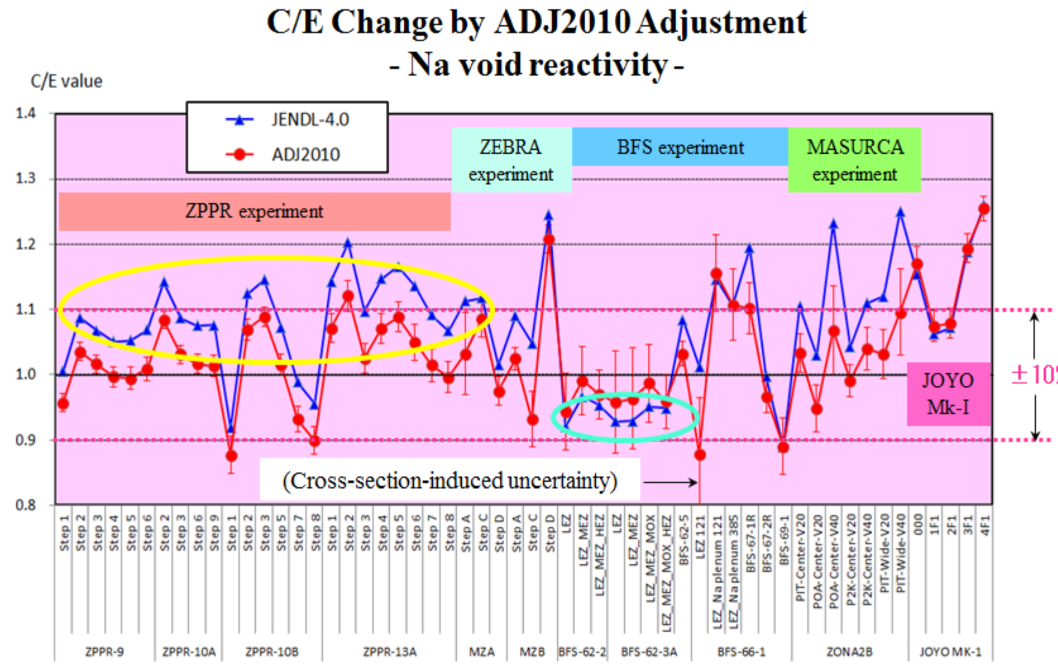


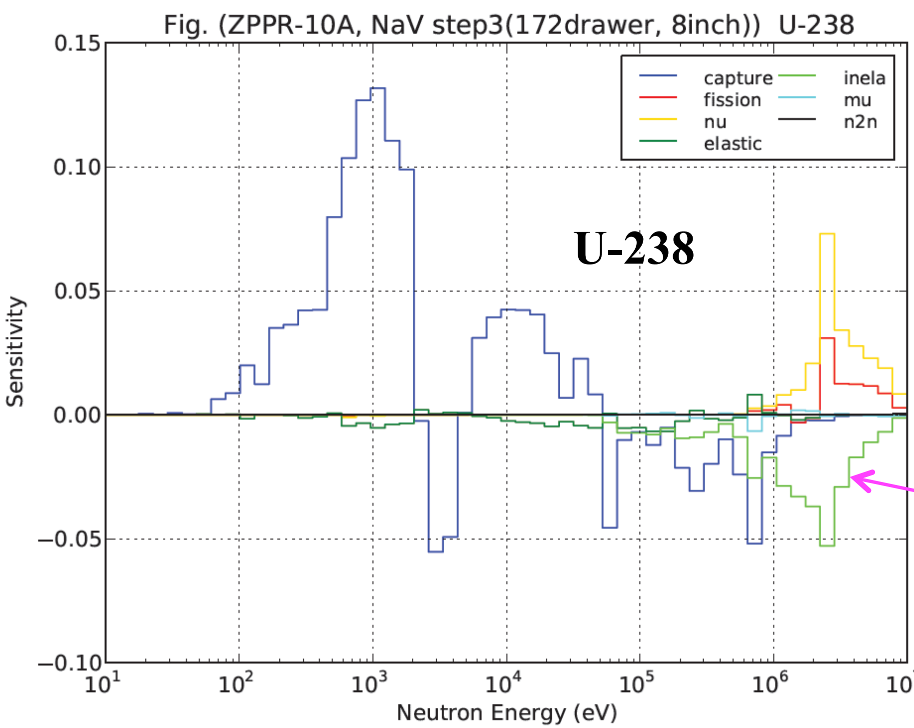


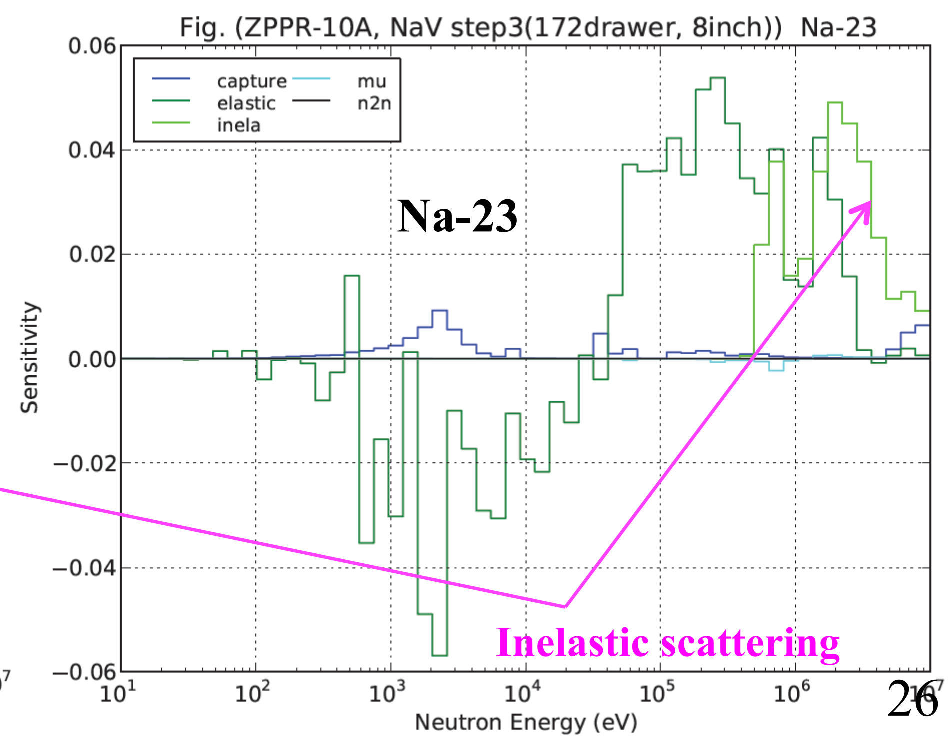


- ADJ2010 largely decreases Na-23 inelastic-scattering cross-section between 5 and 20% over 1MeV. This alteration is at the variance bound of JENDL-4.
- Na-23 inelastic-scattering has a similar sensitivity profile with total (elastic-scattering).
- This decrease of inelastic-scattering is consistent with the overestimation of Na void reactivity for ZPPR, and underestimation for BFS (negative reactivity). -> next slide.

Sensitivity for ZPPR-10A Na Void Reactivity







Concluding Remarks

1. **From ADJ2010 adjustment, we may recommend the followings to nuclear data evaluators:** <*These have high sensitivity to good integral data.*>
   - **Pu-239 capture --> Increase over 3keV by 7 to 9%.**
     - The adjustment mechanism is explainable but complicated and complex.
     - It is necessary to be very careful if use this recommendation because the increase is determined by a combination of integral experiments.
   - **Pu-239 fission --> Keep current data within 0.5% in average.**
   - **Pu-239 nu --> Keep current data within 0.2% in average.**
   - **U-238 capture --> Keep current data within 2%.**
   - **U-235 capture --> Follow JENDL-4.0 within its variance.**

2. **Although large alteration is observed, we cannot make comments:**
   - **Pu-239 fission spectrum and Na-23 inelastic --> should study more as one combined set including U-238 inelastic and Pu-239 inelastic.**
     <*compensation problem exists.*>
   - **U-238 mu-ave. --> Need to be converged among the major libraries.**
   - **U-235 fission --> Current fast-region integral database is not sufficient.**
   - **Fe-56 elastic scattering and Na-23 elastic --> Should be improved in CIELO project.**

Appendix: Theory of Cross-section Adjustment

※ J.B.Dragt, et al.: "Methods of Adjustment and Error Evaluation of Neutron Capture Cross Sections; Application to Fission Product Nuclides," NSE 62, pp.117-129, 1977

- Based on the Bayes theorem, i.e., the conditional probability estimation method
  → To maximize the posterior probability that a cross-section set, ***T***, is true, under the condition that the information of integral experiment, ***Re***, is obtained.

$$J(T) = (T-T_0)^t M^{-1}(T-T_0) + [Re-Rc(T)]^t[Ve+Vm]^{-1}[Re-Rc(T)]$$

Minimize the function $J(T)$. → $dJ(T)/dT = 0$

- The adjusted cross-section set ***T'***, and its uncertainty (covariance), ***M'*** *(Algebra)*

$$T' = T_0 + MG^t[GMG^t+Ve+Vm]^{-1}[Re-Rc(T_0)]$$

$$M' = M - MG^t[GMG^t+Ve+Vm]^{-1}GM$$

✓If $GMG^t << Ve+Vm$, $T' ≒ T_0$ and $GM'G^t ≒ GMG^t$

✓If $GMG^t >> Ve+Vm$, $GM'G^t ≒ Ve+Vm$

✓If $GMG^t ≒ Ve+Vm$, $GM'G^t ≒ 1/2 \times GMG^t$

- Prediction error induced by the cross-section errors

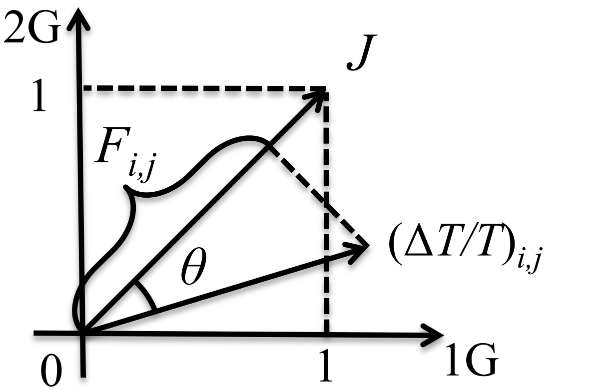
Before adjustment: GMG^t After adjustment: $GM'G^t$

Where, T_0 : Cross-section set before adjustment
M : Covariance before adjustment
Re : Measured values of integral experiments
Rc : Analytical values of integral experiments
Ve : Experimental errors of integral experiments
Vm : Analytical modeling errors of integral experiments
G : Sensitivity coefficients, $(dR/R)/(d\sigma/\sigma)$

Adjustment Motive Force

Motive force: $$F_{i,j} = \frac{\|(\Delta T/T)_{i,j}\|}{\|J\|} \cos\theta$$

where $$\cos\theta = \frac{(\Delta T/T)_{i,j} \cdot J}{\|(\Delta T/T)_{i,j}\| \; \|J\|}$$



Example of 2 energy-group case

$$(\Delta T/T)_{i,j} = M_j G_{i,j}^{\mathrm{T}} [G_{i,j} M_j G_{i,j}^{\mathrm{T}} + V_i]^{-1} [J - R_{c,i}/R_{e,i}]$$

1 – C/E

A special adjustment result, in which only one reaction, *j*, is adjusted by using only one integral experiment, *i*.

- *Motive force* is determined by reaction and integral experiment
  - independent from a combination of integral experiments
- *Motive force* is a scalar value (averaged over all energy group)
  - ±100% alterations for all energy group → *motive force* = ±1
  - 0 % alterations for all energy group → *motive force* = 0

Adjustment Potential

Potential is calculated as well as *motive force* by using

$$(\Delta T/T)'_{i,j} = M_j G^{\mathrm{T}}_{i,j}[G_{i,j} M_j G^{\mathrm{T}}_{i,j} + V_i]^{-1}[J - \overline{R_{c,I}}/\overline{R_{e,I}}]$$

in place of

$$(\Delta T/T)_{i,j} = M_j G^{\mathrm{T}}_{i,j}[G_{i,j} M_j G^{\mathrm{T}}_{i,j} + V_i]^{-1}[J - R_{c,i}/R_{e,i}]$$

Average of 1 – C/E over a set of core parameters related to *i*

1 – C/E of the core parameter *i*

- *Motive force* becomes null in two cases:
  - Not sensitive to the integral experiment: G ~ 0.0

    → There is no *motive force*
  - Sensitive but not necessary to adjust the cross sections: G >> 0.0 and C/E ~ 1.0

    → There is force that keeps the present values, or *frictional force*
- Therefore, *Potential* is needed to distinguish the two cases.
- The amplitude of *Potential* is comparable with that of a different kind of integral experiments, such as criticality and Na void reactivity

JAEA

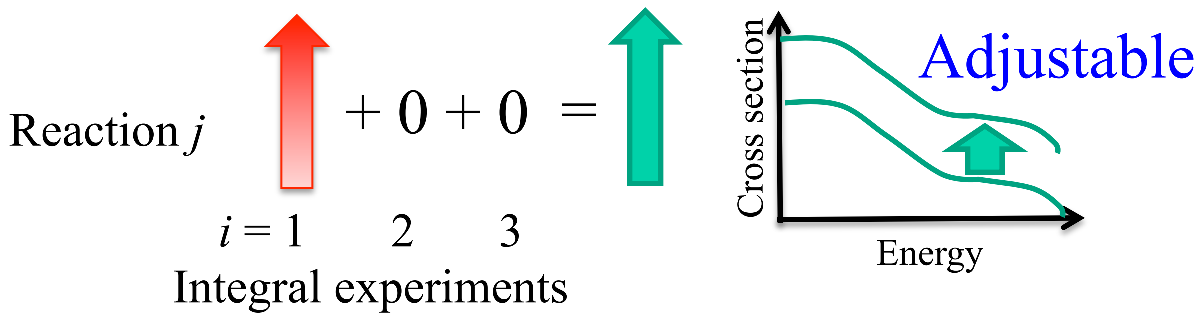
Motive Forces for Pu-239 capture

No.	Motive force	Integra experiments
1	+4.65	BFS-66-1 control rod worth [Ring 1-4]
2 – 8	+4.40 -- +2.60	ZPPR-18A control rod worths (including 7 cases)
9	+2.92	ZPPR-10A criticality
10	**+2.45**	**ZPPR-9 criticality**
	:	:
484, 485	-0.98	ZPPR-18A control rod worths (including 2 cases)
486	-0.99	JOYO MK-I criticality (64 fuel S/As)
487	**-1.06**	**JEZEBEL criticality**
488	-1.07	JOYO MK-I criticality (70 fuel S/As)

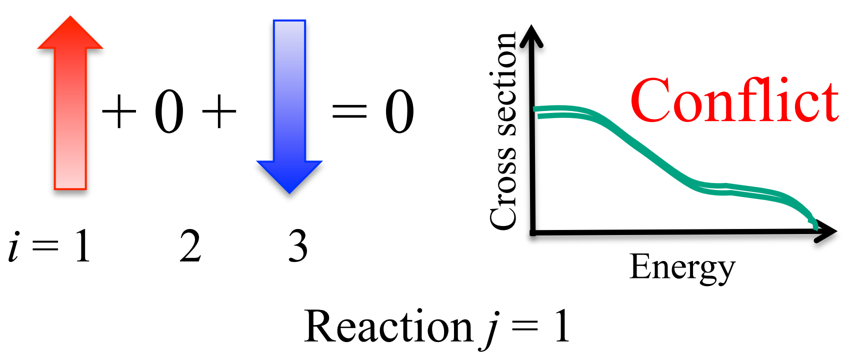
- A lot of experiments have large positive *motive forces*
- Even if some of them are removed, the cross-section alteration of Pu-239 capture is not changed significantly

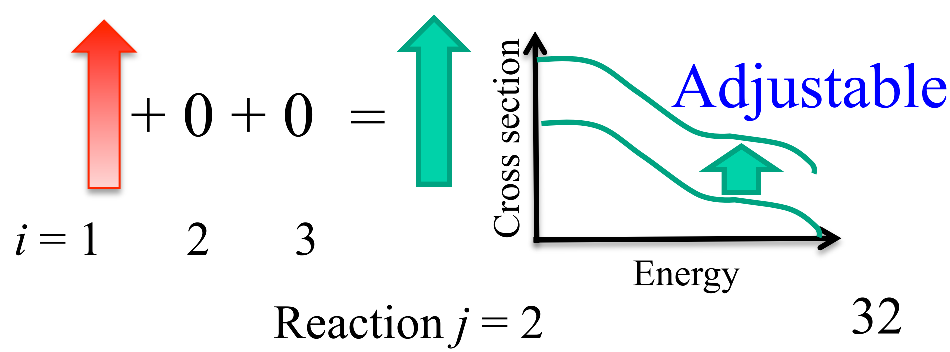
Assumption of Two Situations for Motive Forces

- **<u>F: freely adjustable</u>**
  If only one integral experiment has a large *motive force* for a reaction, the cross section of the reaction is "freely adjustable" and altered.



- **<u>C: conflict</u>**
  If more than two *motive forces* with large potentials have opposite signs, it is considered as a "conflict". In this case, the cross section of the reaction is not significantly adjusted. Then, the other "freely adjustable" cross sections are altered.

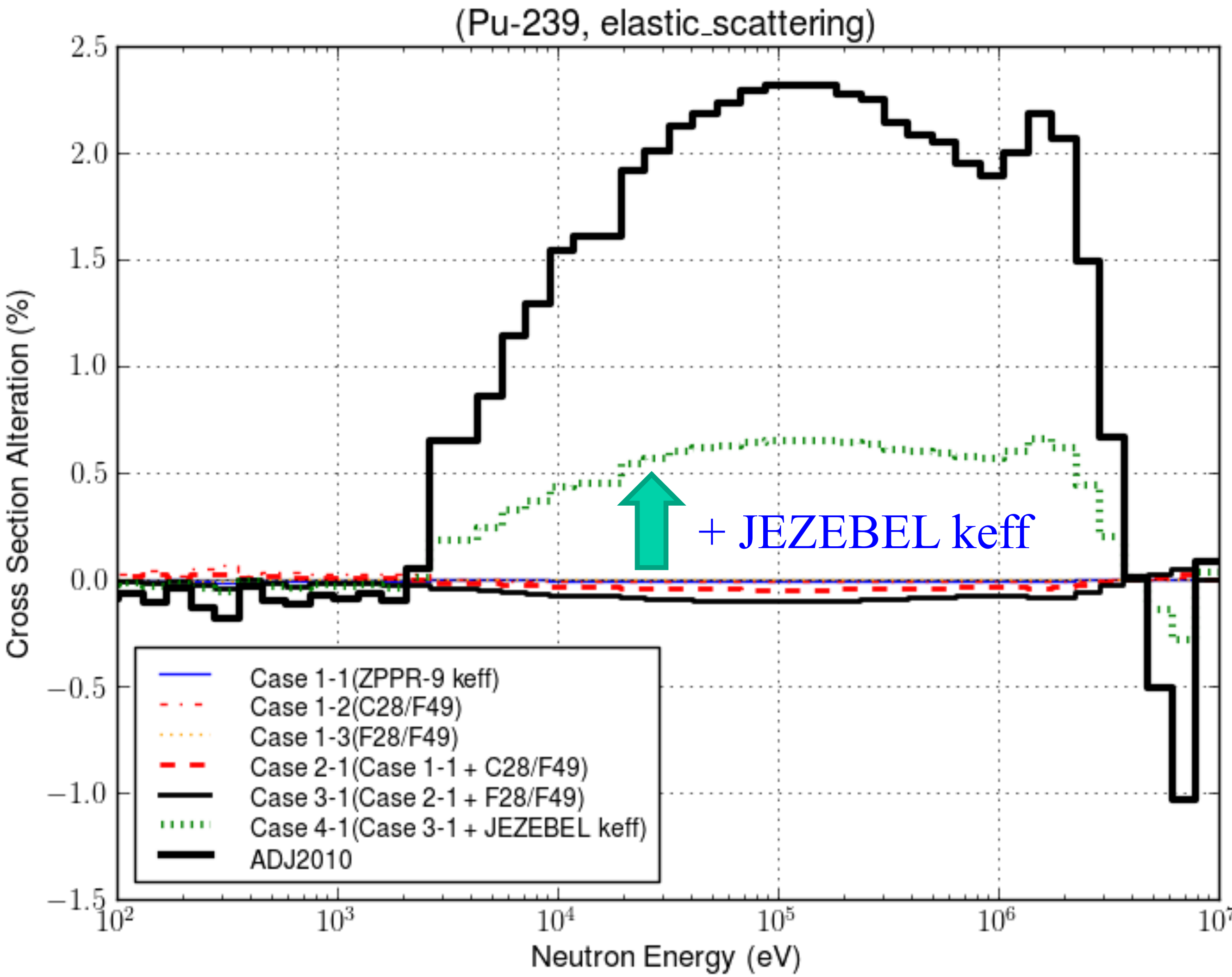




Motive Forces & Potentials for Integral Experiments used for Small Test Cases

	ZPPR-9						JEZEBEL	
	keff		C28/F49		F28/F49		keff	
Pu-239 capture	+2.45 (-1.84)	↑	+0.28 (-0.15)	0	+0.34 (+0.37)	0	-1.06 (-0.94)	↓
Pu-239 fission	-0.24 (+0.18)	↓	+0.18 (-0.10)	↑	-0.07 (-0.07)	0	+0.07 (+0.06)	0
Pu-239 χ	+2.26 (-1.70)	↑	-1.20 (+0.66)	↓	-2.83 (-3.07)	↓	-1.98 (-1.77)	↓
Pu-239 (n, n)	-0.12 (+0.09)	0	-0.01 (+0.00)	0	-0.00 (-0.01)	0	+0.57 (+0.51)	↑
U-238 capture	+0.55 (+1.20)	↑	-1.04 (+0.579	↓	+0.21 (+0.23)	↑	-0.00 (-0.00)	0
U-238 fission	-1.59 (+1.20)	↓	+0.02 (-0.01)	0	+0.62 (+0.67)	↑	+0.00 (+0.00)	0
U-238 (n, n')	+0.57 (-0.43)	↑	-1.13 (+0.62)	↓	-0.39 (-0.43)	↑	+0.00 (+0.00)	0

Cross-section Alteration of Pu-239 (n, n)



- Not moved by using the set of ZPPR-9 keff, C28/F49, and F28/F49
- Begin to move by adding JEZEBEL keff