

# JENDL-4.0 Based Cross-section Adjustment by Adding New Experiments on the Basis of the SG33 Benchmark

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# Integral Experiments of SG33 Benchmark

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- JEZEBEL Pu-239:
  - KEFF, F28/F25, F49/F25, F37/F25
- JEZEBEL Pu-240:
  - KEFF
- FLATTOP-Pu:
  - KEFF, F28/F25, F37/F25
- ZPR6-7:
  - KEFF, F28/F25, F49/F25, C28/F25
- ZRR6-7 high Pu-240 content:
  - KEFF
- ZPPR9:
  - KEFF, F28/F25, F49/F25, C28/F25, SVR(central void), SVR(leakage-dominant)
- JOYO:
  - KEFF

→ Total 20 integral experiments

# Additional New Integral Experiments

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- PROTEUS proposed by PSI
  - HCLWR-PROTEUS
    - Core 7: moderated by water ( $V_m/V_f=0.48$ )
      - KINF
    - Core 8: not moderated
      - KINF
  - Code & Library
    - MCNP6.11 & JEFF-3.1.1
- SNEAK proposed by JSI
  - MOX fuel reflected by metallic depleted uranium
    - 7A: PuO<sub>2</sub>-UO<sub>2</sub>, graphite
      - KEFF
    - 7B: PuO<sub>2</sub>-UO<sub>2</sub>, <sup>nat</sup>UO<sub>2</sub>
      - KEFF
  - Code & Library
    - THREEDANT & ENDF-B/VII.1

→ + 4 integral experiments

# HCLWR-PROTEUS

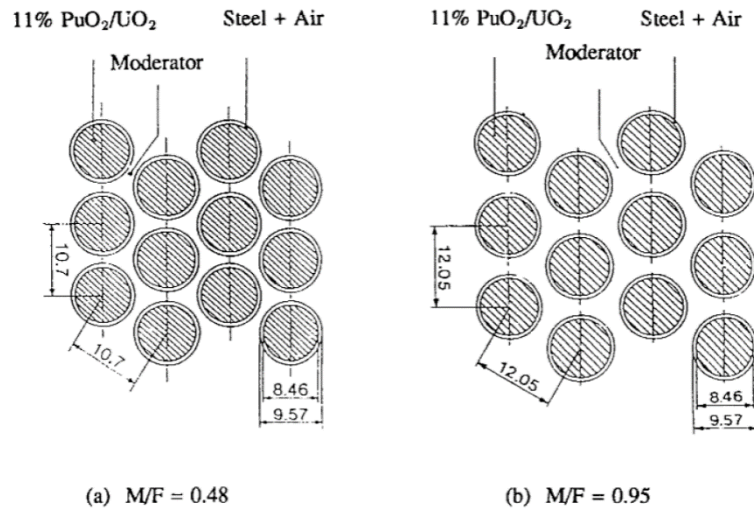
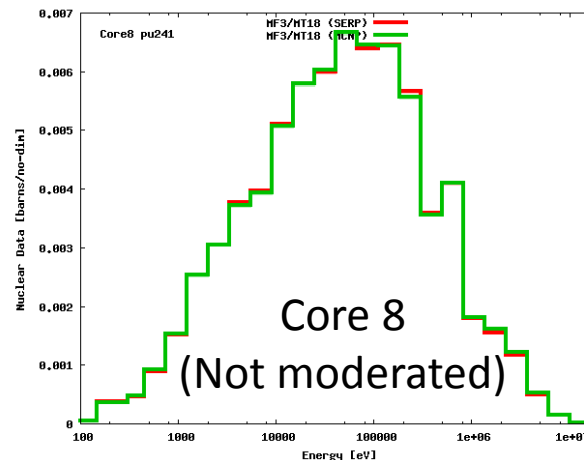
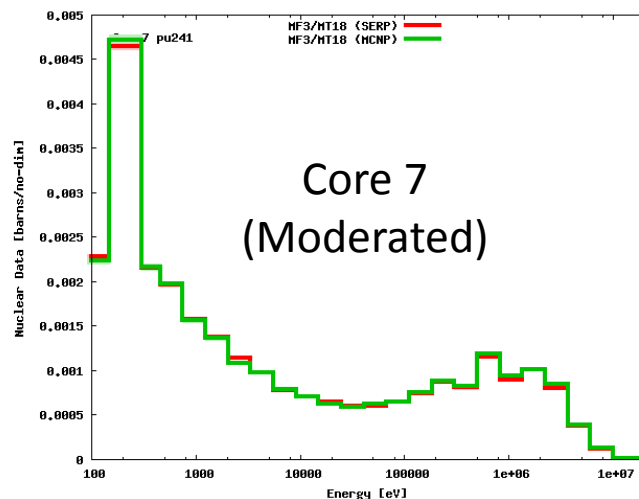


Table: Nominal Pu vector of the reference date (01.01.1986)\*

Isotope	Ratio
Pu-238	1%
Pu-239	64%
Pu-240	23%
Pu-241	8%
Pu-242	4%

Fig.: Lattice description of the a) tight- and b) wide-pitch configuration\*



\*: M. Hursin, et al.,  
“Description of the Data  
provided to the SG39  
with respect to the  
HCLWR experiments at  
Proteus,” AN-41-15-05  
V.1, PSI (2015)

Fig.: Differential sensitivity of Pu-241 fission\*

# Atomic Densities of PROTEUS 7 and 8

Table 2: Fuel Composition for Core 7 and Core 8

Isotope	Core7	Core8	Isotope	Core 7	Core 8
U-234	1.8496E-06	1.9480E-06	O-16	4.5841E-02	4.5841E-02
U-235	1.5996E-04	1.5996E-04	Fe-54	1.7857E-06	1.7857E-06
U-236	2.9158E-07	2.9158E-07	Fe-56	2.8239E-05	2.8239E-05
U-238	2.0492E-02	2.0492E-02	Fe-57	6.7734E-07	6.7734E-07
			Fe-58	8.6206E-08	8.6206E-08
Pu-238	2.3974E-05	2.3876E-05	Ca-40	9.3421E-06	9.3421E-06
Pu-239	1.5364E-03	1.5364E-03	Ca-42	6.2351E-08	6.2351E-08
Pu-240	5.5930E-04	5.5930E-04	Ca-43	1.3010E-08	1.3010E-08
Pu-241	1.7580E-04	1.7142E-04	Ca-44	2.0103E-07	2.0103E-07
Pu-242	8.4588E-05	8.4588E-05	Ca-46	3.8548E-10	3.8548E-10
Am-241	3.3298E-05	3.7678E-05	Ca-48	1.8021E-08	1.8021E-08

M. Hursin, et al., "Description of the Data provided to the SG39 with respect to the HCLWR experiments at Proteus," AN-41-15-05 V.1, PSI (2015)

# SNEAK-7A/7B

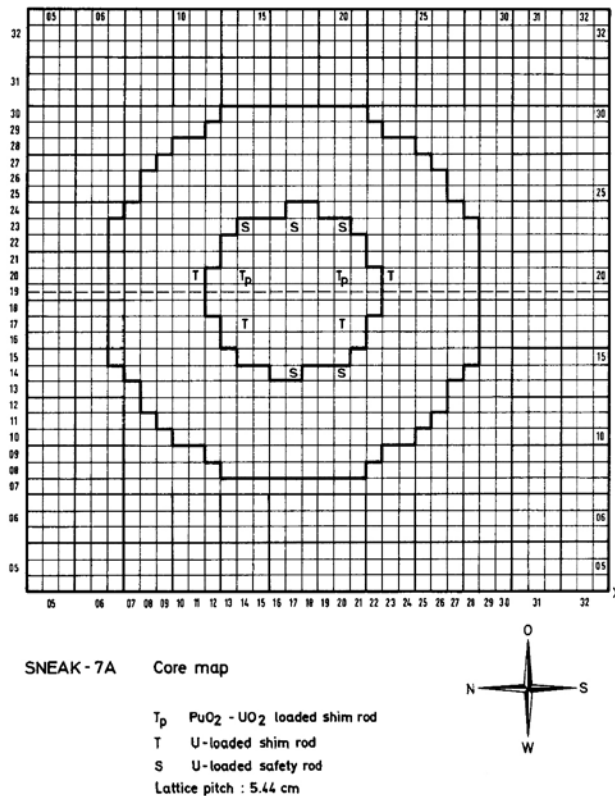


Fig.: SNEAK-7A Core Map\*

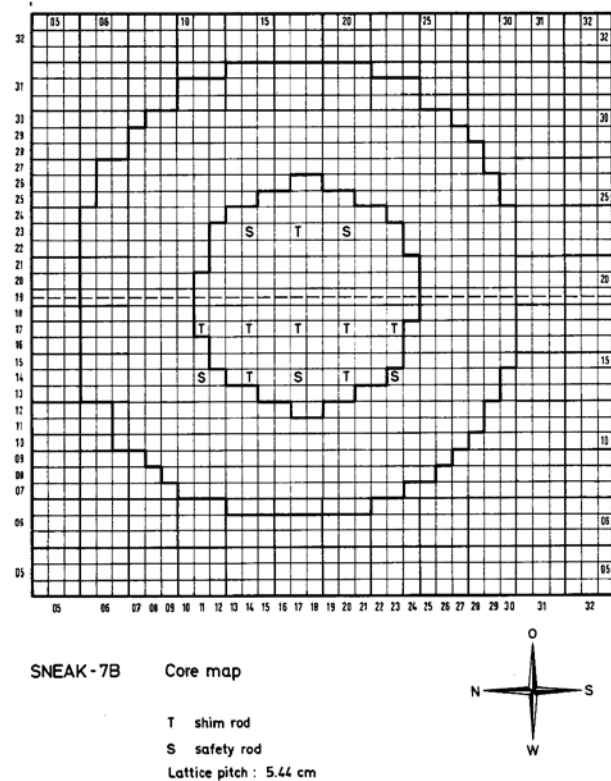


Fig.: SNEAK-7B Core Map\*

\*: E. Ivanov, et al.,  
 “SNEAK 7A and 7B Pu-fueled fast critical assemblies in the Karlsruhe fast critical facility,” International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE), NEA/NSC/DOC(2006)1, March 2015 Edition

Table: Summary of Feature of SNEAK-7A and -7B\*

Assembly	Year	Features	Core Components	Blanket
7A	1970/71	1-zone core	PuO <sub>2</sub> -UO <sub>2</sub> , graphite	Metallic depleted U
7B	1971		PuO <sub>2</sub> -Uo <sub>2</sub> , natUO <sub>2</sub>	

# Atomic Densities of SNEAK-7A and -7B

Table 1.7. Atomic Densities for SNEAK-7A R-Z Model,  $10^{24} \text{ cm}^{-3}$  (Reference 1, p. 69). Table 1.8. Atomic Densities for SNEAK-7B R-Z Model,  $10^{24} \text{ cm}^{-3}$  (Reference 1, p. 71).

Isotope	Inner Core	Outer Core	Blanket
Al	0.0000080	0.0011906 <sup>(a)</sup>	-
C	0.0260987	0.0255387	0.0000135
Cr	0.0022423	0.0022390	0.0011080
Fe	0.0079713	0.0079824	0.0039549
H	-	-	-
Mg	-	-	-
Mn	0.0001109	0.0001178	0.0000875
Mo	0.0000165	0.0000145	0.0000100
Nb	0.0000089	0.0000077	0.0000085
Ni	0.0011664	0.0011818	0.0009845
O	0.0218462	0.0211909	-
<sup>239</sup> Pu	0.0026374	0.0023434	-
<sup>240</sup> Pu	0.0002369	0.0002105	-
<sup>241</sup> Pu	0.0000215	0.0000191	-
<sup>242</sup> Pu	0.0000011	0.0000010	-
Si	0.0000933	0.0000932	0.0000453
<sup>235</sup> U	0.0000586	0.0002958 <sup>(b)</sup>	0.0001624
<sup>238</sup> U	0.0079604	0.0080456	0.0399401

- (a) This value is 7.2% higher than the value calculated from stretched-platelet atom densities (Table 1.9).  
(b) Note that this value is 5.9% higher than the value calculated using the described method for obtaining outer-core atom densities.

Isotope	Core	Blanket
Al	0.0012112	-
C	0.0000631	0.0000135
Cr	0.0027560	0.0011080
Fe	0.0098021	0.0039549
H	0.0000071	-
Mg	0.0000095	-
Mn	0.0000646 <sup>(a)</sup>	0.0000875
Mo	0.0000184	0.0000010 <sup>(b)</sup>
Nb	0.0000084	0.0000085
Ni	0.0014594	0.0009845
O	0.0331936	-
<sup>239</sup> Pu	0.0018312	-
<sup>240</sup> Pu	0.0001645	-
<sup>241</sup> Pu	0.0000149	-
<sup>242</sup> Pu	0.0000007	-
Si	0.0001174	0.0000453
<sup>235</sup> U	0.0002663	0.0001624
<sup>238</sup> U	0.0145794	0.0399401

- (a) The calculated value for Mn using the method described in the previous paragraph is 94% larger than this value.  
(b) This value was given as 0.0000100 for SNEAK 7A. All other blanket values are the same for both cores.

\*: E. Ivanov, et al., "SNEAK 7A and 7B Pu-fueled fast critical assemblies in the Karlsruhe fast critical facility," International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE), NEA/NSC/DOC(2006)1, March 2015 Edition

# Missing Sensitivity Coefficients

Adjusted nuclides and reactions		Sensitivity coefficients	
		PROTEUS 7 & 8	SNEAK 7A & 7B
U-235	capture	●	●
	fission	●	●
	nu	●	●
	elastic scattering	●	●
	inelastic scattering	●	●
	mu average		
	fission spectrum		●
U-238	capture	●	●
	fission	●	●
	nu	●	●
	elastic scattering	●	●
	inelastic scattering	●	●
	mu average		●
Pu-239	capture	●	●
	fission	●	●
	nu	●	●
	elastic scattering	●	●
	inelastic scattering	●	●
	mu average		●
	fission spectrum		●
Pu-240	capture	●	●
	fission	●	●
	nu	●	●
	elastic scattering	●	●
	inelastic scattering	●	●
	mu average		
Pu-241	capture	●	●
	fission	●	●
	nu	●	●
	elastic scattering	●	●
	inelastic scattering	●	●
	mu average		

Adjusted nuclides and reactions		Sensitivity coefficients	
		PROTEUS 7 & 8	SNEAK 7A & 7B
B-10	capture	●	
	elastic scattering	●	
	inelastic scattering	●	
	mu average		
O-16	capture	●	
	elastic scattering	●	
	inelastic scattering	●	
	mu average		
Na-23	capture	●	
	elastic scattering	●	
	inelastic scattering	●	
	mu average		
Cr-52	capture	●	
	elastic scattering	●	
	inelastic scattering	●	
	mu average		
Fe-56	capture	●	●
	elastic scattering	●	●
	inelastic scattering	●	●
	mu average		●
Ni-58	capture	●	
	elastic scattering	●	
	inelastic scattering	●	
	mu average		

- For PROTEUS, sensitivity coefficients of fission spectrum and mu-average are missing
- For SNEAK, sensitivity coefficients of C-12, O-16, Cr-52 and Ni-58 are missing



# Input Data for Additional Integral Experiments

- C/E values

- Calculated values with a nuclear data library,  $x$ , are converted into those with JENDL-4.0 by using sensitivity coefficients:

$$C_{JENDL-4.0} = C_x \times S_x \frac{\sigma_{JENDL-4.0} - \sigma_x}{\sigma_x}$$

- Sensitivity coefficients

- Given 33-group sensitivity coefficients are used without any modifications because the sensitivity coefficients are little sensitive to the nuclear data libraries

- Uncertainty and correlation

- Experimental uncertainty:
    - Given data are used as they are
  - Analytical model uncertainty:
    - Ignored (set to zero)
  - Correlation factor:
    - Correlation factors between the other experiments are ignored (set to zero)

# HCLWR-PROTEUS

Table: C/E and experimental uncertainty on  $k_{inf}$  for PROTEUS Core7 and 8

Core #	Calculations	Experiments		C/E	
		Cell method	Buckling method	Cell method	Buckling method
7	1.12136	$1.115 \pm 0.006$	$1.121 \pm 0.005$	$1.006 \pm 0.006$	$1.000 \pm 0.005$
8	1.13465	$1.178 \pm 0.004$	$1.185 \pm 0.012$	$0.963 \pm 0.004$	$0.958 \pm 0.012$

M. Hursin, et al., “Description of the Data provided to the SG39 with respect to the HCLWR experiments at Proteus,” AN-41-15-05 V.1, PSI (2015)

- Conversion of C/E value (JEFF-3.1.1 → JENDL-4.0)
  - Core 7: +0.372% (C/E = 1.006 → 1.0097)
  - Core 8: +0.439% (C/E = 0.963 → 0.9672)

# SNEAK-7A/7B

Table: C/E and experimental uncertainty on keff for SNEAK-7A and 7B

	Calculation	Experiment	C/E
SNEAK-7A KEFF	1.0064 <sub>97</sub>	1.0010 +- 0.0029	1.0054 <sub>9</sub> +- 0.0029
SNEAK-7B KEFF	1.0058 <sub>63</sub>	1.0016 +- 0.0035	1.0042 <sub>6</sub> +- 0.0035

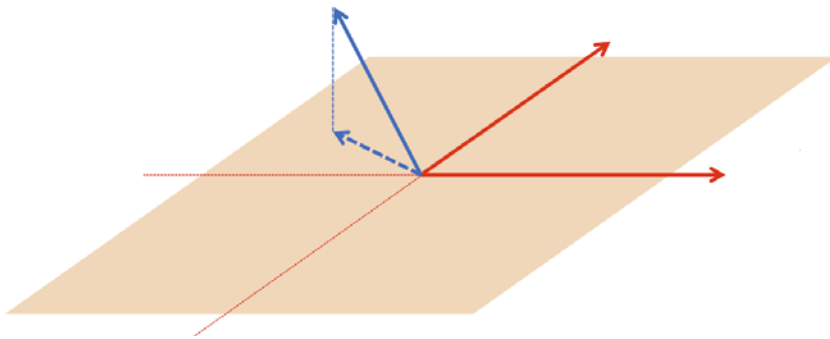
I. Kodeli, "Sensitivities profiles: Flattop-Pu, SNEAK-7A, SNEAK-7B, ASPIS-FE88," WPEC/SG39 website, <https://www.oecd-neo.org/science/wpec/sg39/>

- Conversion of C/E value (ENDF/B-VII.1 → JENDL-4.0)
  - Core 7: +0.398% (C/E = 1.0054<sub>9</sub> → 1.0094<sub>9</sub>)
  - Core 8: +0.479% (C/E = 1.0042<sub>6</sub> → 1.0090<sub>6</sub>)

# Trial Application of Sub-space Method

## Sub-space decomposition nuclear data space

If a unit nuclear data vector is NOT on this plane, this nuclear data cannot be reconstructed by a set of sensitivity vectors; the norm of the projected vector on this sub-space corresponds to usefulness of the integral data set to validate this nuclear data.



## SVD to sensitivity matrix

$$\mathbf{S} = \mathbf{U}\mathbf{D}\mathbf{V}^T$$

Sensitivity matrix

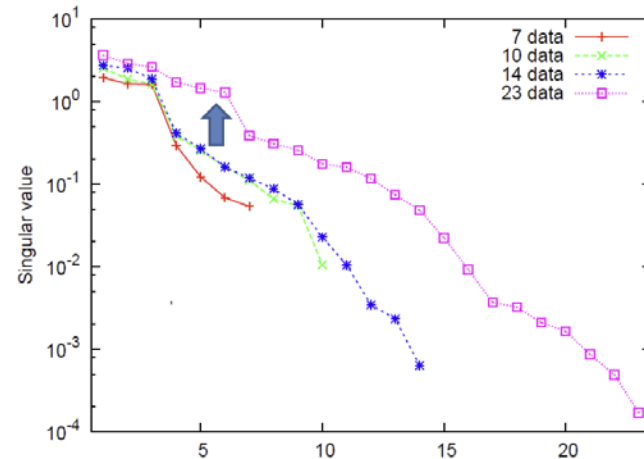
$$\mathbf{D} = \text{diag}(\sigma_1, \sigma_2, \dots)$$

$$\mathbf{U} = (\mathbf{u}_1, \mathbf{u}_2, \dots)$$

Left-hand singular vectors

A orthonormal set of vectors  $\mathbf{S} = \{\mathbf{u}_1, \mathbf{u}_2, \dots\}$  spans a sensitivity sub-space.

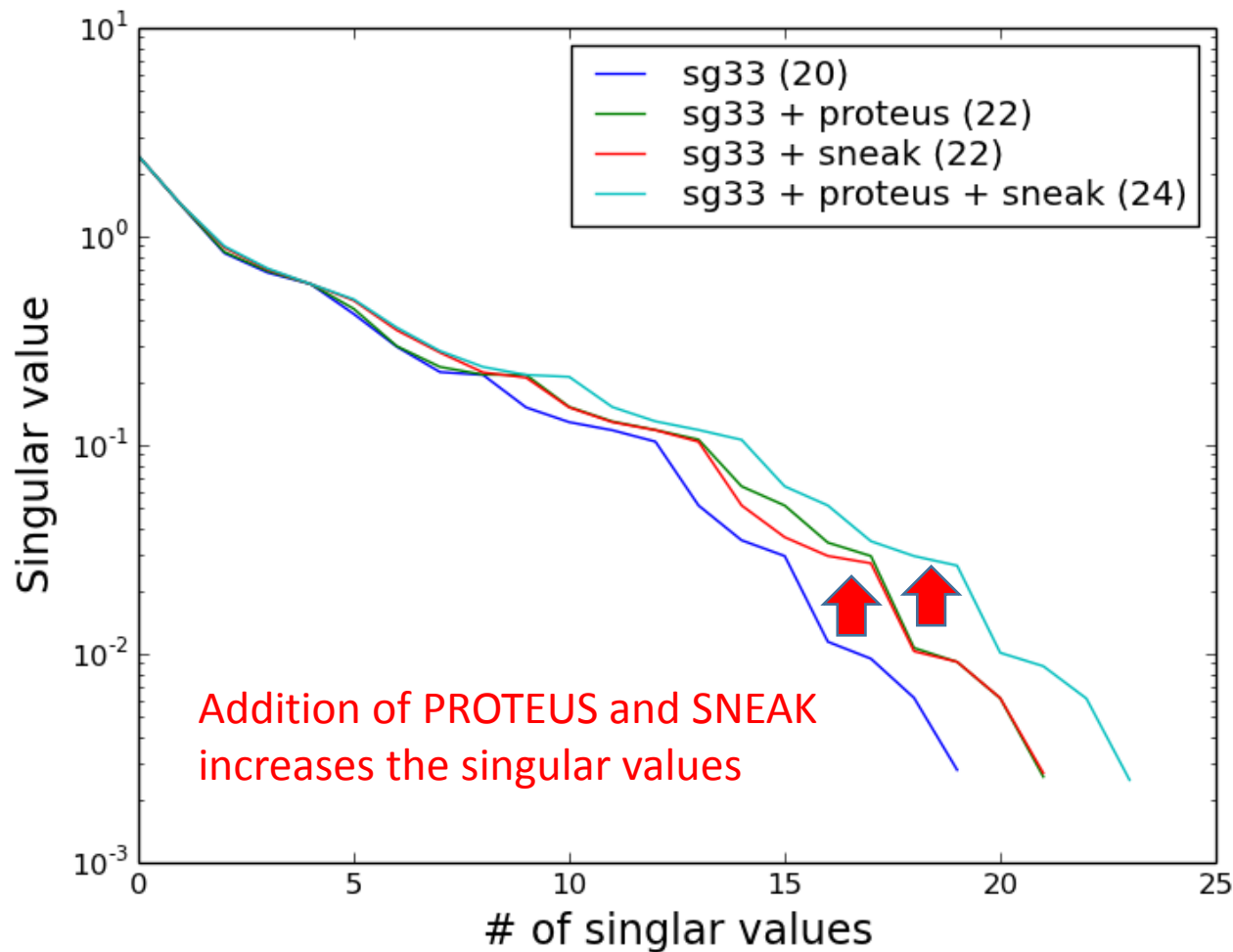
## Singular values



Consideration of the RRR data contributes to increase dimensions of the sensitivity sub-space.

\*: G. Chiba, "Application of sub-space method for nuclear data validation," Consultants' Meeting on "Compensating Effects due to Nuclear Reaction and Material Cross Correlations in Integral Benchmarks," IAEA Headquarters, Vienna (2015)

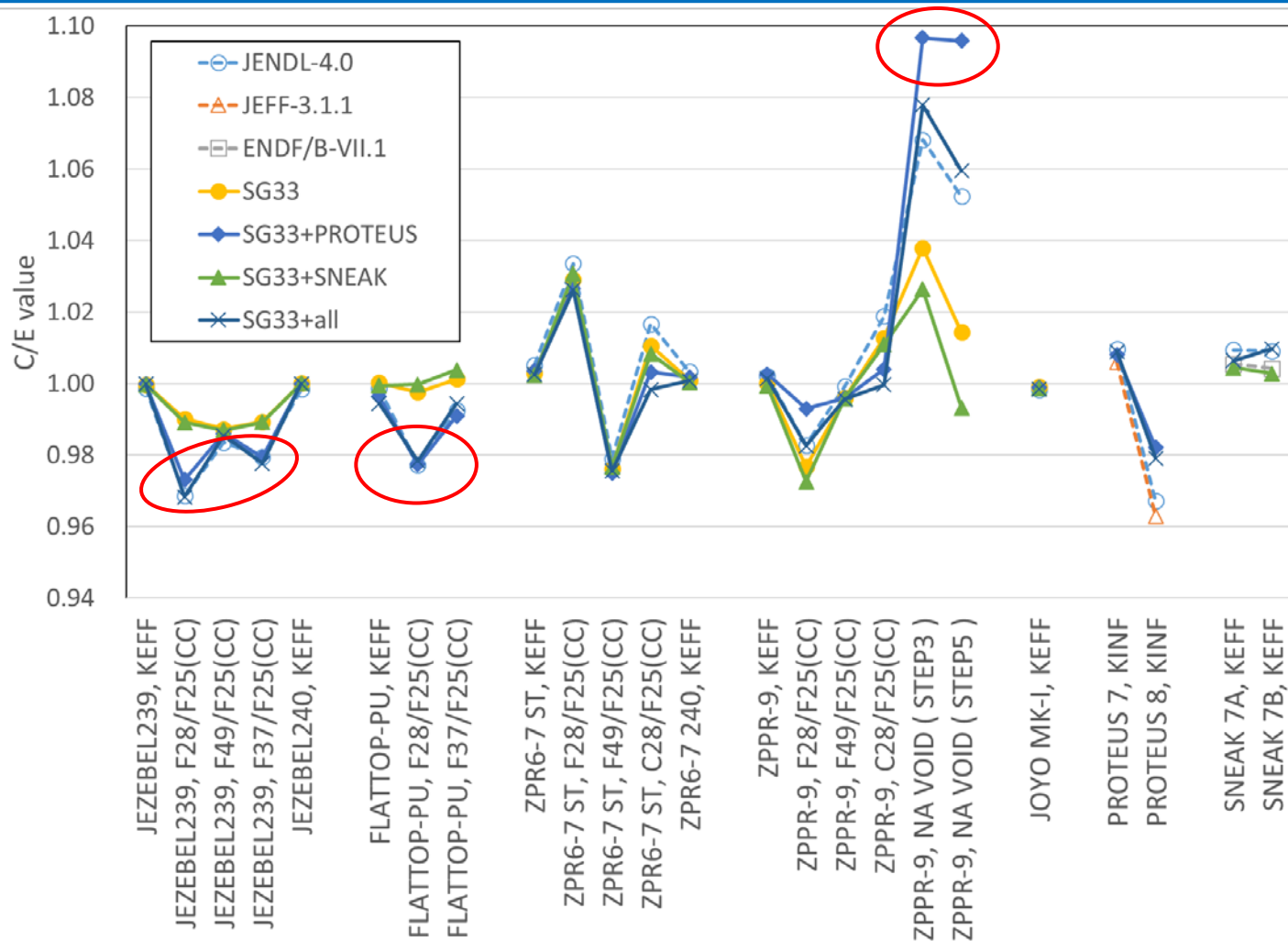
# Singular Values of Sensitivity Matrix



- Consideration of PROTEUS and SNEAK data contributes to an increase in dimensions of the sensitivity sub-space\*

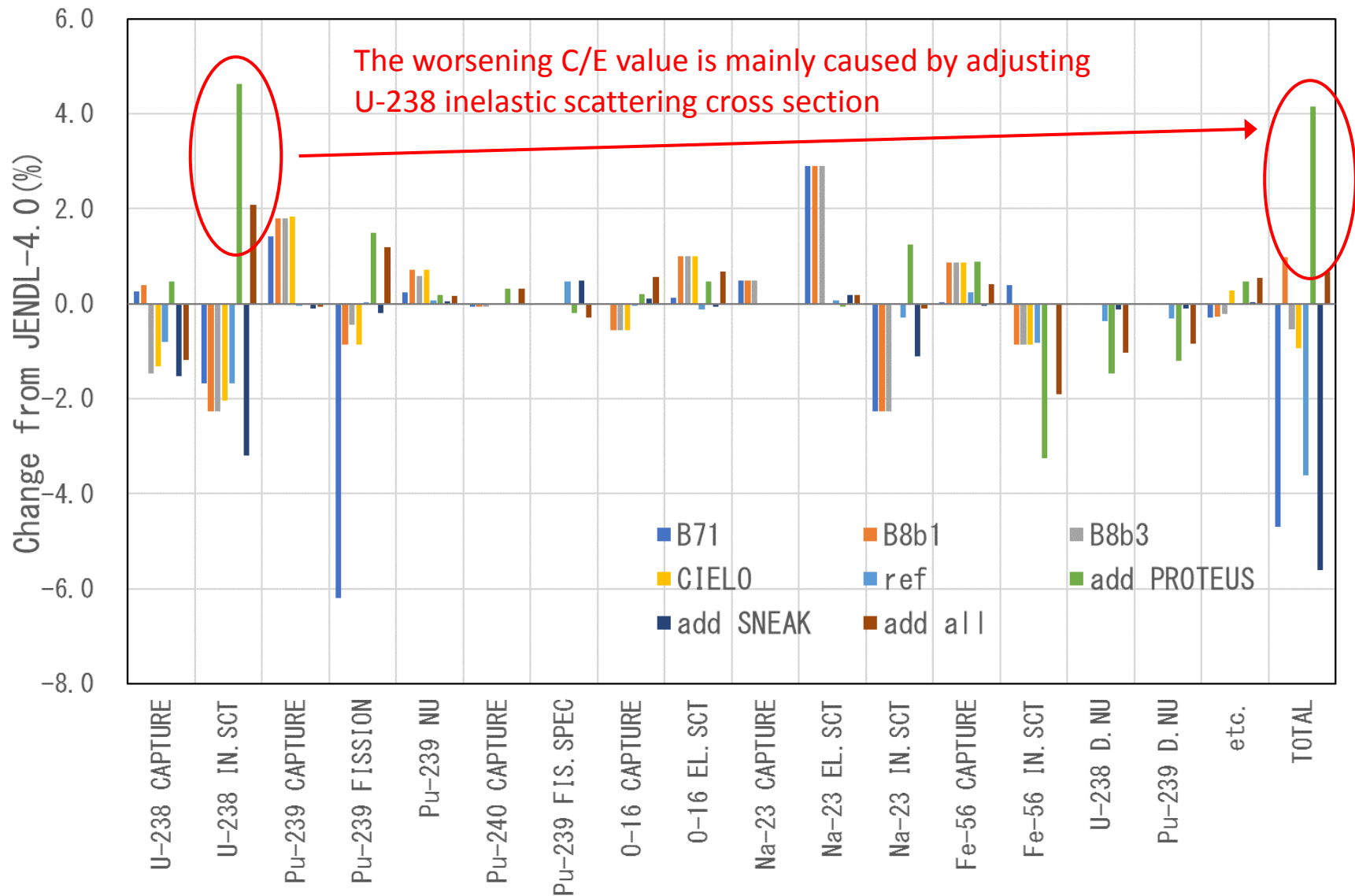
→ This result means that they have additional information

# C/E Values

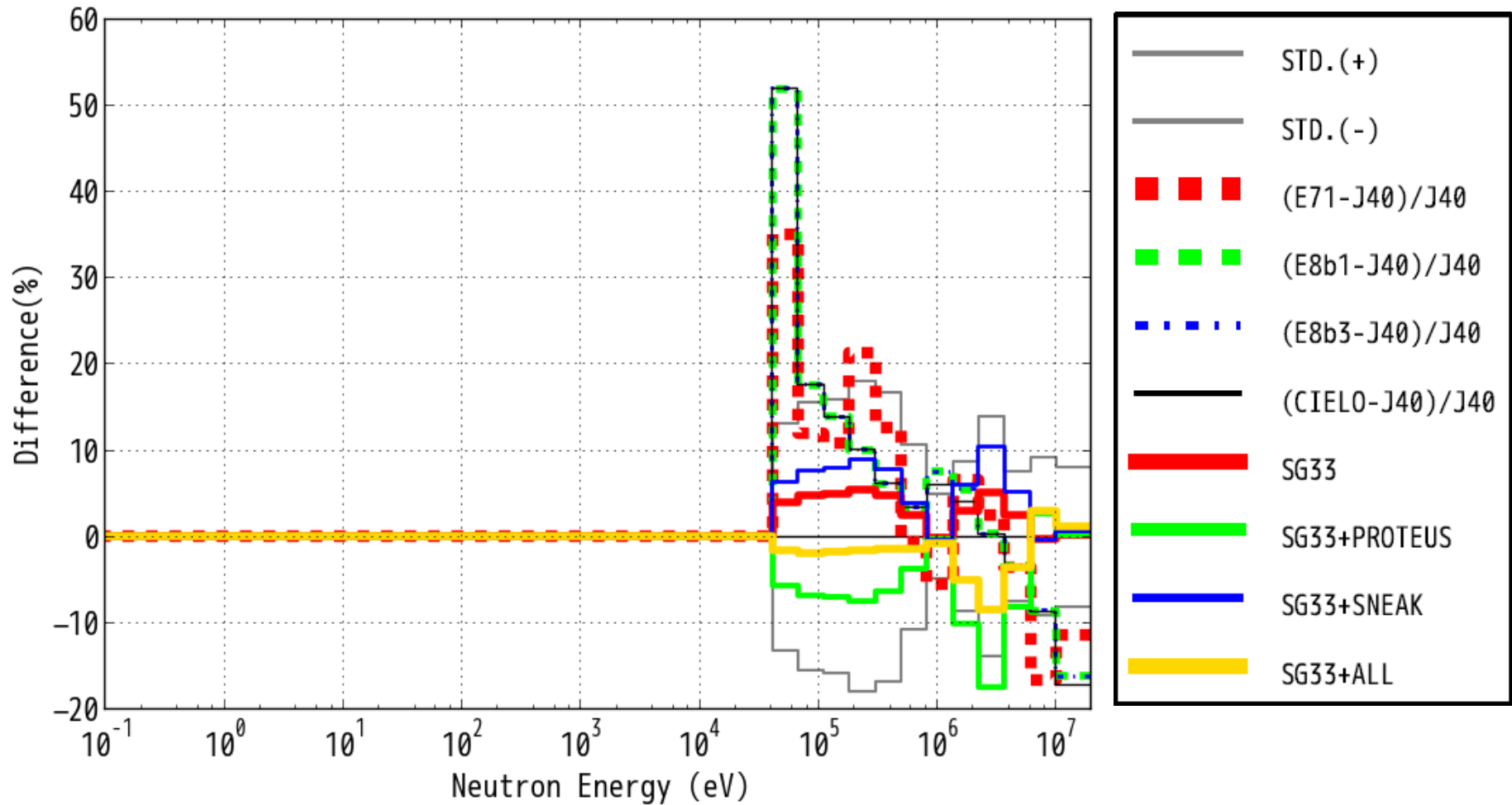


- C/E values of JEZEBEL and FLATTOP-PU are not improved when adding PROTEUS
- Addition of PROTEUS worsens the C/E values of ZPPR-9 sodium void worth

# ZPPR-9 Sodium Void Reactivity (Step5)



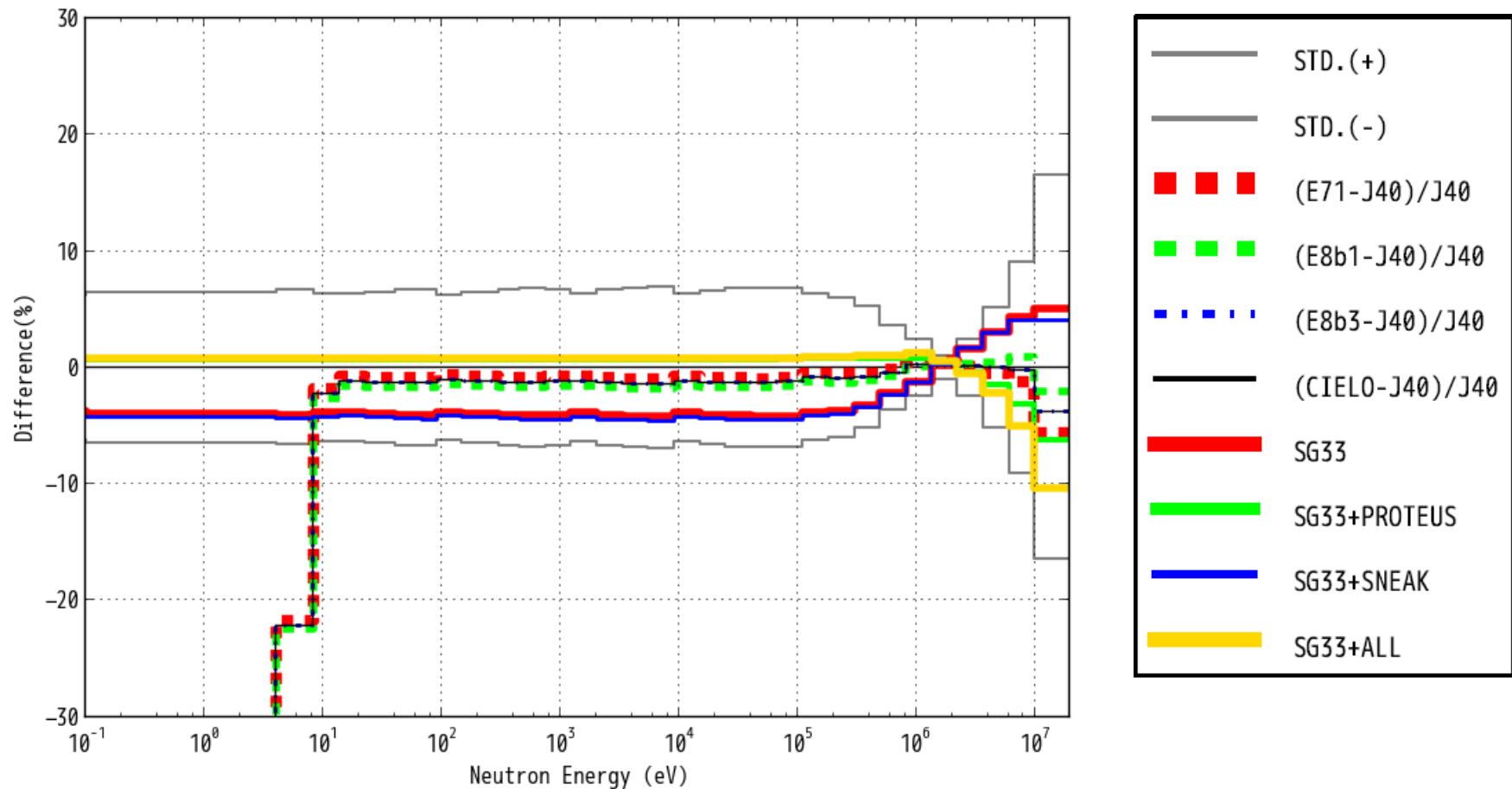
# U-238 inelastic scattering cross sections



- SG33 and SNEAK increase U-238 inelastic scattering cross section but PROTEUS reduces it → There is a contradiction



# Pu-239 fission spectrum



- Since the sensitivity coefficients of fission spectrum for PROTEUS are not available, this result must include a compensation effect
- According to the adjusted result of U-238 inelastic, PROTEUS prefers harder spectrum → But Pu-239 fission spectrum is adjusted to be softer

# Detailed Versions of CIELO

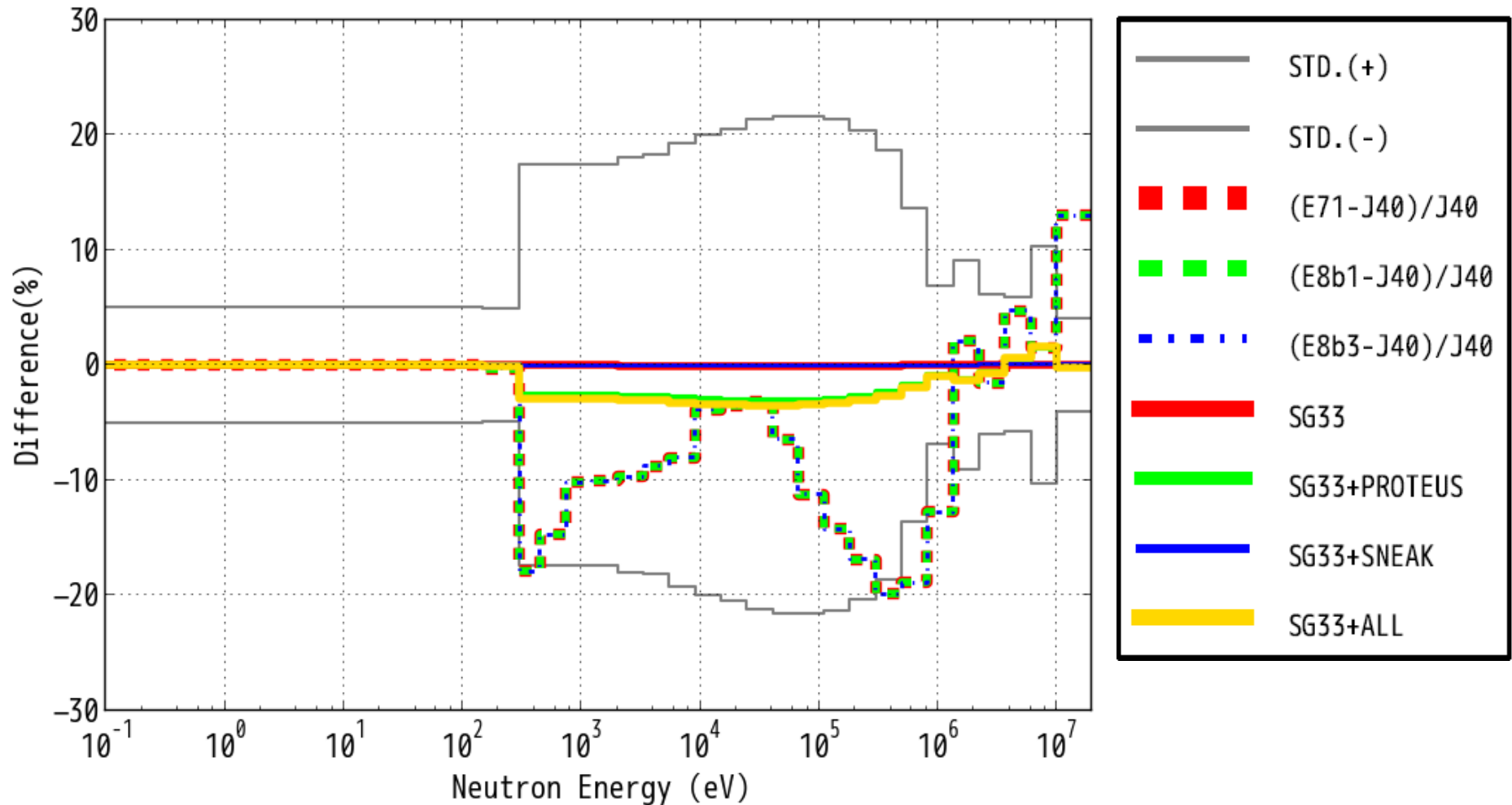
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All the CIELO files were downloaded from

<https://www-nds.iaea.org/CIELO/>

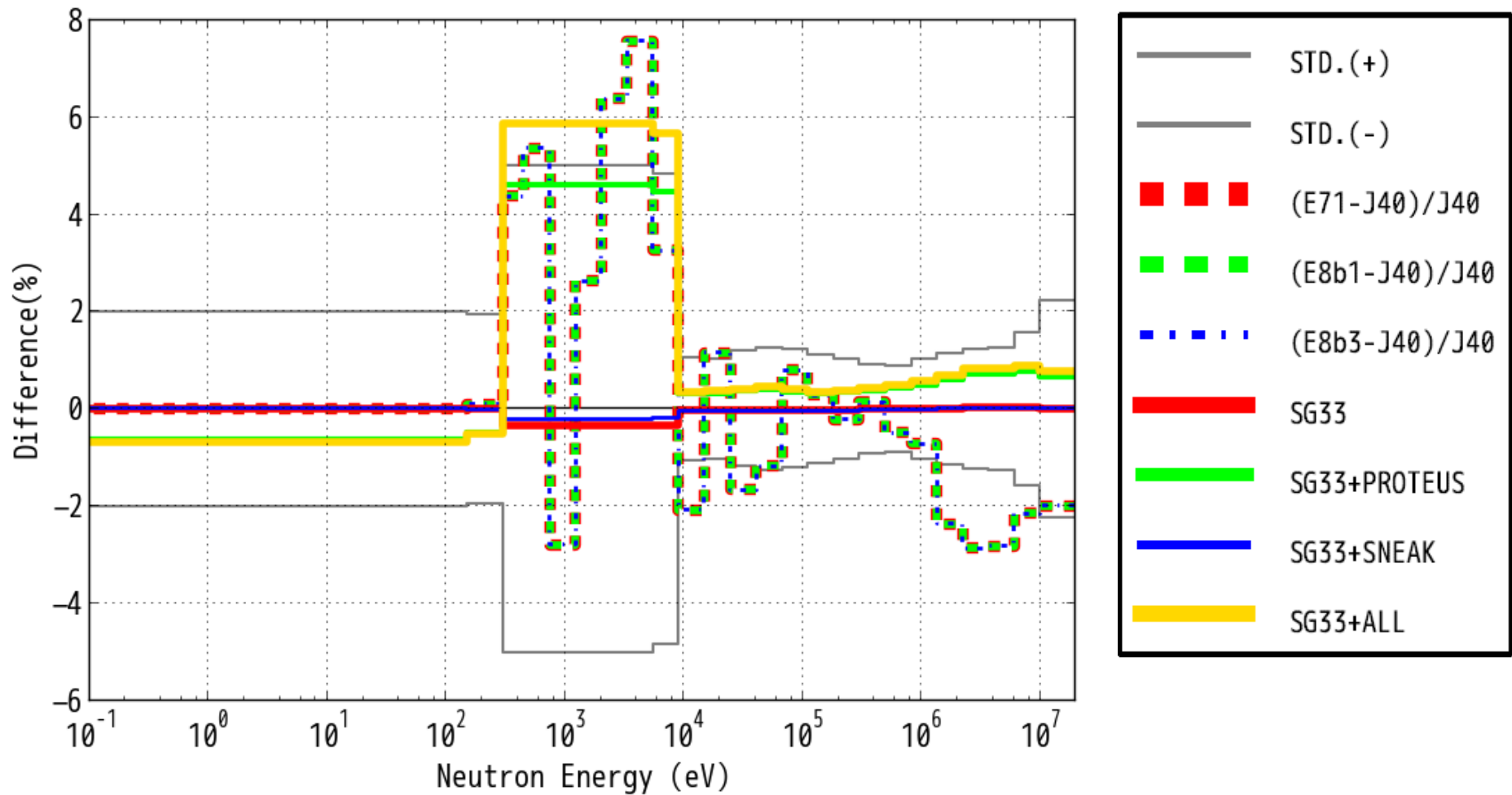
- IAEA-CIELO as of 5 Nov. 2016
  - **U-238** Version: u238beta2STD compressed ENDF file (internal IAEA designation u238ib51brlFsST1)
  - **U-235** Version: u235beta2STD compressed ENDF file (internal IAEA designation u235ib25o23g6DNcnu5ef4)
- IAEA-CIELO as of 8 Aug. 2016 (+ update 18 Aug. 2016)
  - **Pu-239** Version: lanlmbc2v; ENDF/B-VIII beta2 candidate file (mbc2) provided by A.C.(Skip) Kahler
  - **O-16** ENDF/B-VIII beta1 candidate file (o16e80b1) downloaded from NNDC
  - **Fe-56** Empire "ib15", complex file assembly using JEFF-3.2, JENDL-4.0 and EXFOR (Gforge version 219). Tuned P2 and P4 Legendre coefficients of elastic scattering to improve performance in iron-reflected benchmarks.

# Pu-241 elastic scattering cross sections



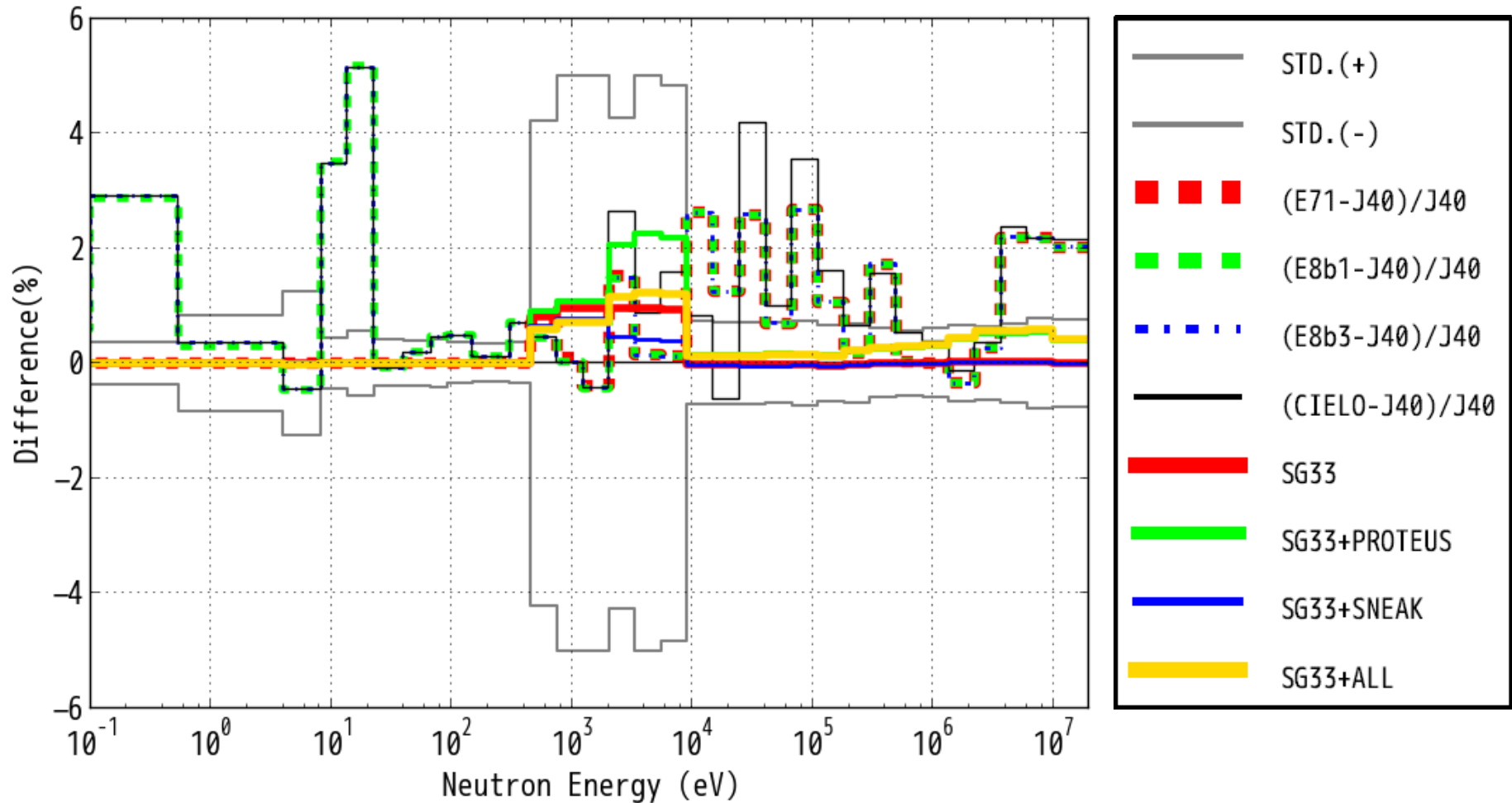
- SG33 and SNEAK give no change on Pu-241 cross section
- Addition of PROTEUS makes changes → new information

# Pu-241 fission cross sections



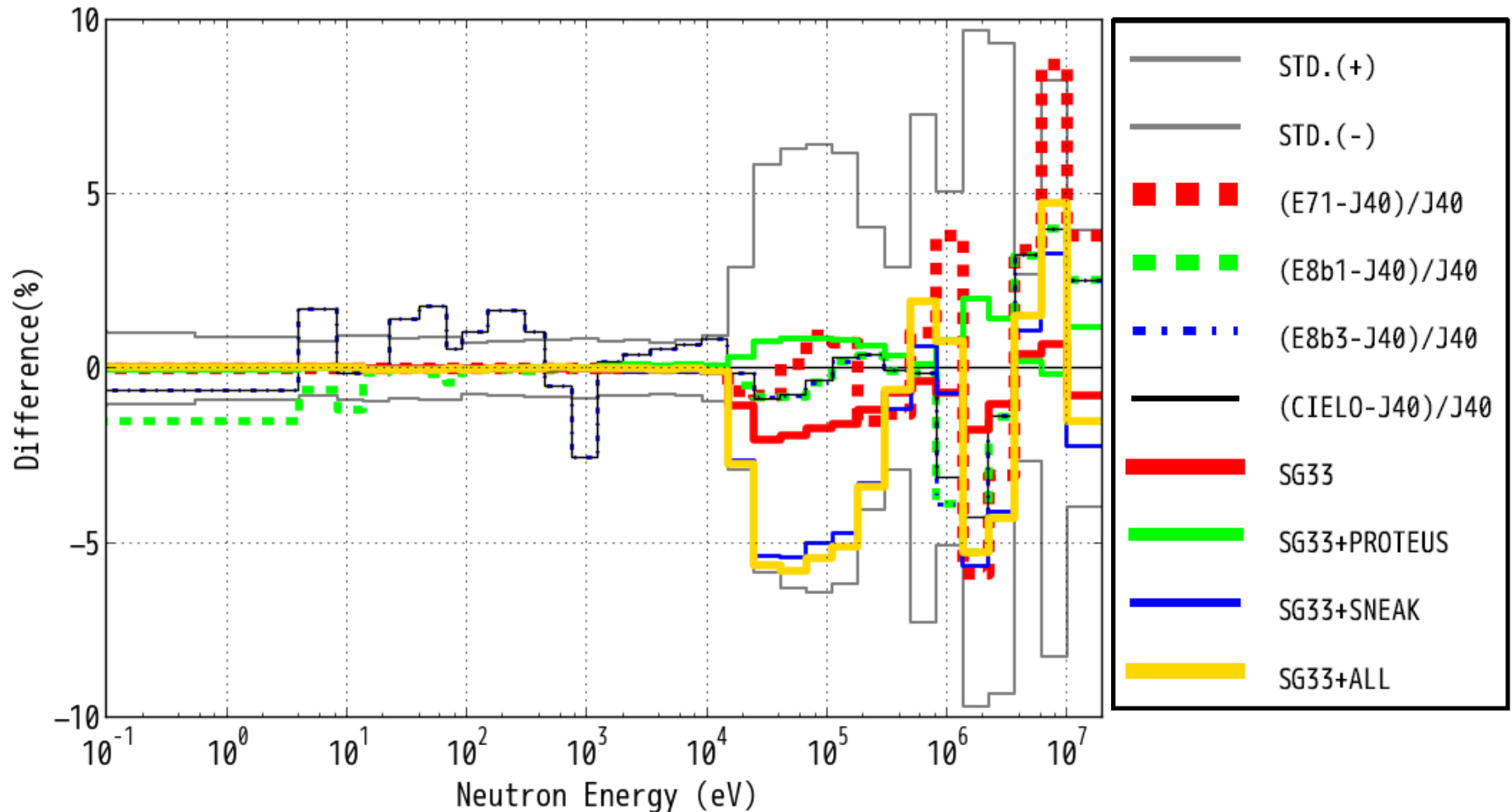
- PROTEUS increases Pu-241 fission cross section in above keV ranges
- PROTEUS supports ENDF-B/VIII.0 beta1 & 3 in keV ranges ?

# U-235 fission cross sections



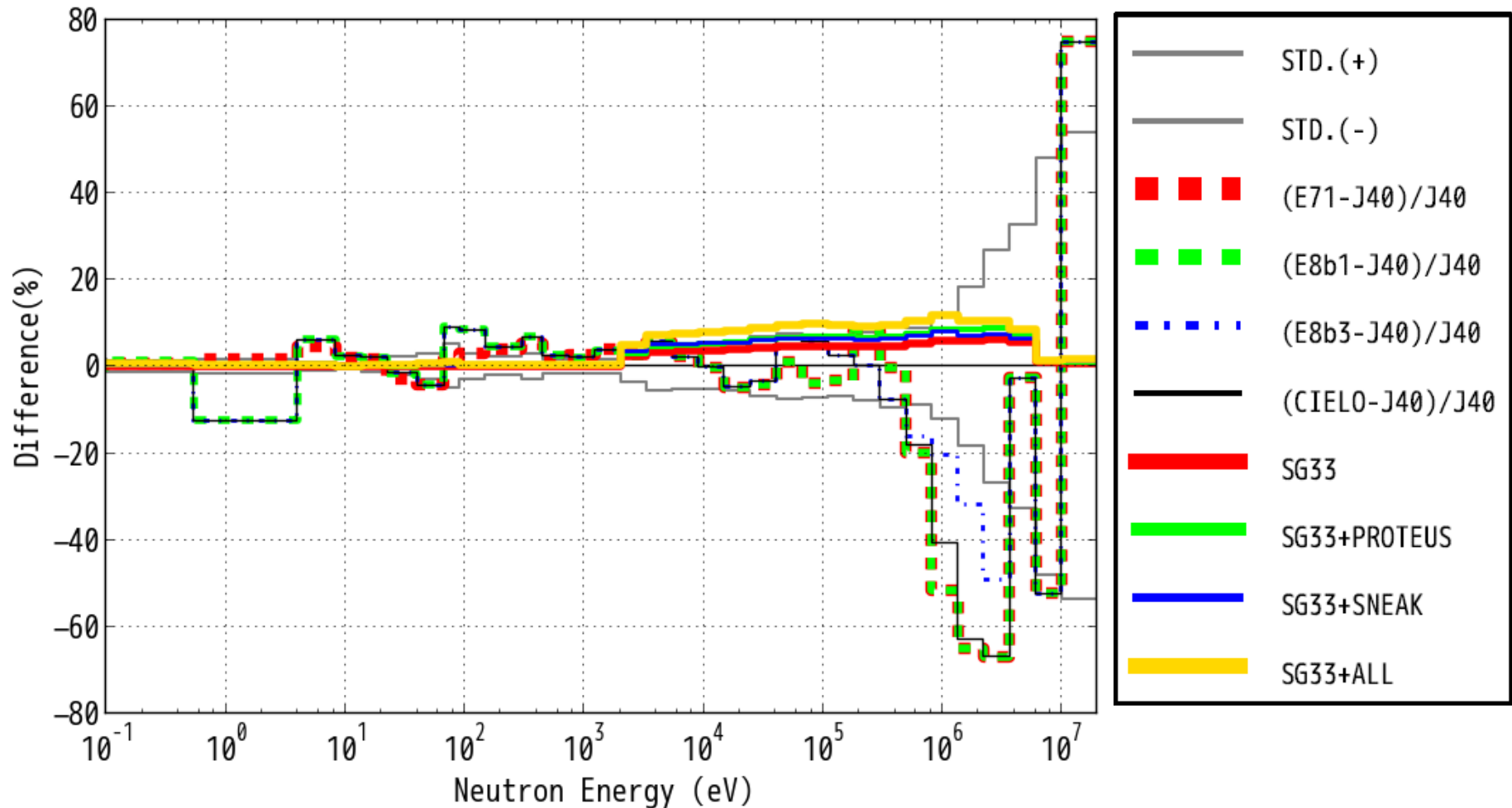
- PROTEUS increases U-235 fission cross section
- SNEAK seems to constrain the increment

# U-238 elastic scattering cross sections



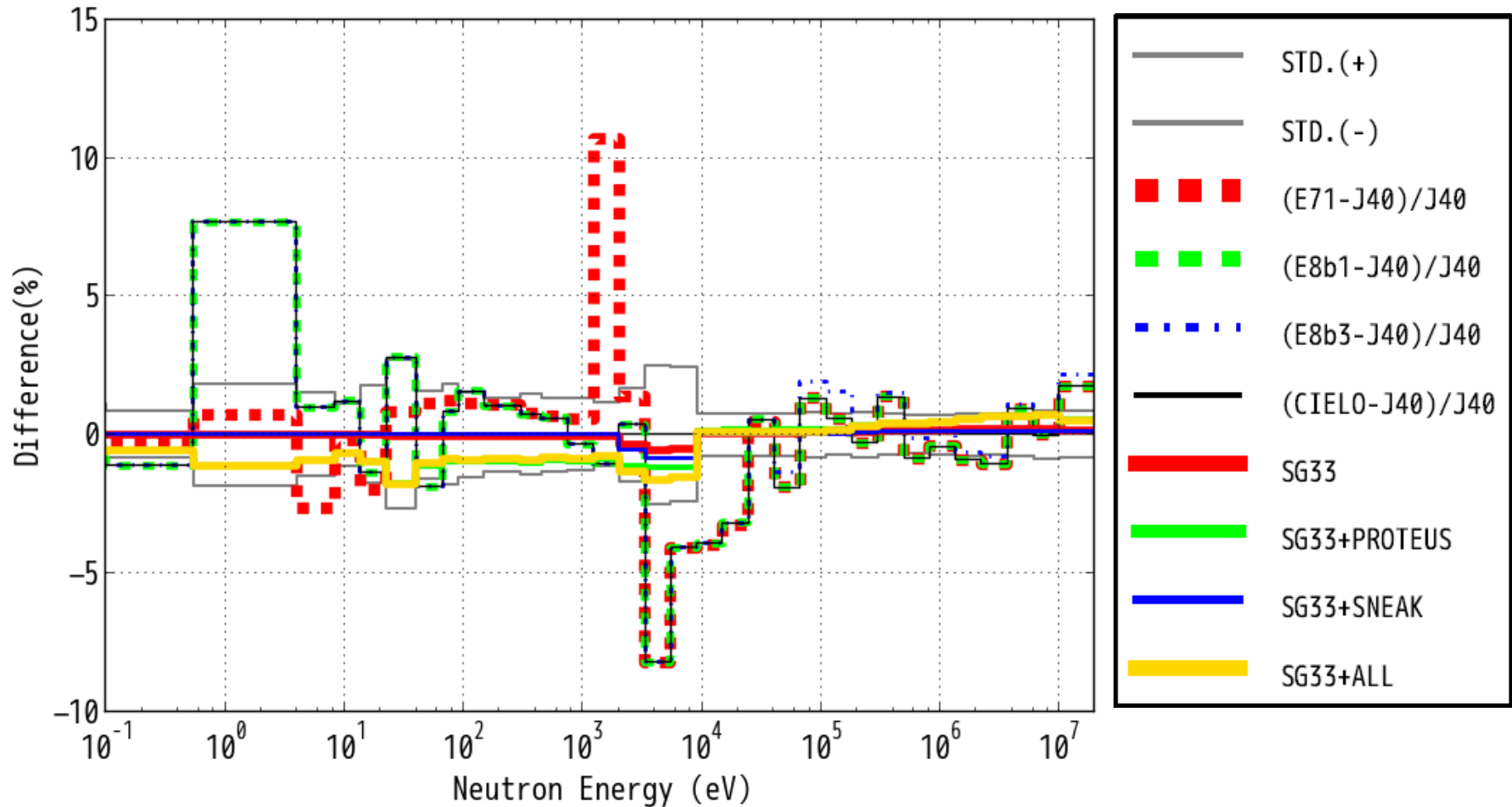
- PROTEUS and SNEAK seem to conflict with each other
- Changes by SNEAK seem to be dominant

# Pu-239 capture cross sections



- All integral experiments increase Pu-239 capture cross section → There is no contradiction

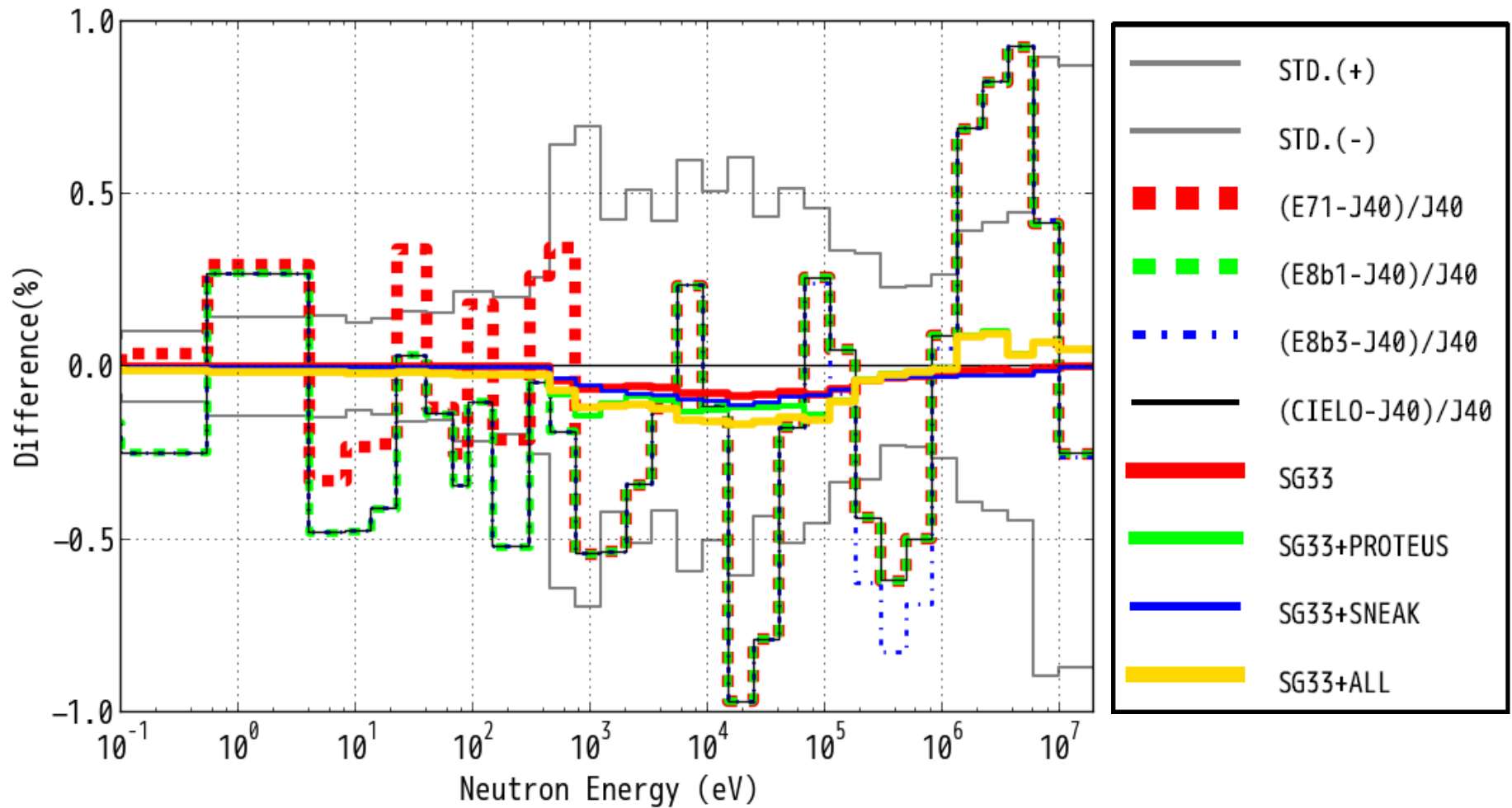
# Pu-239 fission cross sections



- PROTEUS decreases Pu-239 fission cross section in lower energy ranges

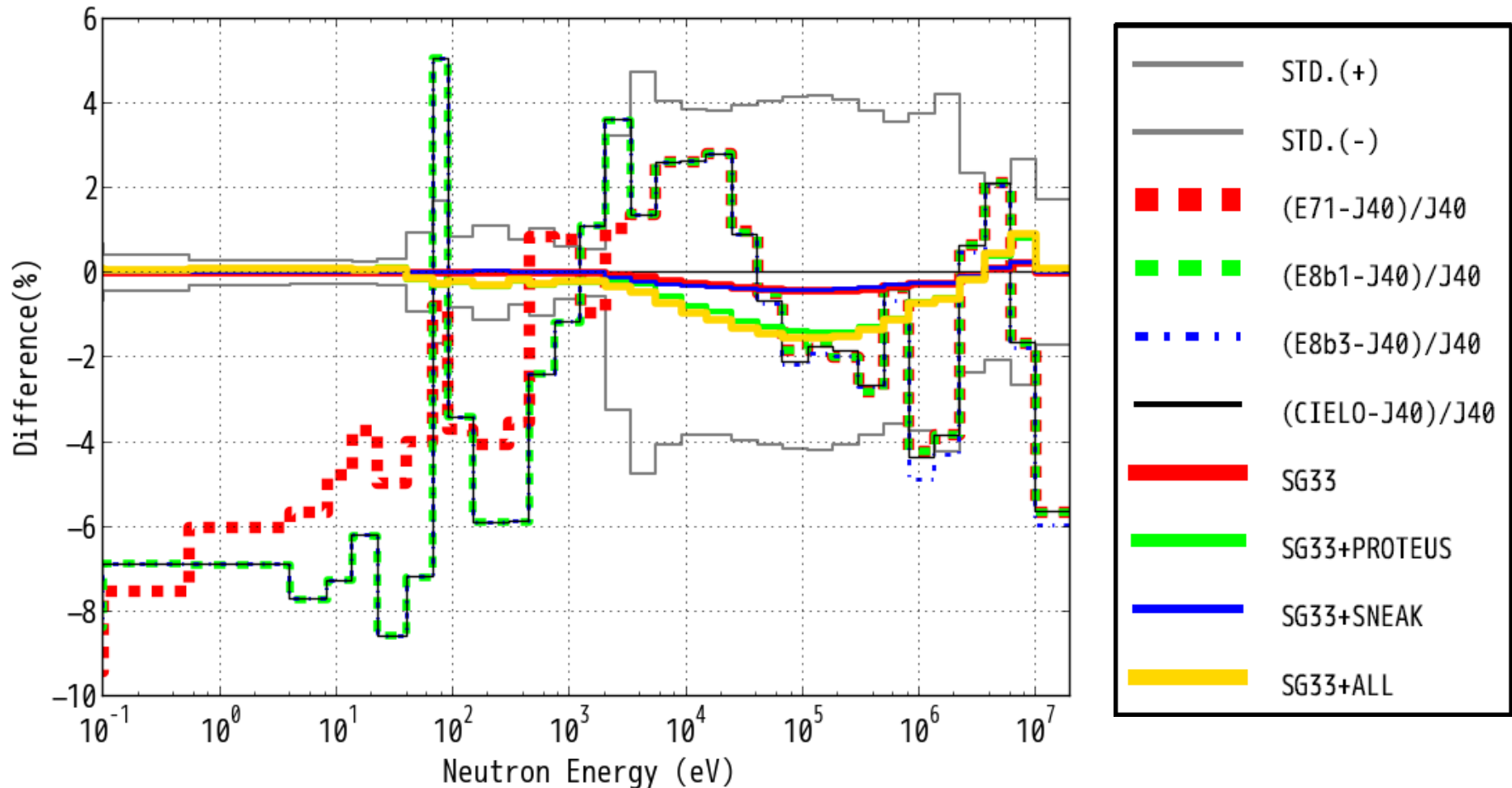


# Pu-239 nu-bar



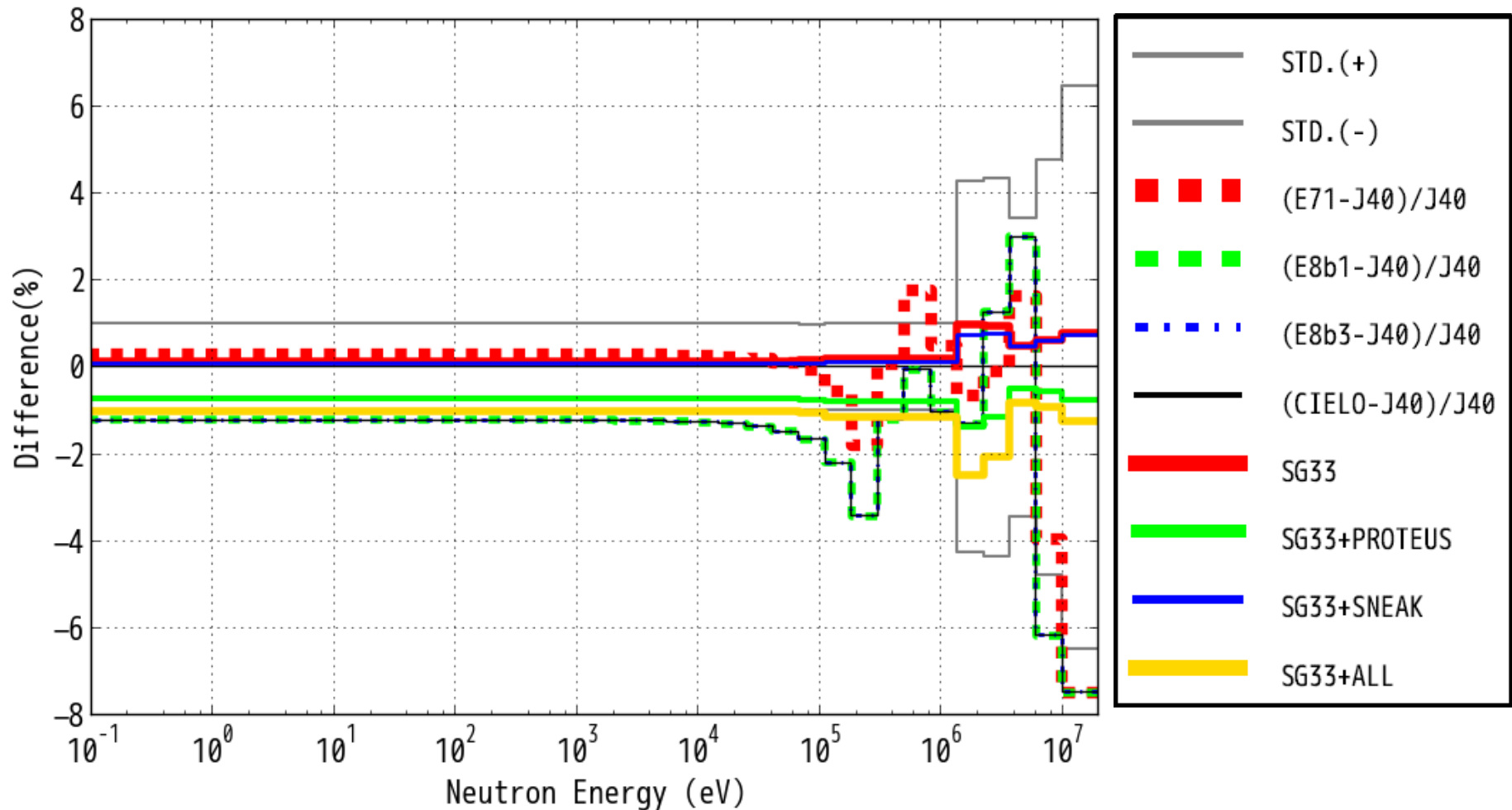
- There is no contradiction among all integral experiments

# Pu-239 elastic scattering cross sections



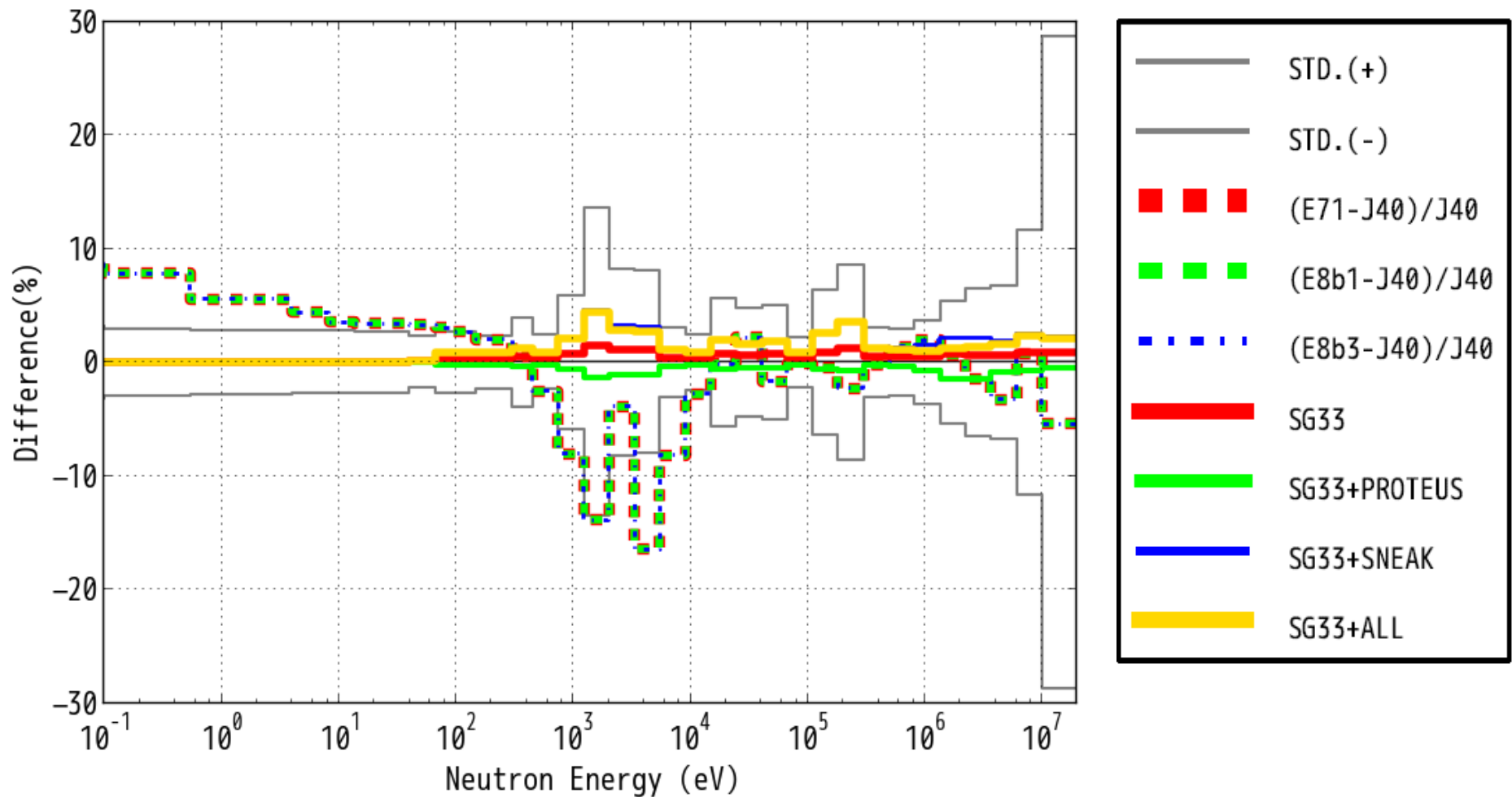
- There is no contradiction among all integral experiments
- PROTEUS makes further reduction of Pu-239 elastic scattering cross section

# O-16 elastic scattering cross sections



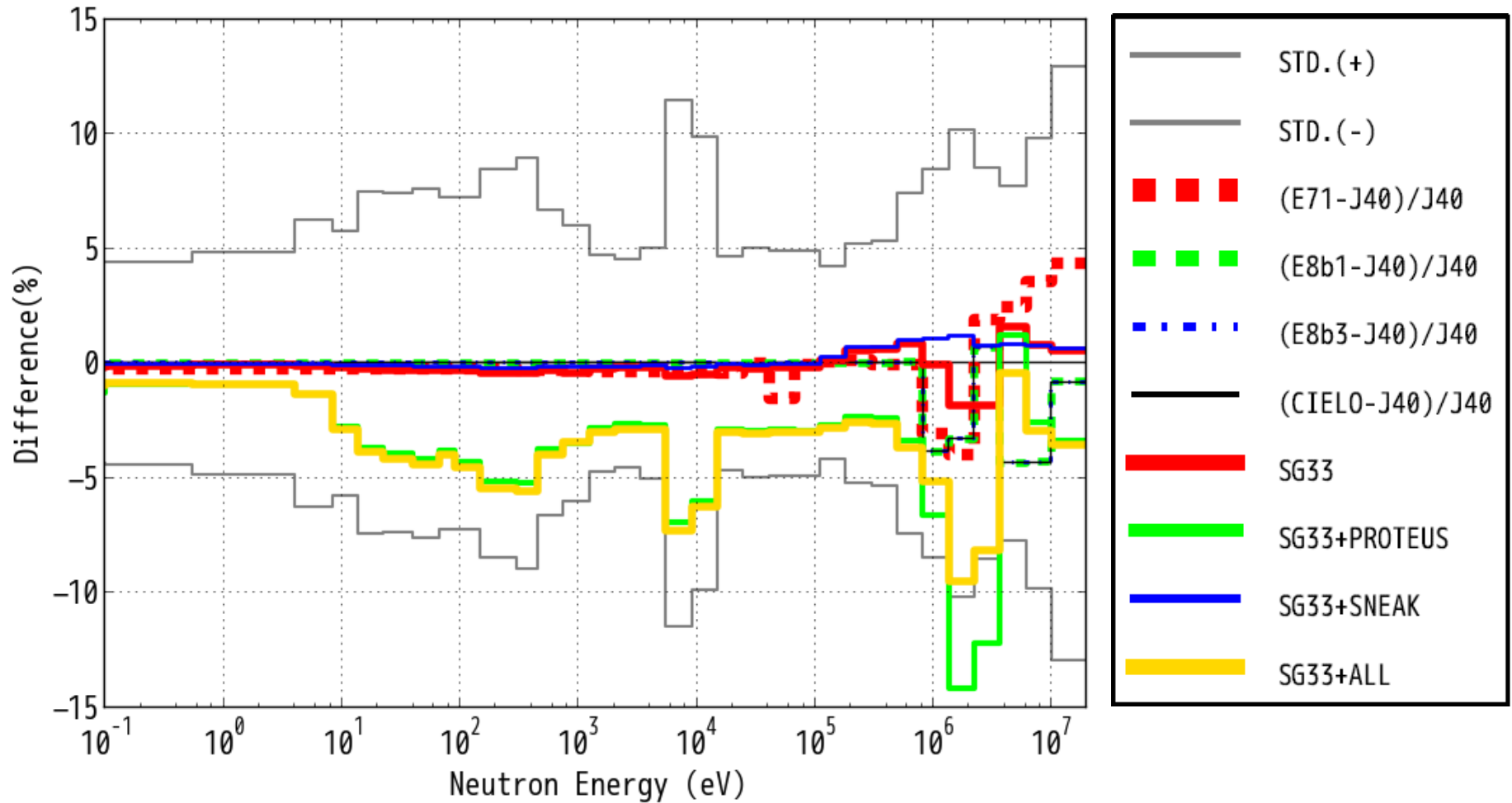
- PROTEUS reduces O-16 elastic scattering cross section
- Can we say that PROTEUS supports CIELO?

# Na-23 elastic scattering cross sections



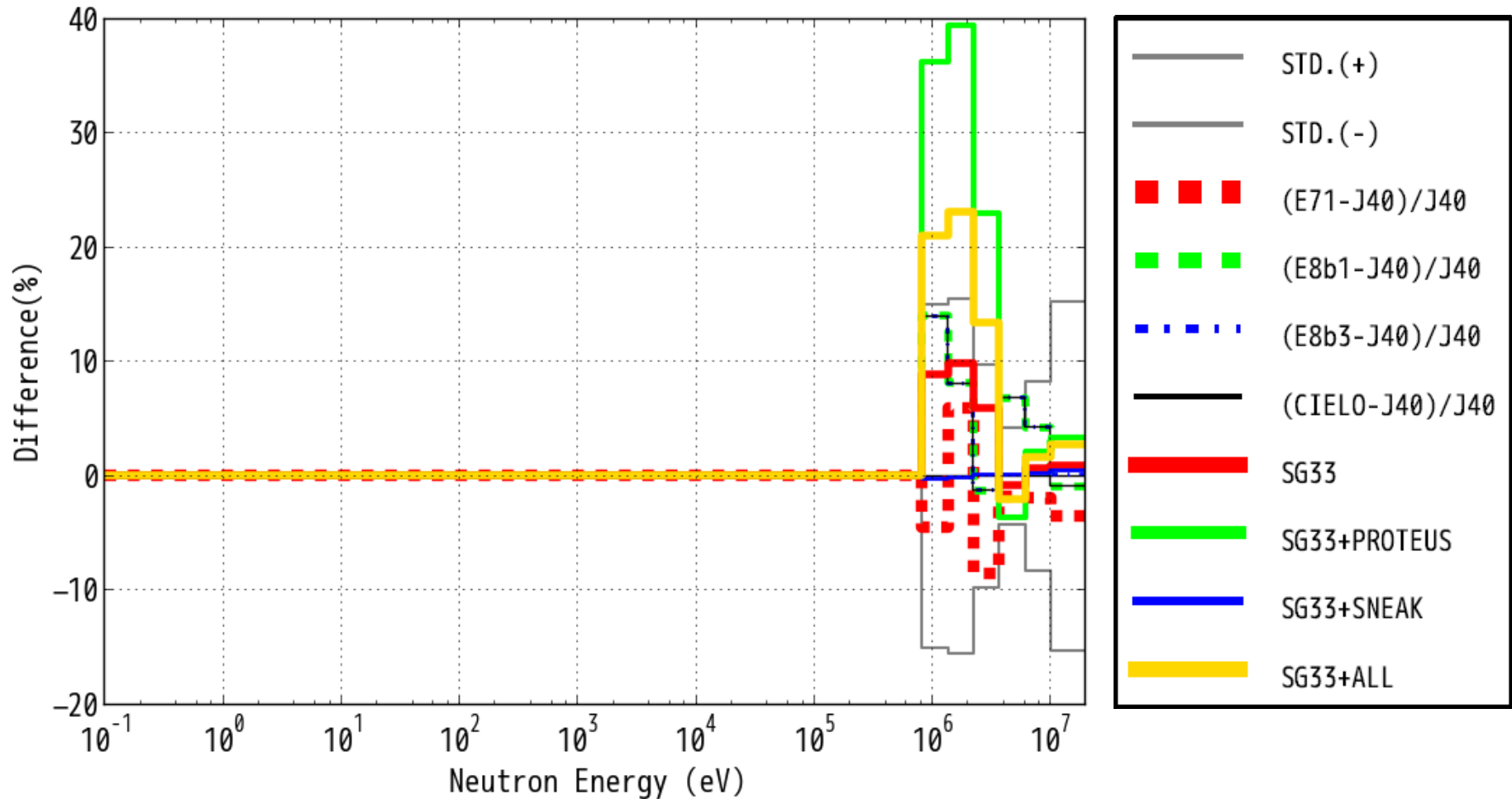
- PROTEUS reduces Na-23 elastic scattering although it does not include sodium
- There must have strong contradiction in the other reactions

# Fe-56 elastic scattering cross sections



- PROTEUS reduces Fe-56 elastic cross section

# Fe-56 inelastic scattering cross sections



- PROTEUS increases Fe-56 inelastic cross section too much ( $> 2$ -sigma) but this reaction only