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Comparison of PIA sequences by using the UR ^{238}U capture cross-section as a standard

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This study:

- Data assimilation: 4 configurations + 14 integral experiments.

- 10 nuclides considered in adjustment:
  ^{16}O, ^{23}Na, ^{52}Cr, ^{56}Fe, ^{58}Ni, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu.

- 33 group JEFF-3.1 a priori cross-sections (ECCO: ERANOS-2.2-N)

+

33 group a priori COMMARA-2.0 based variance/covariance data.
^{238}U capture cross-section in the unresolved resonance region: standard i.e. variance ≡ 0.

Asymptotic Progressive Incremental Adjustment

Configuration	❖ Integral parameters to assimilate	
GODIVA	*F28/F25, F49/F25, F37/F25*	At core center
JEZEBEL-Pu239	*F28/F25, F49/F25, F37/F25*	
ZPR6-7	*F28/F25, F49/F25, C28/F25*	
ZPPR9	*F28/F25, F49/F25, C28/F25,* Na Void -Step 3, -Step 5: coolant density effects	

- Sequence: GODIVA spectral indices → ZPPR9 coolant density effects → ZPPR9 spectral indices → ZPR6-7 spectral indices → JEZEBEL-Pu239 spectral indices.

❖**Asymptotic PIA: k_{eff} needs to be excluded from the assimilation.**

Asymptotic PIA methodology

Iterative procedure used in individual incremental steps:

For $i = 0, 1, 2, \ ...$ **$\boldsymbol{i = 0}$: a priori, starting point:**

$$\boldsymbol{\Delta T_i = M_i G_i^T \left(G_i M_i G_i^T + V_E + V_M\right)^{-1} CE_i \ , \ CE_i = \left(CE_{i,k}\right) = \left(\frac{R_{E,k} - (R_c(T_i))_{,k}}{(R_c(T_i))_{,k}}\right)} \qquad \textbf{(1)}$$

with

$M_i = \left(M_{i,j,j'}\right) = cov\left(T_{i,j}, T_{i,j'}\right) / \left(T_{i,j} T_{i,j'}\right)$: nuclear data variance/covariance matrix in relative terms.

$i = 0$: M_0: derived from COMMARA-2.0, this study.

$$\boldsymbol{M_{i+1} = \left(M_{i+1,j,j'}\right) = M_i - M_i G_i^T \left(G_i M_i G_i^T + V_E + V_M\right)^{-1} G_i M_i} \qquad \textbf{(2.1)}$$

Will be discarded

$$\boldsymbol{M_{i+1} = \left(M_{i+1,j,j'}\right) = M_0 - M_0 G_i^T \left(G_i M_0 G_i^T + V_E + V_M\right)^{-1} G_i M_0} \qquad \textbf{(2.2)}$$

Asymptotic PIA methodology (continued)

Additionally, Eq. (1):

$$\Delta T_i = (\Delta T_{i,j}) = \left(\frac{T_{i+1,j} - T_{i,j}}{T_{i,j}}\right) = \left(\frac{T_{i+1,j}}{T_{i,j}} - 1\right) = (F_{i,j} - 1) \qquad \Rightarrow$$

$$\boldsymbol{T_{i+1}} = (\boldsymbol{T_{i+1,j}}) = (\boldsymbol{T_{i,j}F_{i,j}}), \qquad \boldsymbol{F_i} = (\boldsymbol{F_{i,j}}) = (\mathbf{1} + \boldsymbol{\Delta T_{i,j}}) \qquad \textbf{(3)}$$

$T_i = (T_{i,j})$: data set vector. Starting from JEFF-3.1, this study.

$R_C(T_i) = \left((R_C(T_i))_{,k}\right)$: analytical values vector. Through ERANOS (2.2-N), this study. **Asymptotic PIA: for integral parameters $\boldsymbol{k}$ dealt with in specific step.**

$F_i = (F_{i,j})$: adjustment factor vector i.e. $\boldsymbol{T_{i+1,j}} = \left(\prod_{\boldsymbol{m=0}}^{\boldsymbol{i}} \boldsymbol{F_{m,j}}\right)\boldsymbol{T_{0,j}}$.

$R_E = (R_{E,k})$: vector of the central values of the experimental integral parameters.

Asymptotic PIA methodology (continued)

$$G_i = \left(G_{i,k,j}\right) = \left(\frac{d\left(\left(R_c(T_i)\right)_{,k}\right)}{\left(R_c(T_i)\right)_{,k}} \Bigg/ \frac{dT_{i,j}}{T_{i,j}} \right)$$

: in the form of sensitivity coefficient vector by using appropriate indexing.

$$V_E = \left(V_{E,k,k'}\right) = cov\left(R_{E,k}, R_{E,k'}\right) / \left(R_{E,k} R_{E,k'}\right)$$

: experimental variance/covariance matrix.

$$V_M = \left(V_{M,k,k'}\right) = cov\left(\left(R_c(T)\right)_{,k}, \left(R_c(T)\right)_{,k'}\right) / \left(\left(R_c(T)\right)_{,k} \left(R_c(T)\right)_{,k'}\right)$$

: analytical modeling matrix.

Iterations loop

From iteration i to $i+1$, two steps:

(1) $M_i, G_i, V_E, V_M, R_E, R_C(T_i) \xRightarrow{\text{Eq. 1}} \Delta T_i \xRightarrow{\text{Eq. 3}} F_i, T_{i+1}$

$M_i, G_i, V_E, V_M \xRightarrow{\text{Eq. 2}} M_{i+1}$

In house tool GLLS

(2) $T_{i+1} \xrightarrow{\text{In house tool MICADJ}}$ ERANOS (2.2-N) $\Rightarrow$ $R_C(T_{i+1}), G_{i+1};$

together with M_{i+1}: go to (1)

and replace i by $i+1$.

(1), (2) until $F_n = 1 \rightarrow n$ iterations needed to converge.

Practical reason: $0.99 < F_{n,j} < 1.01$, this study.

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Results (C/Es)

Configuration	Integral parameter	Experimental uncertainty (%)	PIA-Simulation		
			1	**1ST**	**1STm**
			C/E		
GODIVA	*F28/F25*	1.1	0.998	0.998	1.002
	F49/F25	1.0	1.001	1.001	1.004
	F37/F25	1.4	0.996	0.995	0.997
	k_{eff}	0.1	0.977	0.977	0.977
JEZEBEL-Pu239	*F28/F25*	1.1	0.997	0.998	1.000
	F49/F25	0.9	0.999	1.000	1.000
	F37/F25	1.4	1.005	1.004	1.001
	k_{eff}	0.2	0.995	0.996	0.997
ZPR6-7	*F28/F25*	3.0	1.020	1.019	1.011
	F49/F25	2.1	0.977	0.978	0.983
	C28/F25	2.4	1.001	1.003	1.000
	k_{eff}	0.2	1.007	1.006	1.001
ZPPR9	*F28/F25*	2.7	0.951	0.948	0.931
	F49/F25	2.0	0.997	0.997	1.001
	C28/F25	1.9	0.994	0.995	0.994
	Na Void Step 3	1.9	1.033	1.030	1.014
	Na Void Step 5	1.9	0.975	0.973	0.955
	k_{eff}	0.1	1.006	1.005	1.004
JEZEBEL-Pu240	k_{eff}	0.2	0.999	1.000	1.001
ZPR6-7_Pu240	k_{eff}	0.2	1.007	1.006	1.006
JOYO	k_{eff}	0.2	0.993	0.993	0.993
FLATTOP-Pu	*F28/F25*	1.1	0.981	0.982	0.995
	F37/F25	1.4	1.004	1.005	1.010
	k_{eff}	0.3	0.991	0.991	0.984
FLATTOP-25	*F28/F25*	1.1	0.996	0.996	1.003
	F49/F25	0.9	1.005	1.005	1.008
	F37/F25	1.3	1.005	1.005	1.008
	k_{eff}	0.1	0.972	0.972	0.967
MIX-MET-FAST-001	k_{eff}	0.2	0.993	0.994	0.995
PU-MET-FAST-010	k_{eff}	0.2	0.985	0.986	0.985
PU-MET-FAST-009	k_{eff}	0.3	0.988	0.988	0.986

- **1**: Reference solution.
- **1ST**: similar to **1**, UR ^{238}U capture cross-section: standard.
- **1STm**: similar to **1ST**, however:

$$M_{i+1} = \left(M_{i+1,j,j'}\right) = M_0 - M_0 G_i^T \left(G_i M_0 G_i^T + V_E + V_M\right)^{-1} G_i M_0$$

instead of

$$M_{i+1} = \left(M_{i+1,j,j'}\right) = M_i - M_i G_i^T \left(G_i M_i G_i^T + V_E + V_M\right)^{-1} G_i M_i$$

- **1-1ST**: *C/E*s similar: The COMMARA-2.0 uncertainty of the UR ^{238}U capture cross-section is only ~1-3%.
- **1ST-1STm**: also comparable.

Results (nuclear data caused uncertainties)

Configuration	Integral parameter	Experimental uncertainty (%)	PIA-Simulation		
			1	**1ST**	**1STm**
			Uncertainty (%)		
GODIVA	*F28/F25*	1.1	0.6	0.6	0.9
	F49/F25	1.0	0.2	0.2	0.5
	F37/F25	1.4	0.5	0.5	0.7
	k_{eff}	0.1	0.7	0.7	0.7
JEZEBEL-Pu239	*F28/F25*	1.1	0.3	0.2	1.0
	F49/F25	0.9	0.2	0.2	0.5
	F37/F25	1.4	0.3	0.3	0.8
	k_{eff}	0.2	0.3	0.3	0.4
ZPR6-7	*F28/F25*	3.0	0.9	0.9	1.9
	F49/F25	2.1	0.4	0.4	0.6
	C28/F25	2.4	0.7	0.6	0.9
	k_{eff}	0.2	0.6	0.6	0.6
ZPPR9	*F28/F25*	2.7	1.2	1.2	2.3
	F49/F25	2.0	0.4	0.4	0.6
	C28/F25	1.9	0.7	0.6	0.9
	Na Void Step 3	1.9	1.9	1.9	2.5
	Na Void Step 5	1.9	2.2	2.2	3.0
	k_{eff}	0.1	0.6	0.6	0.6
JEZEBEL-Pu240	k_{eff}	0.2	0.5	0.5	0.5
ZPR6-7_Pu240	k_{eff}	0.2	0.6	0.6	0.6
JOYO	k_{eff}	0.2	0.9	0.9	0.9
FLATTOP-Pu	*F28/F25*	1.1	0.4	0.3	0.8
	F37/F25	1.4	0.4	0.4	0.8
	k_{eff}	0.3	0.4	0.4	0.5
FLATTOP-25	*F28/F25*	1.1	0.6	0.6	0.9
	F49/F25	0.9	0.2	0.2	0.5
	F37/F25	1.3	0.6	0.6	0.8
	k_{eff}	0.1	0.9	0.9	0.9
MIX-MET-FAST-001	k_{eff}	0.2	0.2	0.2	0.3
PU-MET-FAST-010	k_{eff}	0.2	0.4	0.4	0.5
PU-MET-FAST-009	k_{eff}	0.3	0.3	0.3	0.4

- **1**: Reference solution.
- **1ST**: similar to **1**, UR ^{238}U capture cross-section: standard.
- **1STm**: similar to **1ST**, however:

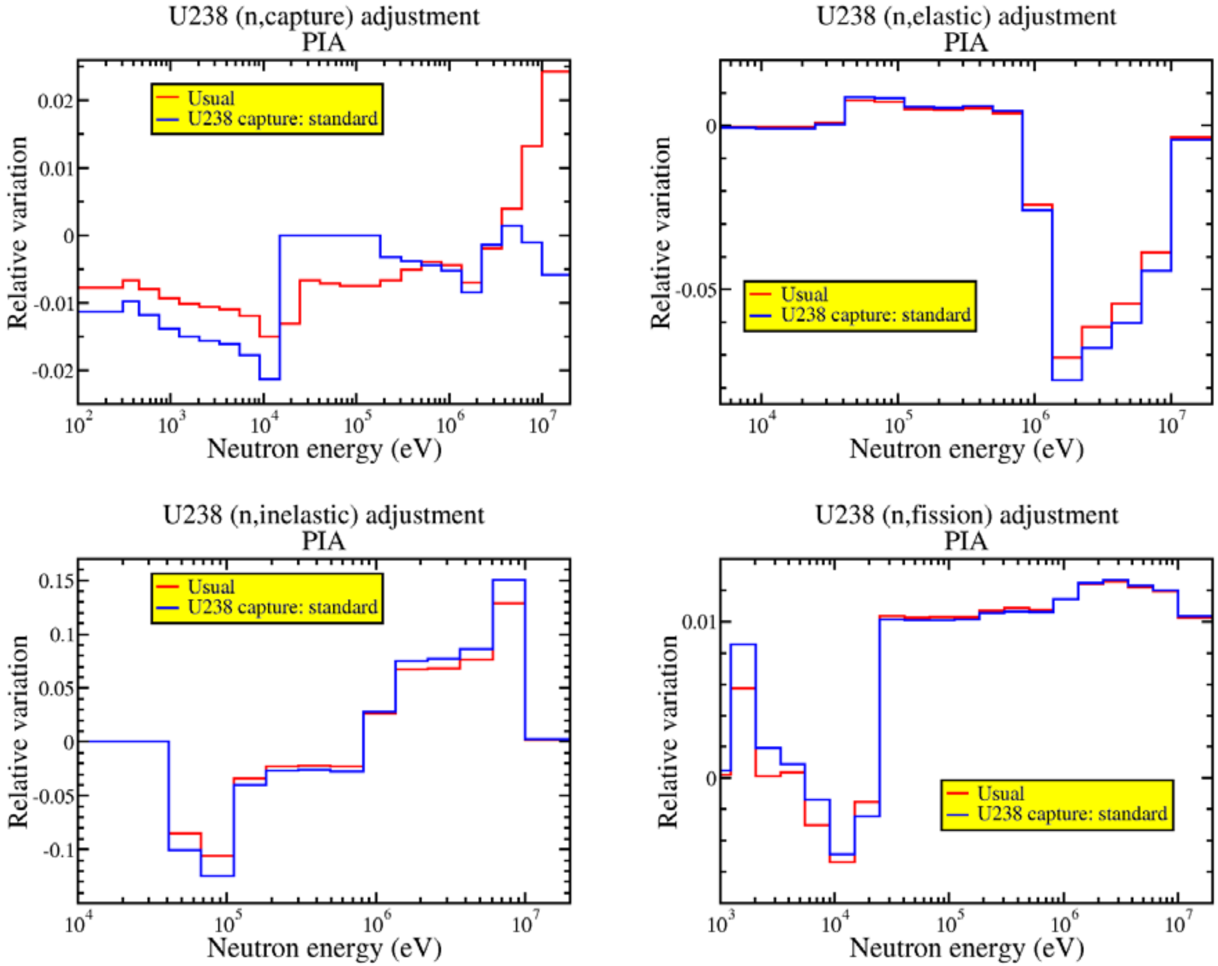
$$M_{i+1} = (M_{i+1,j,j'}) = M_0 - M_0 G_i^T (G_i M_0 G_i^T + V_E + V_M)^{-1} G_i M_0$$

instead of

$$M_{i+1} = (M_{i+1,j,j'}) = M_i - M_i G_i^T (G_i M_i G_i^T + V_E + V_M)^{-1} G_i M_i$$

- **1-1ST**: uncertainties similar. The COMMARA-2.0 uncertainty of the UR ^{238}U capture cross-section is only ~1-3%.
- **1STm**: as expected, uncertainties larger, though smaller than a priori values.

Adjustment of ^{238}U with respect to JEFF-3.1 (1, 1ST)

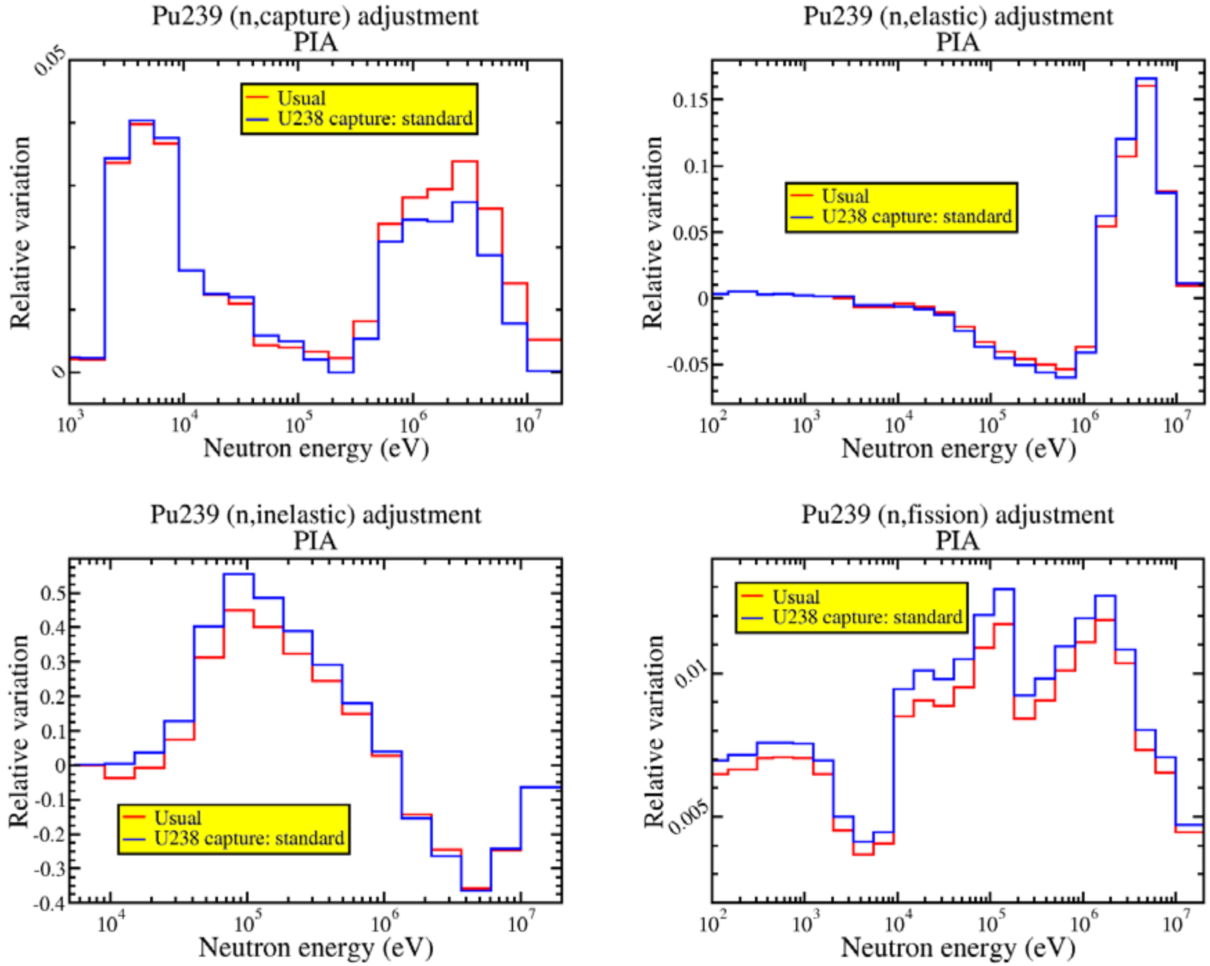


- The adjustment of the capture cross-section is different for high energies > 1MeV.
- Indeed: COMMARA-2.0 correlations for capture cross-section between UR and fast energy range large.

Relative variation:

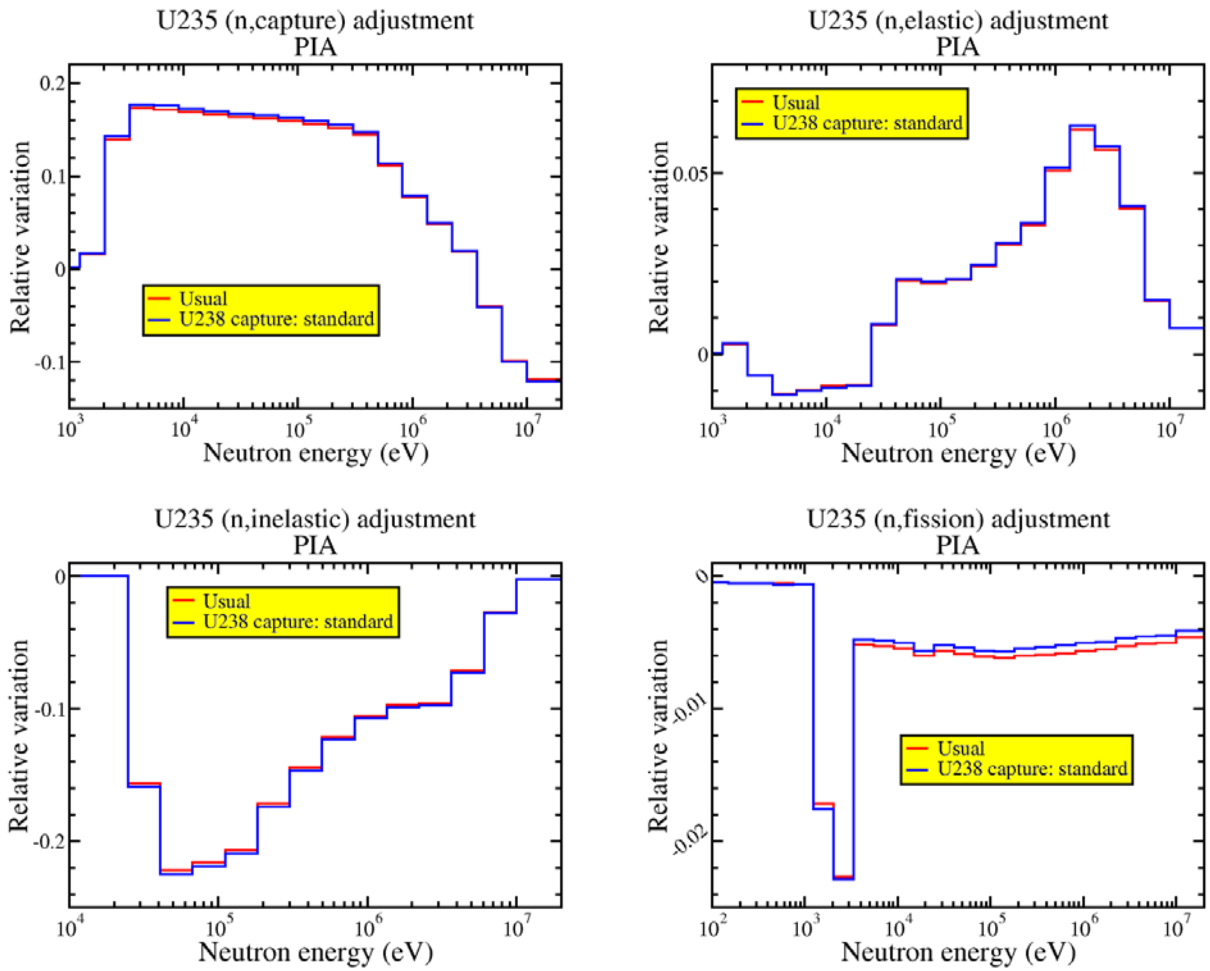
$$\frac{\sigma_{adj} - \sigma_{jeff}}{\sigma_{jeff}}$$

Adjustment of ^{239}Pu with respect to JEFF-3.1 (1, 1ST)



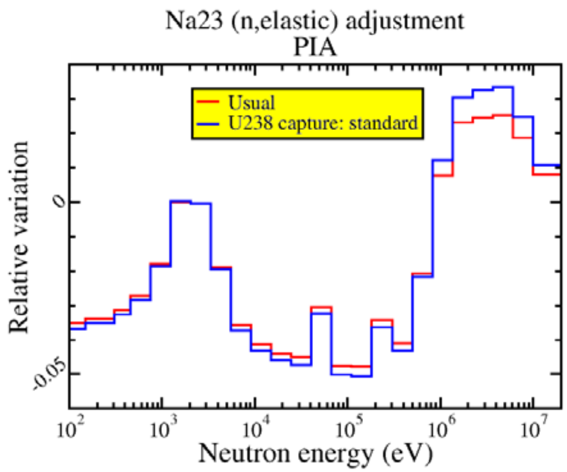
- The adjustment of the scattering and fission cross-sections is somewhat stronger if the UR capture cross-section of ^{238}U has no uncertainty.

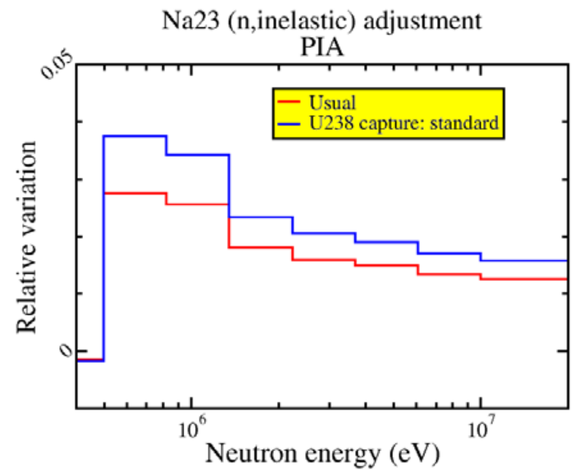
Adjustment of ^{235}U with respect to JEFF-3.1 (1, 1ST)



- Almost no effects coming from ^{238}U.

Adjustment of ^{23}Na with respect to JEFF-3.1 (1, 1ST)

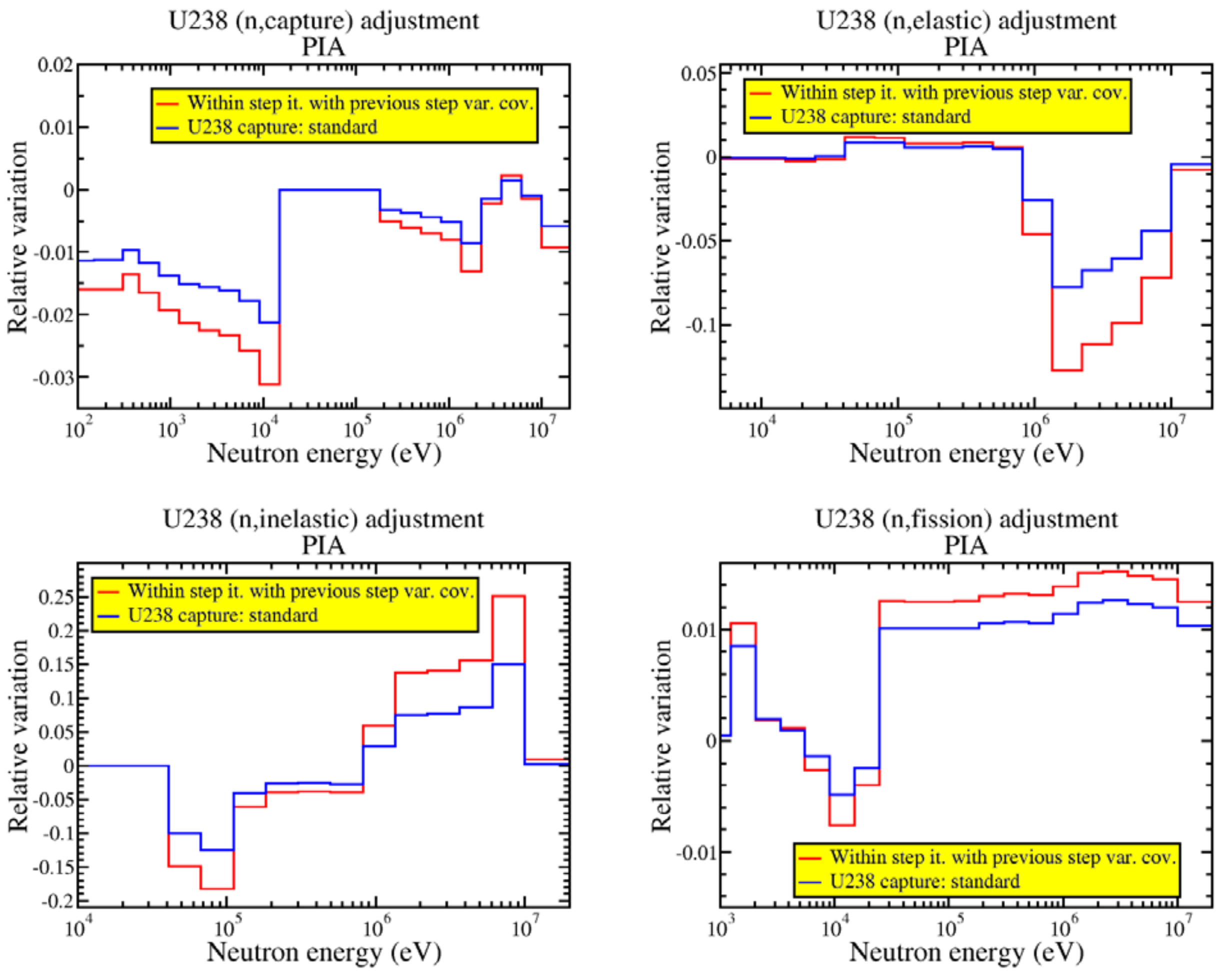




- The adjustment of the scattering cross-sections is somewhat stronger if the UR capture cross-section of ^{238}U has no uncertainty.

However: adjustments for ^{23}Na and ^{238}U not reliable: asymptotic sensitivity coefficients to ^{23}Na and ^{238}U of the integral parameters to assimilate dependent on the PIA sequence.

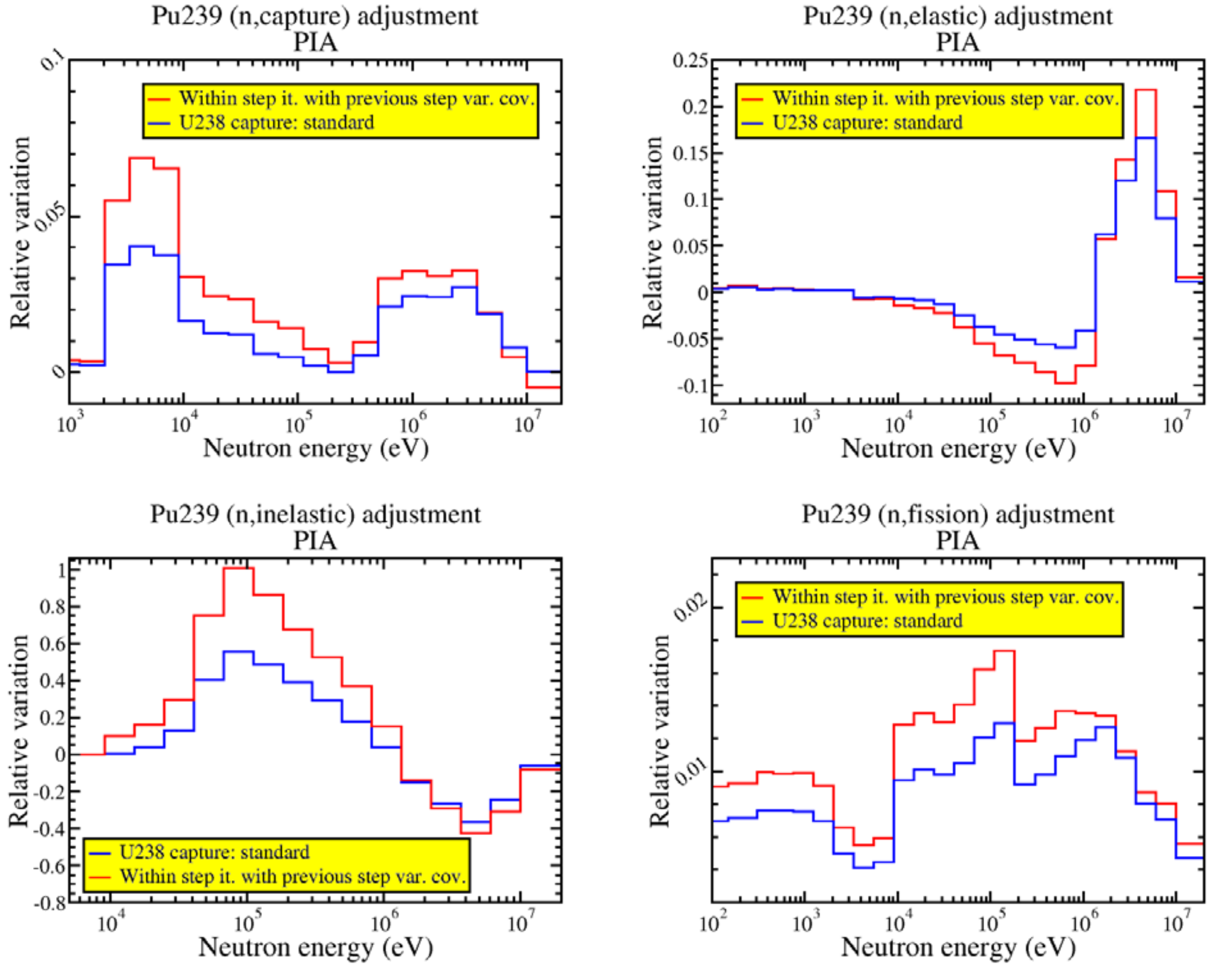
Adjustment of ^{238}U with respect to JEFF-3.1 (1ST, 1STm)



- Adjustment similar trends, however, as expected, stronger when using a priori variance/ covariance matrix at beginning of each incremental step.

Blue: $\boldsymbol{M_i}$ (Eq. (2.1))
Red: $\boldsymbol{M_0}$ (Eq. (2.2))

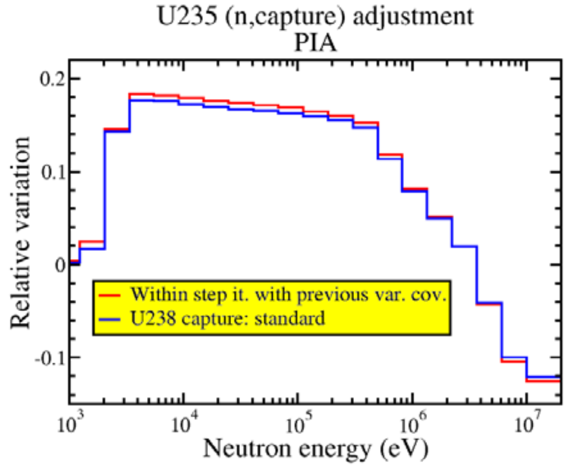
Adjustment of ^{239}Pu with respect to JEFF-3.1 (1ST, 1STm)

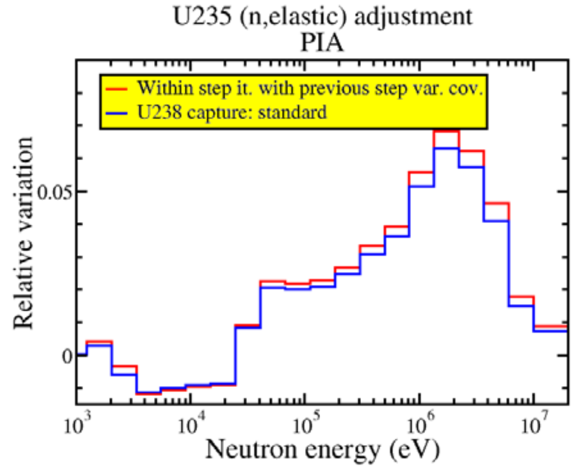


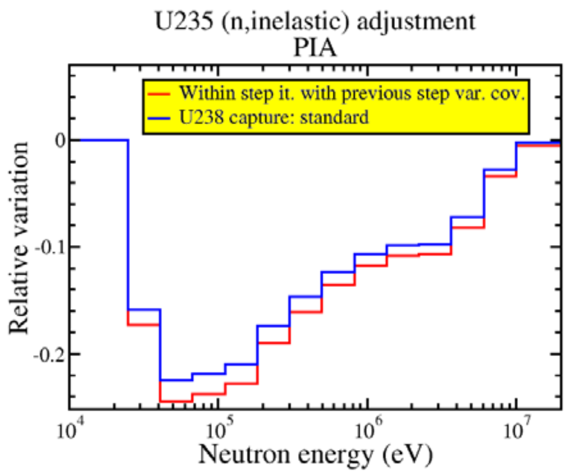
- Adjustment similar trends, however **>> 1σ changes** with a priori variance/ covariance matrix at beginning of each incremental step.

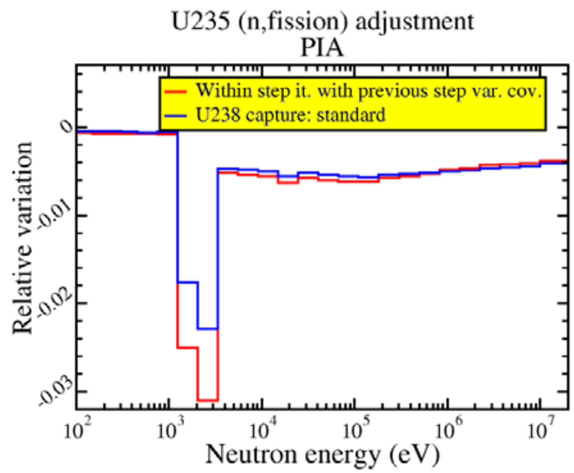
Blue: $\boldsymbol{M_i}$ (Eq. (2.1))
Red: $\boldsymbol{M_0}$ (Eq. (2.2))

Adjustment of ^{235}U with respect to JEFF-3.1 (1ST, 1STm)





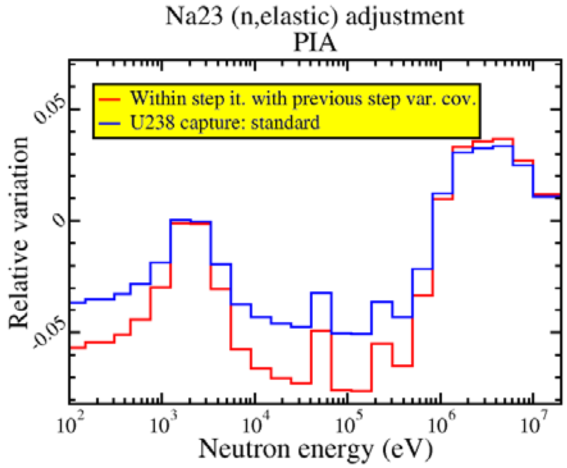


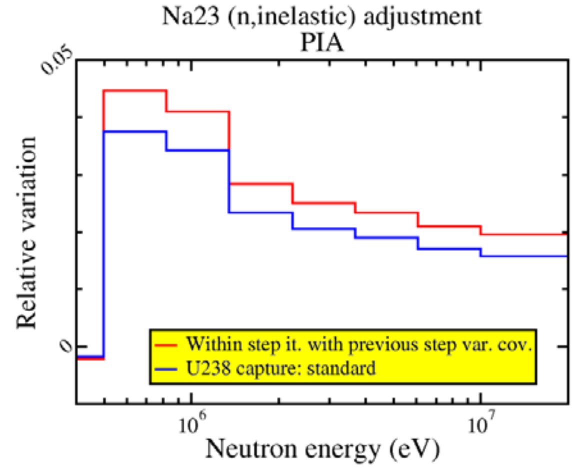


- Adjustment: similar trends.

Blue: $\boldsymbol{M_i}$ (Eq. (2.1))
Red: $\boldsymbol{M_0}$ (Eq. (2.2))

Adjustment of ^{23}Na with respect to JEFF-3.1 (1ST, 1STm)





- Adjustment: similar trends. however, as expected, stronger when using a priori variance/ covariance matrix at beginning of each incremental step.

Blue: $\boldsymbol{M_i}$ (Eq. (2.1))
Red: $\boldsymbol{M_0}$ (Eq. (2.2))