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Detailed comparison of Progressive Incremental Adjustment (PIA) sequence results involving adjustments of spectral indices and coolant density effects on the basis of the SG33 benchmark

NEA Nuclear Data Week, WPEC/SG-39

In this study: 14 integral parameters to assimilate

Experimental configurations with integral parameters part of the data assimilation

Configuration	Integral parameters
GODIVA	<i>F28/F25, F49/F25, F37/F25</i>
JEZEBEL-Pu239	<i>F28/F25, F49/F25, F37/F25</i>
ZPR6-7	<i>F28/F25, F49/F25, C28/F25</i>
ZPPR9	<i>F28/F25, F49/F25, C28/F25, Na Void Step 3, Na Void Step 5</i>

- *F28, F25, F49*, and *F37*: respectively used for ^{238}U , ^{235}U , ^{239}Pu , and ^{237}Np microscopic fission reaction rates per atom.
- *C28*: ^{238}U capture reaction rate per ^{238}U atom.
All spectral indices, Table, at core center.
- Na Void Step 3 and Na Void Step 5: reactivity effects (ZPPR9) due to Na removal from small zone near core center and from leakage dominated larger configuration.
- 10 nuclides adjusted: ^{16}O , ^{23}Na , ^{52}Cr , ^{56}Fe , ^{58}Ni , ^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu , ^{241}Pu .

12 target configurations

Target experimental configurations with integral parameters

Configuration	Integral parameters
GODIVA	$F28/F25, F49/F25, F37/F25, k_{eff}^{(a)}$
JEZEBEL-Pu239	$F28/F25, F49/F25, F37/F25, k_{eff}^{(a)}$
ZPR6-7	$F28/F25, F49/F25, C28/F25, k_{eff}^{(a)}$
ZPPR9	$F28/F25, F49/F25, C28/F25, \text{Na Void Step 3, Na Void Step 5}, k_{eff}^{(a)}$
JEZEBEL-Pu240	k_{eff}
ZPR6-7 Pu240	k_{eff}
JOYO	k_{eff}
FLATTOP-Pu	$F28/F25, F37/F25, k_{eff}$
FLATTOP-25	$F28/F25, F49/F25, F37/F25, k_{eff}$
MIX-MET-FAST-001	k_{eff}
PU-MET-FAST-010	k_{eff}
PU-MET-FAST-009	k_{eff}

^(a)Also part of the adjustment in one of the simulations.

8 configurations not part of the data assimilation

- JEZEBEL-Pu240, ZPR6-7 Pu240, JOYO.
- FLATTOP-Pu: Pu sphere reflected by natural U.
- FLATTOP-25: ^{235}U sphere reflected by natural U.
- MIX-MET-FAST-001: Pu sphere surrounded by highly enriched U.
- PU-MET-FAST-010: Pu sphere surrounded by Al.
- PU-MET-FAST-009: δ -phase Pu sphere reflected by natural U.

Sensitivity coefficients

- ERANOS (2.2-N), explicit, 33 group by means of flux, adjoint flux, generalized importance.
- Generalized Perturbation Theory (GPT) : spectral indices.
- Equivalent Generalized Perturbation Theory (EGPT): reactivity effects.
- [Standard Perturbation Theory (SPT) : k_{eff} , limited use.]

Data adjustment: Asymptotic GLLS method

Iterative procedure used in individual incremental steps within PIA:

For $i = 0, 1, 2, \dots$

$i = 0$: a priori, starting point:

$$\Delta T_i = M_i G_i^T (G_i M_i G_i^T + V_E + V_M)^{-1} C E_i, \quad C E_i = (C E_{i,k}) = \left(\frac{R_{E,k} - (R_c(T_i))_{,k}}{(R_c(T_i))_{,k}} \right) \quad (1)$$

with

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

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

$$M_{i+1} = (M_{i+1,j,j'}) = M_i - M_i G_i^T (G_i M_i G_i^T + V_E + V_M)^{-1} G_i M_i \quad (2)$$

GLS method

Additionally, Eq. (1):

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

$$\mathbf{T}_{i+1} = (\mathbf{T}_{i+1,j}) = (\mathbf{T}_{i,j} \mathbf{F}_{i,j}), \quad \mathbf{F}_i = (\mathbf{F}_{i,j}) = (\mathbf{1} + \Delta \mathbf{T}_{i,j}) \quad (3)$$

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

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

$F_i = (F_{i,j})$: adjustment factor vector i.e. $\mathbf{T}_{i+1,j} = (\prod_{m=0}^i \mathbf{F}_{m,j}) \mathbf{T}_{0,j}$.

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

GLS method

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

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

$$V_E = (V_{E,k,k'}) = cov(R_{E,k}, R_{E,k'}) / (R_{E,k} R_{E,k'}) : \text{experimental variance/covariance matrix.}$$

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

: analytical modeling matrix.

Iterations loop

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

$$(1) \quad M_i, G_i, V_E, V_M, R_E, R_C(T_i) \xrightarrow{\text{Eq. 1}} \Delta T_i \xrightarrow{\text{Eq. 3}} F_i, T_{i+1} \quad \left. \begin{array}{l} \\ \xrightarrow{\text{Eq. 2}} M_{i+1} \end{array} \right\} \text{In house tool GLLS}$$

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

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.

Adjustment: this study, 6 cases

- Simulation 1: integral parameters assimilated simultaneously.

PIA: Simulations 2, 2A, 2B, 3, 3A, 3B:

- 2:

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

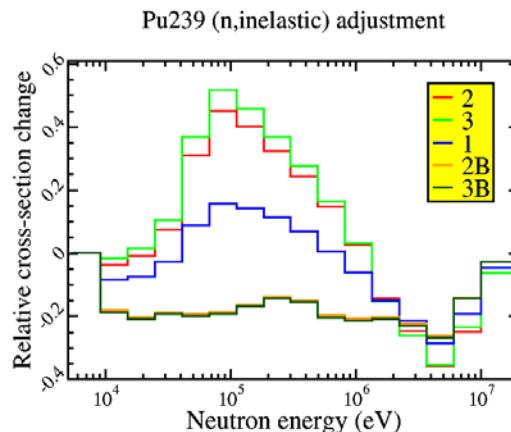
- 2A: Simulation 2 → k_{eff} of the 4 configurations just for $\bar{\nu}$.

- 2B: Similar to Simulation 2: no iterations.

- 3 : Reversed order as compared to Simulation 2: JEZEBEL-Pu239 first.

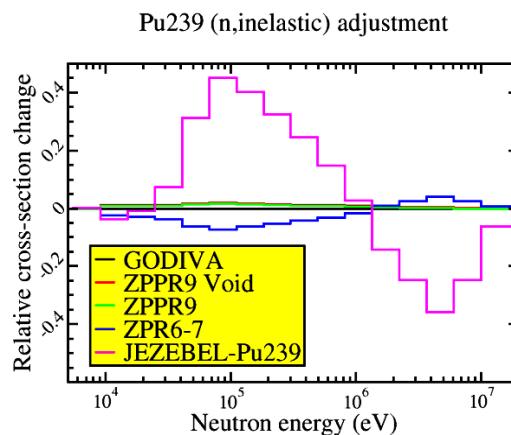
- 3B: Similar to Simulation 3: no iterations.

Adjustment of the ^{239}Pu inelastic scattering cross-section with respect to JEFF-3.1 a priori data in 33 groups

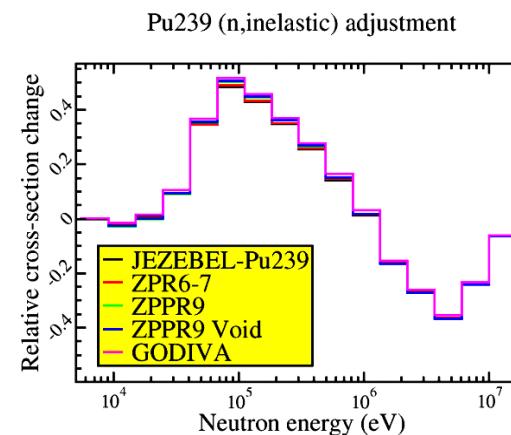


Adjustment: strong, max. 1σ COMMARA-2.0.

- $2 \equiv 3; 2B \equiv 3B$: sequence independent.
- $2 \neq 2B$: important role of iterations.
- 1 similar to 2,
smaller magnitude: compensations.



Simulation 2 (steps)

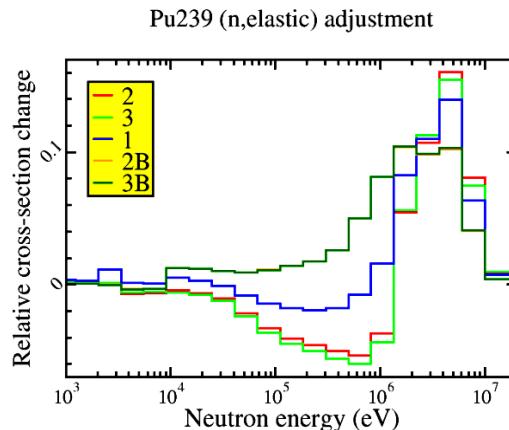


Simulation 3 (steps)

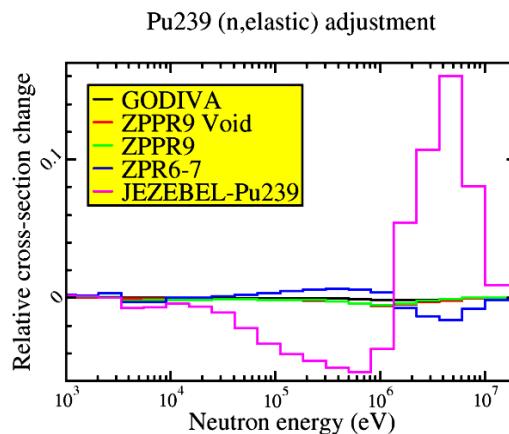
Adjustment, PIA:

- Coming from assimilating JEZEBEL-Pu239 data.

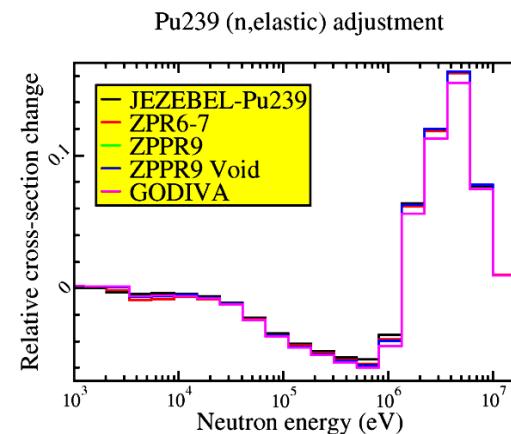
Adjustment of the ^{239}Pu elastic scattering cross-section



- $2 \equiv 3.$ $2\text{B} \equiv 3\text{B}.$
- $2 \neq 2\text{B}.$
- 1: between 2 and 2B having partly different sign.



Simulation 2 (steps)

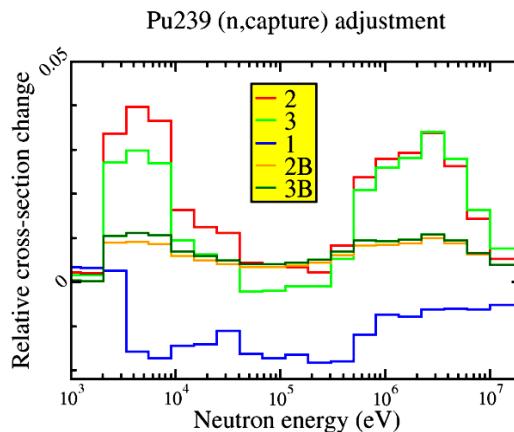


Simulation 3 (steps)

Adjustment, PIA:

- JEZEBEL-Pu239.

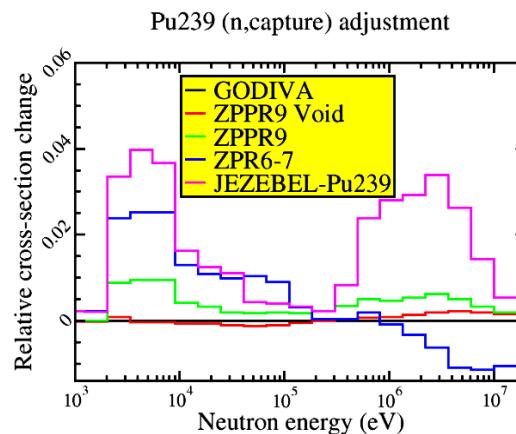
Adjustment of the ^{239}Pu capture cross-section



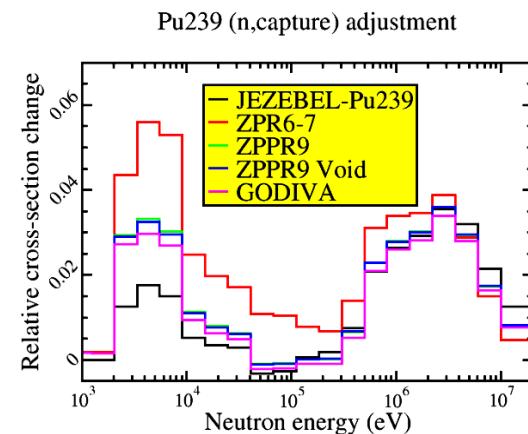
Adjustment, PIA:

- Fission source range: JEZEBEL-Pu239.
- Near main Na resonance 2.85keV: ZPR6-7.
- ZPPR9: seems unimportant or redundant.

- $2 \equiv 3$. $2B \equiv 3B$.
- $2 \neq 2B \neq 1$.



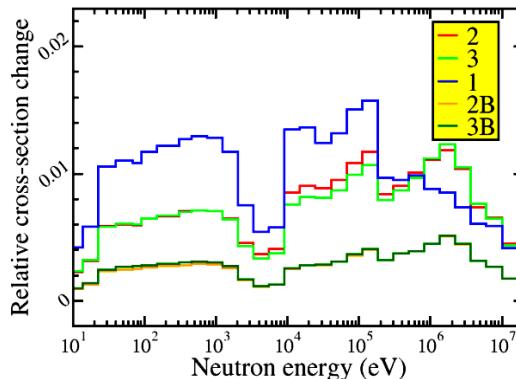
Simulation 2 (steps)



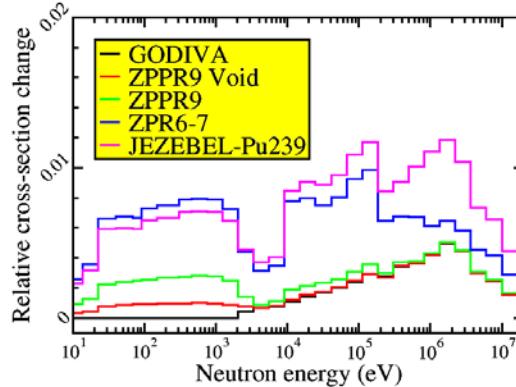
Simulation 3 (steps)

Adjustment of the ^{239}Pu fission cross-section

Pu239 (n,fission) adjustment



Pu239 (n,fission) adjustment

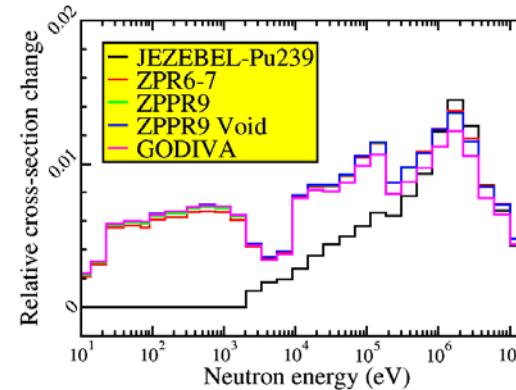


Simulation 2 (steps)

Adjustment: weak.

- $2 \equiv 3$. $2\text{B} \equiv 3\text{B}$.
- $2 \neq 2\text{B} \neq 1$.

Pu239 (n,fission) adjustment

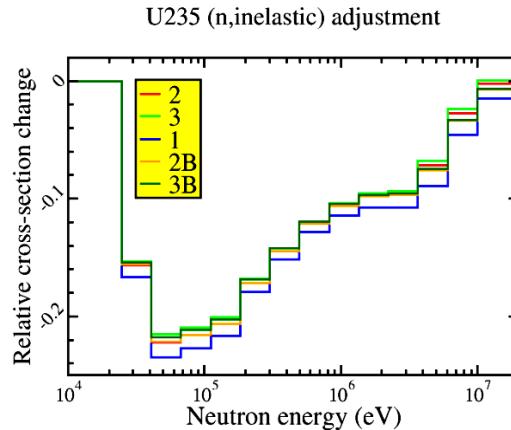


Simulation 3 (steps)

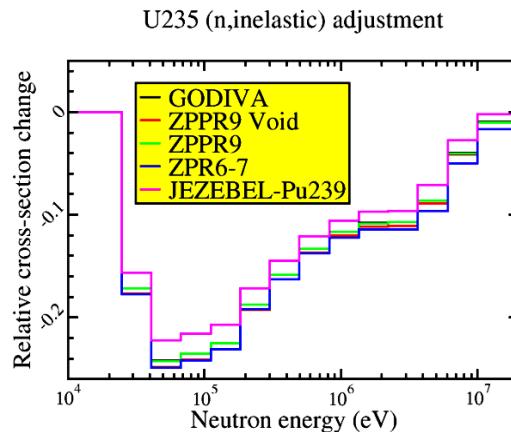
Adjustment, PIA:

- JEZEBEL-Pu239, super fast range.
- ZPR6-7 < 100keV.

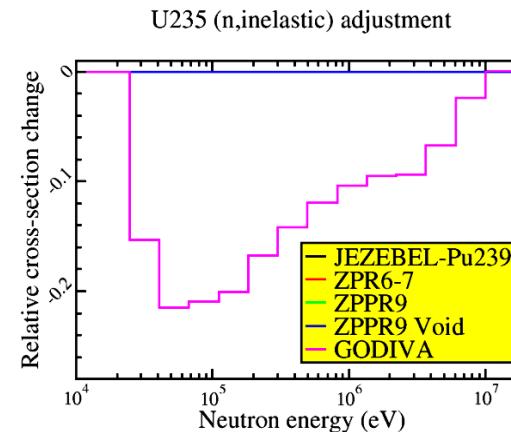
Adjustment of the ^{235}U inelastic scattering cross-section



- $2 \equiv 2B \equiv 3 \equiv 3B \equiv 1$.



Simulation 2 (steps)

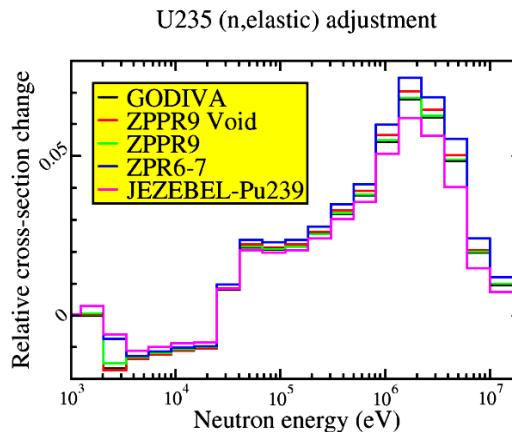
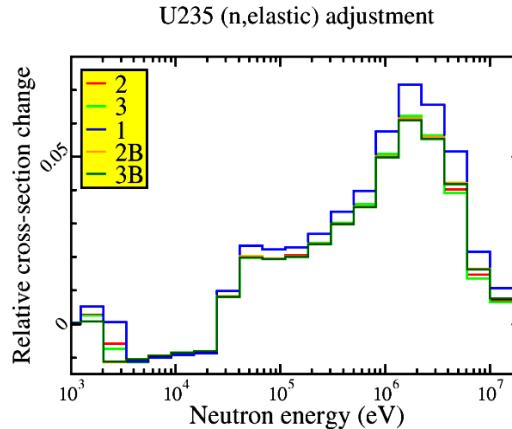


Simulation 3 (steps)

Adjustment, PIA:

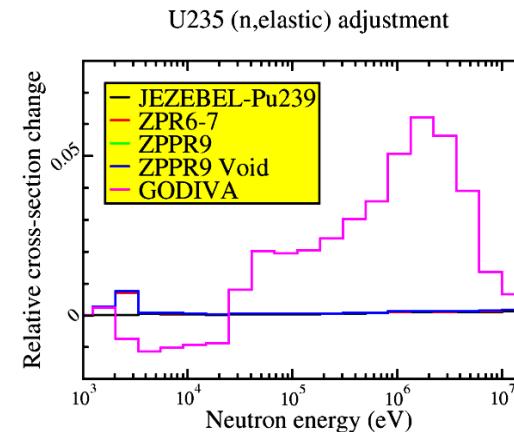
- GODIVA.

Adjustment of the ^{235}U elastic scattering cross-section



Simulation 2 (steps)

- $2 \equiv 2\text{B} \equiv 3 \equiv 3\text{B} \equiv 1.$

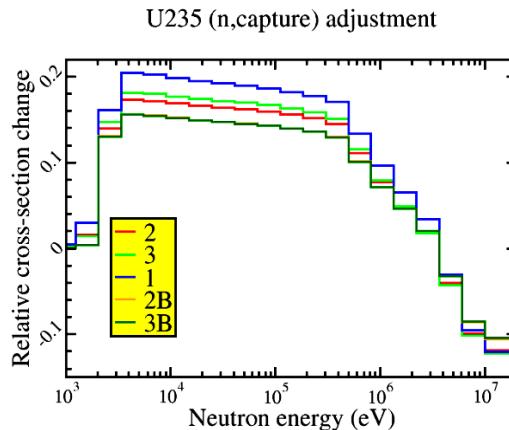


Simulation 3 (steps)

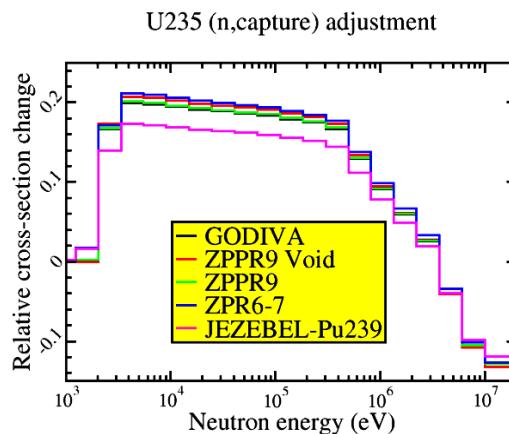
Adjustment, PIA:

- GODIVA.

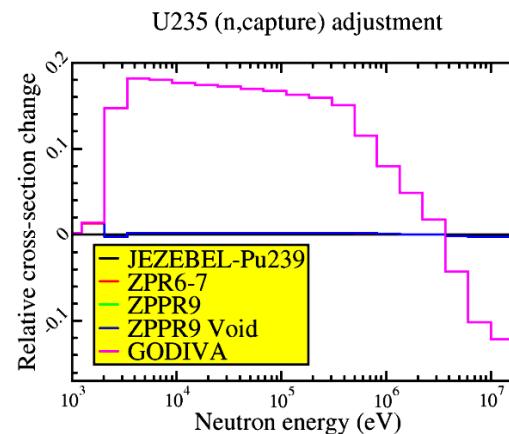
Adjustment of the ^{235}U capture cross-section



- $2 \equiv 3.$ $2\text{B} \equiv 3\text{B}.$
- $2 \approx 2\text{B} \approx 1.$



Simulation 2 (steps)

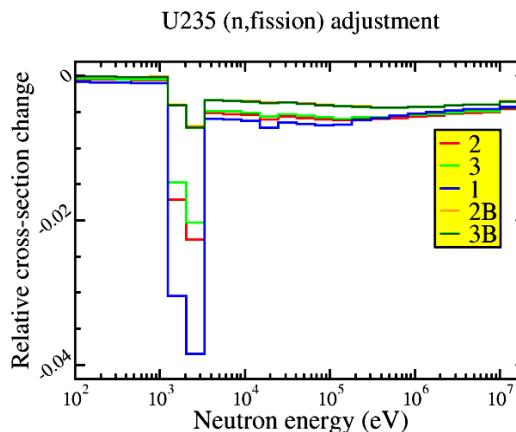


Simulation 3 (steps)

Adjustment, PIA:

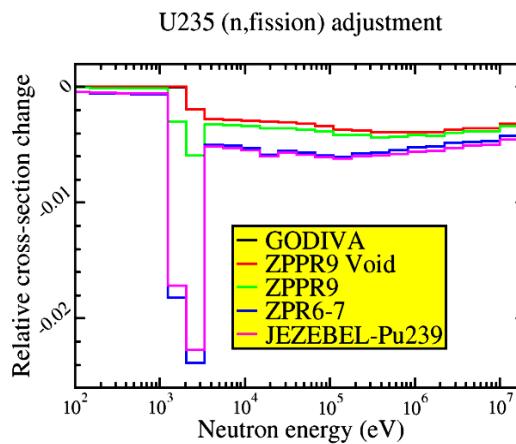
- GODIVA.

Adjustment of the ^{235}U fission cross-section

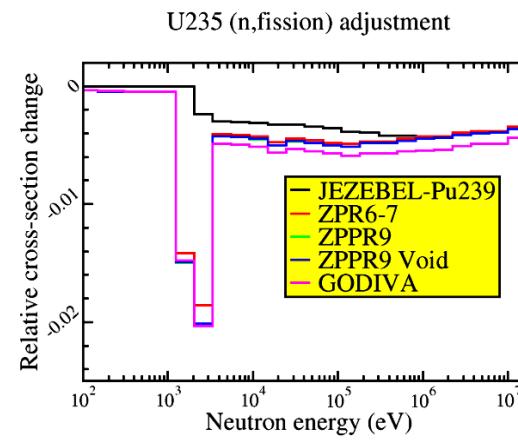


Adjustment: weak.

- $2 \equiv 3$. $2\text{B} \equiv 3\text{B}$.
- $2 \neq 2\text{B} \neq 1$.



Simulation 2 (steps)

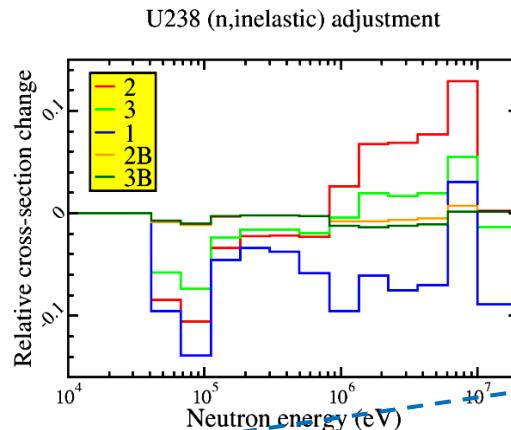


Simulation 3 (steps)

Adjustment, PIA:

- ZPR6-7, main Na resonance.

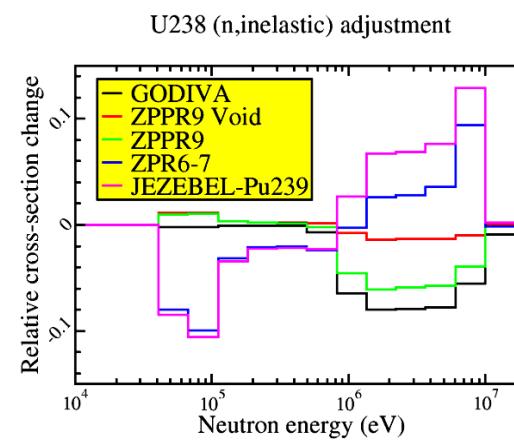
Adjustment of the ^{238}U inelastic scattering cross-section



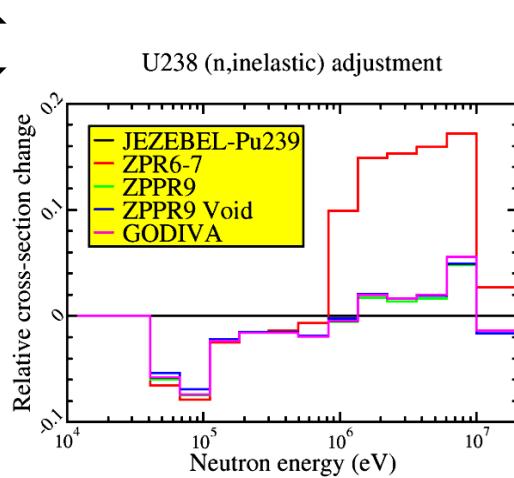
- $2 \neq 3 \neq 1$ with different trends.
- $2\text{B} \equiv 3\text{B}$, almost no adjustment.

Adjustment unreliable, PIA:

- Inconsistent, contradictory separation of effects e.g. between GODIVA and ZPPR9.

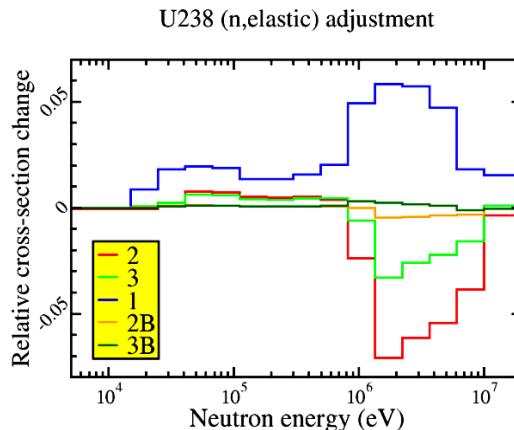


Simulation 2 (steps)



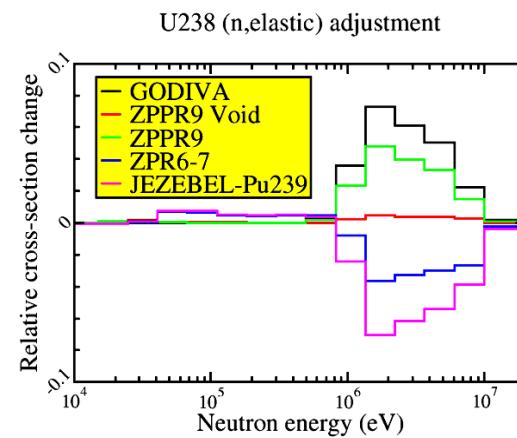
Simulation 3 (steps)

Adjustment of the ^{238}U elastic scattering cross-section

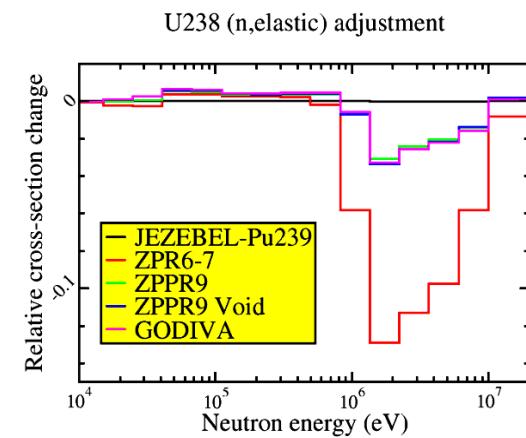


Adjustment: inconsistent, PIA.

- $2 \neq 3 \neq 1$, high energy.
- $2\text{B}, 3\text{B}$: weak.
- $2 \neq 2\text{B}$.

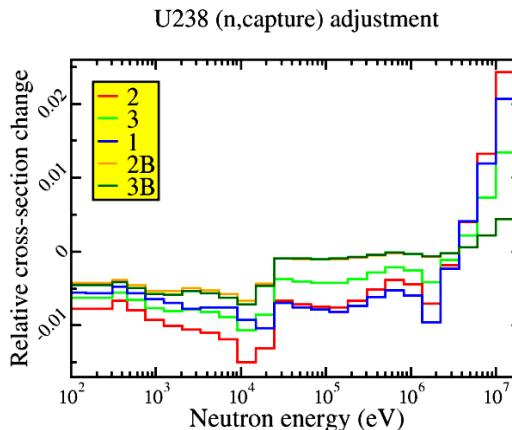


Simulation 2 (steps)



Simulation 3 (steps)

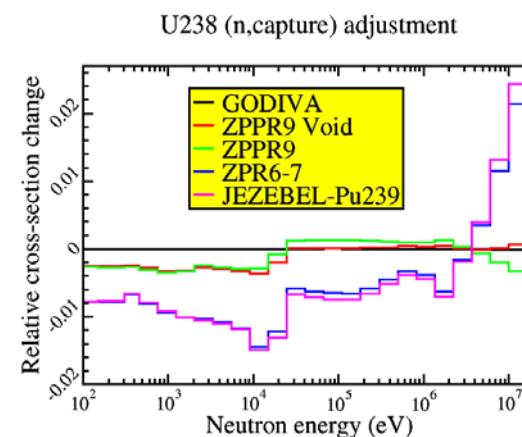
Adjustment of the ^{238}U capture cross-section



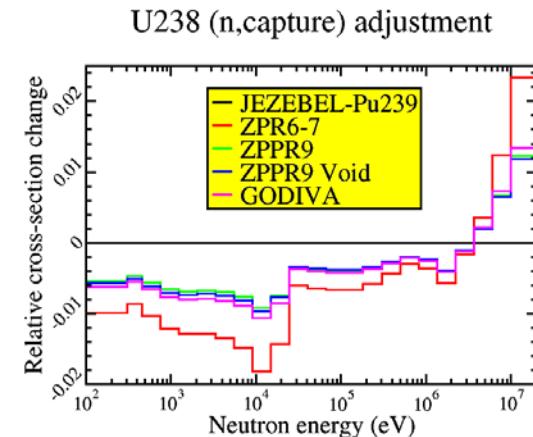
Adjustment, weak:

- Conflicting between ZPPR9 and ZPR6-7, PIA: unreliable.

- $2 \neq 3 \neq 1$.
- $2\text{B} \equiv 3\text{B}$: almost no adjustment.

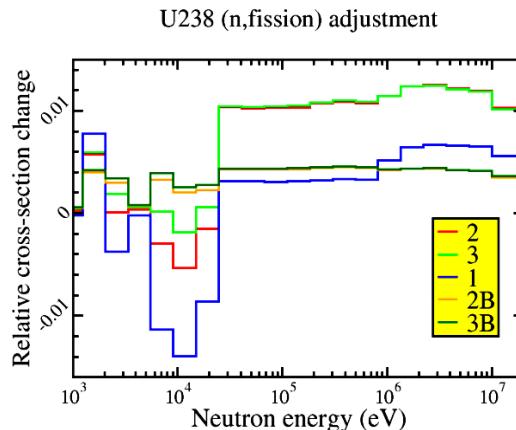


Simulation 2 (steps)



Simulation 3 (steps)

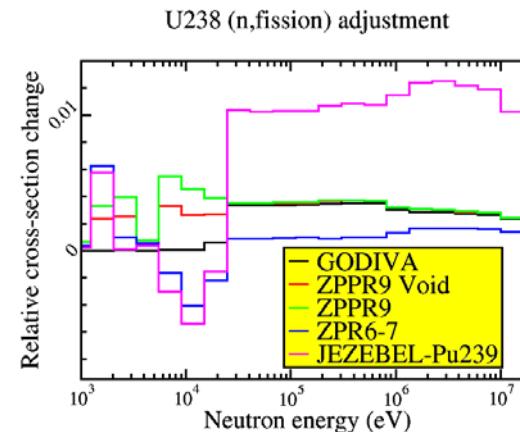
Adjustment of the ^{238}U fission cross-section



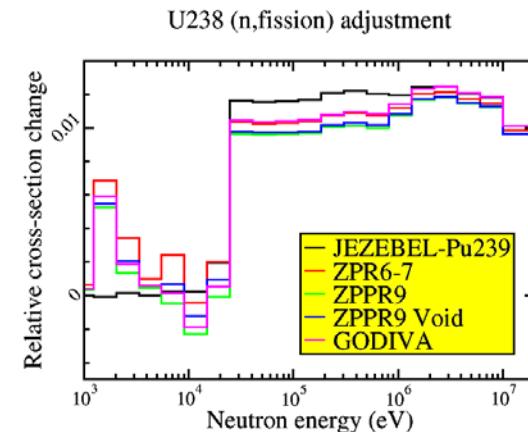
- $2 \equiv 3, E > 30\text{keV}.$
- $2 \neq 3, E < 30\text{keV}.$
- $2\text{B} \equiv 3\text{B}.$

Adjustment, weak:

- $E > 30\text{keV}: \text{JEZEBEL-Pu239, reliable, PIA.}$
- $E < 30\text{keV}: \text{Conflicting between ZPPR9 and ZPR6-7, unreliable, PIA.}$

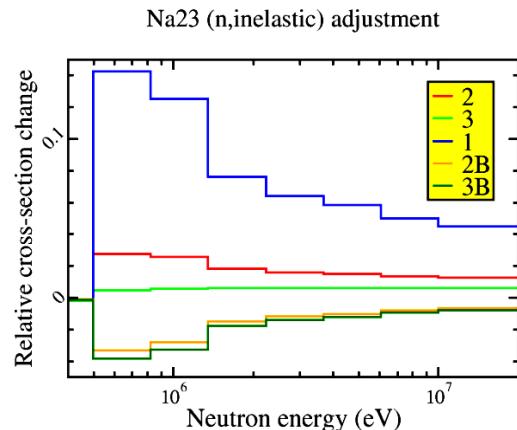


Simulation 2 (steps)



Simulation 3 (steps)

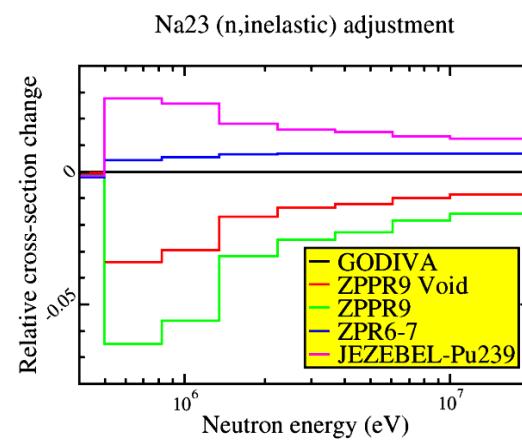
Adjustment of the ^{23}Na inelastic scattering cross-section



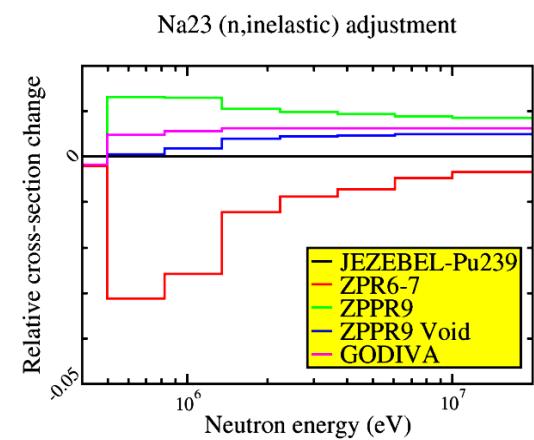
Adjustment: stronger without PIA.

- Conflicting between ZPPR9 and ZPR6-7, PIA.

- $2 \neq 3 \neq 1$.
- $2\text{B} \equiv 3\text{B}$.

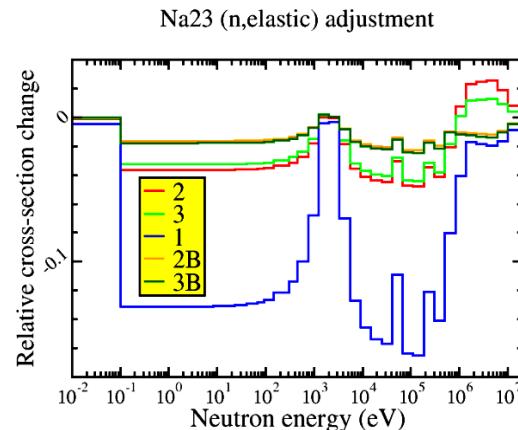


Simulation 2 (steps)



Simulation 3 (steps)

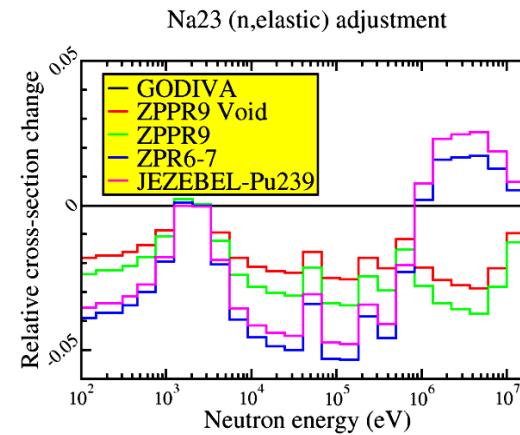
Adjustment of the ^{23}Na elastic scattering cross-section



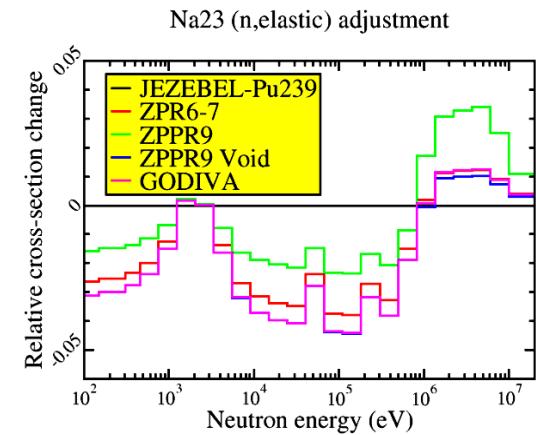
- $E > 1\text{MeV}$: $2 \neq 3$.
- $E < 1\text{MeV}$: $2 \equiv 3$.
- $2\text{B} \equiv 3\text{B}$.

Adjustment without PIA stronger, different trend.

- $E > 1\text{MeV}$: conflicting between ZPPR9 and ZPR6-7.
- $E < 1\text{MeV}$: ZPPR9 coolant density effects + ZPR6-7, PIA.

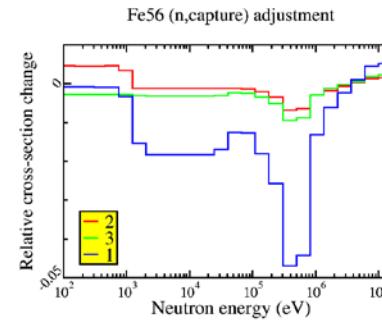
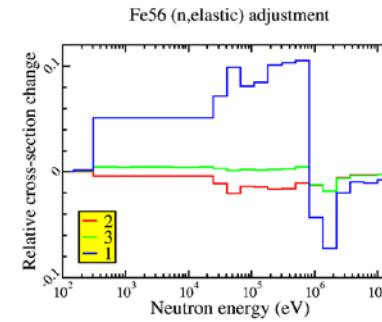
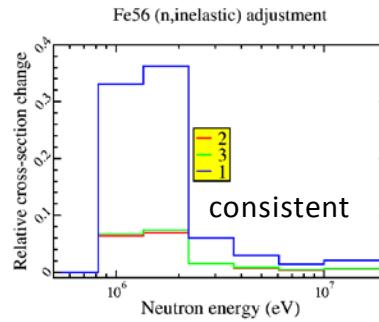
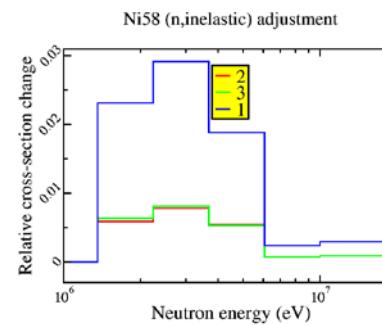
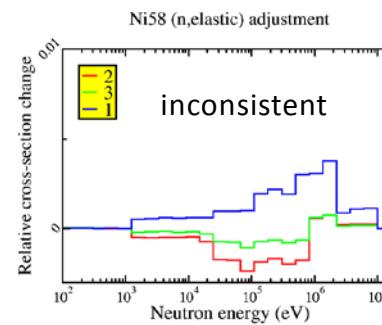
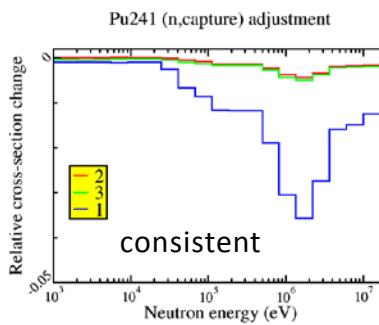
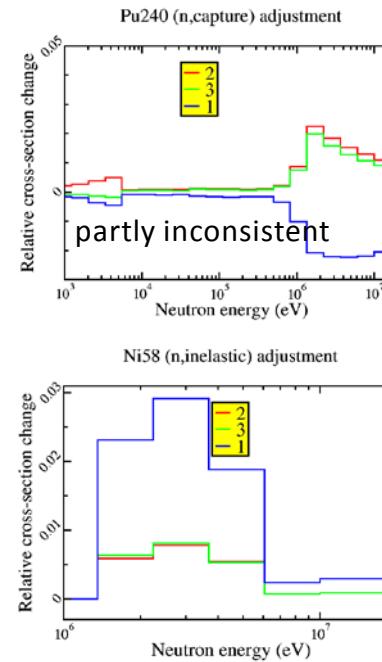
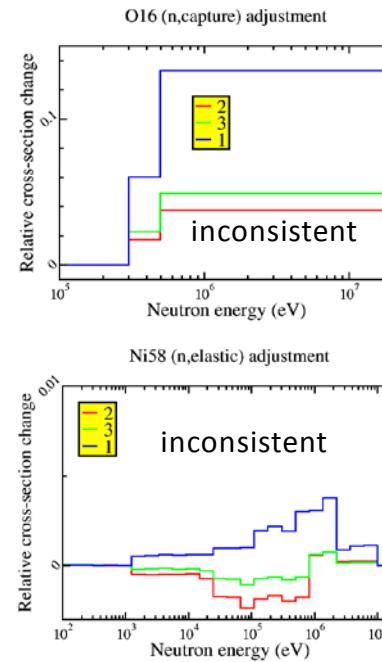
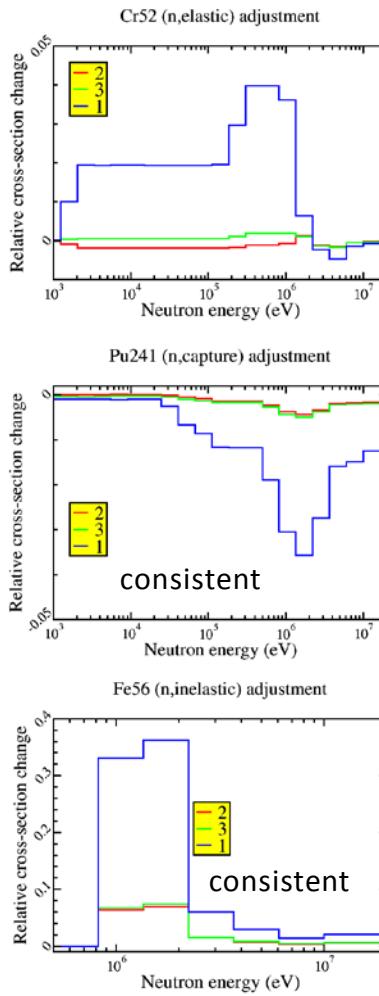


Simulation 2 (steps)

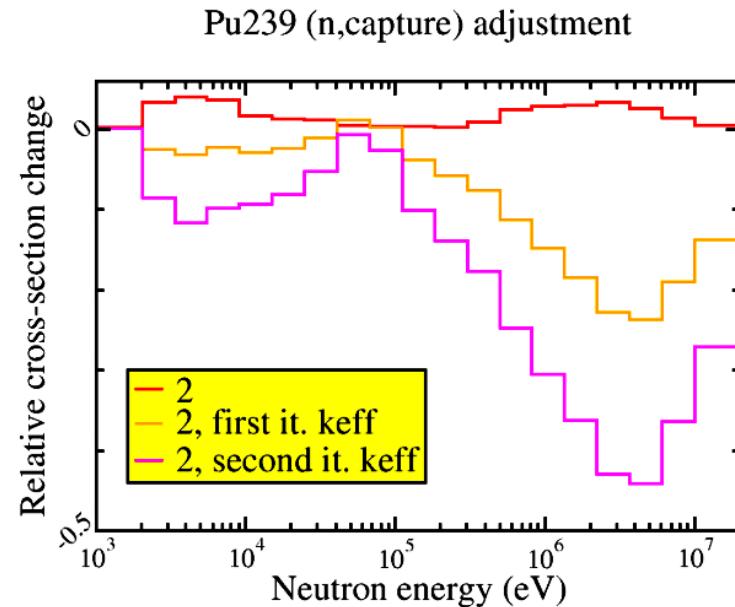
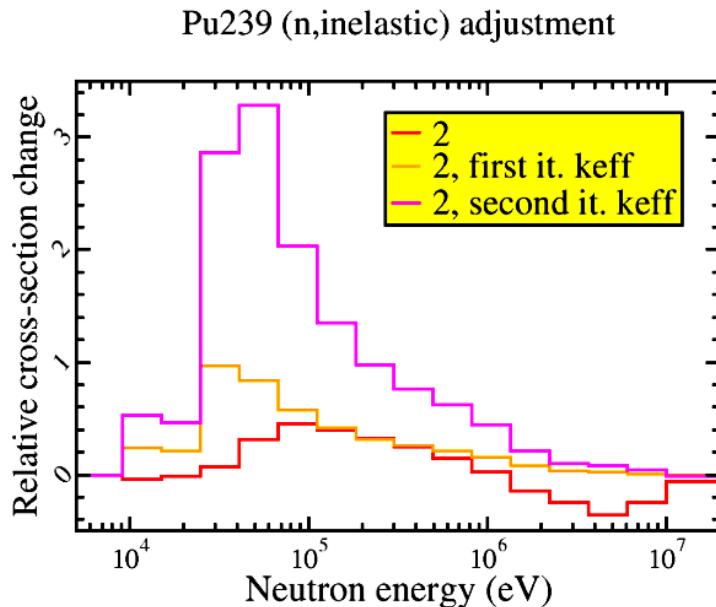


Simulation 3 (steps)

Additional stronger adjustments



PIA: adjusting k_{eff}



- Divergence, “Tsunami” effect reversing trends → Adjusting k_{eff} should be avoided.

Summary, 1

- I. PIA, integral parameters to assimilate: spectral indices and local reactivity effects.
- II. PIA, reject adjustment for cross-section of given isotope, data type and energy group or range when:



Adjustment depends on sequence, inconsistent ↔

- Conflicting effects between different steps.
- A posteriori sensitivity coefficients of the integral parameters to this cross-section also sequence dependent.

Summary, 2

III. Conversely, PIA reliable adjustment:

Largely independent of sequence, consistent.



- Clear separation of effects coming from individual steps without inconsistencies: though some integral parameters may be unneeded in cases where their assimilation does not have any impact on the adjustment, redundancy.
- The a posteriori sensitivity coefficients to the cross section under study independent of the sequence.

Summary, 3

IV. Limited data base, this study: ^{238}U and ^{23}Na cross-sections not adjustable. Needs considering additional experiments.