PAUL SCHERRER INSTITUT

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Additional PSI adjustment studies accounting for nonlinearity

General framework of this study: SG33 benchmark

Focus on the French deterministic code system ERANOS and the associated data libraries which form a reference deterministic tool for fast –spectrum system calculations.

In addition to the original SG33 benchmark specifications:

- **Use of "best" ERANOS options to adjust system-oriented multi-group libraries** (consisting of available cross-sections and variance/covariance data), **specific to ERANOS.**

  These "best" options with respect to the benchmark (homogeneous cells):
  -Slowing-down calculations: 1968 groups (subgroup method, probability tables) to get broad group cross- sections.
  -Core simulations: P_1S_{16} approximations (higher order anisotropic cross-sections not provided in 1968 groups), 33 groups. Enough accurate for sodium systems,
  however: not always accurate for metallic fueled spheres, e.g. Flattop-Pu.
  -Mesh thickness of less than 1mm in view of accurate calculations ($k_{direct} = k_{adjoint}$, proper convergence of generalized importance function) for
  -Standard , Equivalent and Generalized Perturbation theory to obtain sensitivity coefficients for k_{eff}, reactivity effects and reaction rate ratios: Nuclear data uncertainty analysis, data adjustment.

- **Account for nonlinearity by means of iterative procedure : Repeated calculation of sensitivity coefficients with adjusted cross-sections; multiple, stepwise adjustment.**

Analysis of benchmark and other experiments carried out in spherical, metallic fueled configurations using various approximations (JEFF-3.1 data)

Configuration	Integral parameter	Experimental error (%)	Prior *C/E* (S_{16}) Anisotropic scattering P_1[a]	P_1[b]	P_3[b]	P_5[b]	Prior *C/E* (P_5S_{100})[b,c]
Flattop-Pu	k_{eff}	**0.300**	**0.980**	**0.982**	**0.999**	**1.001**	**0.999**
	F28/F25	1.100	0.951	0.968	0.987	0.990	0.989
	F37/F25	1.400	0.993	1.003	1.014	1.015	1.014
Flattop-25	k_{eff}	0.100	0.987	0.988	1.000	1.000	0.999
	F28/F25	1.072	0.951	0.950	0.963	0.964	0.963
	F49/F25	0.867	0.984	0.984	0.986	0.986	0.986
	F37/F25	1.281	0.977	0.984	0.991	0.992	0.991
MIX-MET-FAST-001	k_{eff}	0.160	0.987	0.988	0.998	0.998	0.996
PU-MET-FAST-010	k_{eff}	0.180	0.982	0.984	1.001	1.002	1.000
PU-MET-FAST-009	k_{eff}	0.270	0.971	0.991	1.008	1.008	1.006
Jezebel-Pu239	k_{eff}	0.200	0.993	0.993	1.000	1.000	0.998
	F28/F25	1.100	0.956	0.974	0.984	0.984	0.984
	F49/F25	0.900	0.983	0.983	0.984	0.984	0.984
	F37/F25	1.400	0.990	1.000	1.004	1.004	1.004
Jezebel-Pu240	k_{eff}	0.200	0.997	0.997	1.004	1.004	1.002
Godiva	k_{eff}	0.100	0.991	0.992	0.997	0.997	0.995
	F28/F25	1.096	0.950	0.950	0.958	0.958	0.957
	F49/F25	0.989	0.979	0.980	0.981	0.981	0.981
	F37/F25	1.409	0.966	0.975	0.978	0.978	0.978

[a]Calculations performed using standard 33 neutron broad group cross-sections.
[b]Calculations performed on the basis of 175 neutron broad group cross-sections in the VITAMIN-J structure.
[c]The associated quadrature set to this S_{100} approximation corresponds to the P_{99} method.

***k*$_{eff}$ for Flattop-Pu excluded from the adjustment: Thus 19 experiments considered:**

Much more dependent on the use of more refined approximations as compared to the other experiments.

Larger orders of angular flux representation (than 16) and higher scattering cross-section anisotropies (than 1) needed.

Analytical modeling error ~2% >> Experimental error 0.3%
would override nuclear data error and make experiment useless for adjustment.

The effect of using more than 33 groups appears in general less important.

S. Pelloni, "Application of an iterative methodology for cross-section and variance/covariance data adjustment to the analysis of fast spectrum systems accounting for non-linearity,"
Annals of Nuclear Energy, **72**, p. 373-390 (October 2014).

Nonlinear adjustment methodology (iterations index *i* = 0, 1, 2, …)

ERANOS Edition 2.2-N: JEFF-3.1/COMMARA-2.0 or ENDF/B-VI.8/BOLNA.
COMAC (JEFF based) would have been more suitable than COMMARA.
Format for variance/covariance data: AMERE, generated using simple reformatting in-house code.

Prior, before adjustment: $i = 0$.
Posterior, after adjustment: $i = 1$ **(Linear approach),** $i > 1$ **(Nonlinearity).**
Adjustment from **Generalized Linear Least Squares (GLLS)** in-house code using **JAEA methodology**.
Matrix inversion routine: AMARA code (Gandini) available from the NEADB.
GLLS: Reproduces ERANOS module SENSITIVITY_ANALYSIS (prior uncertainties with their decompositions):
Additionally generates

- prior and posterior variance/covariance matrices of the analytical values of the integral parameters (Matrices U_i, Eqs (1)-(2)), *guessed* posterior C-values (Eq. 6, *linear approximation*) with their *1-σ* uncertainties (Eq. (7)),
- minimum χ square,
- relative cross-section changes ΔT_i (Eqs 3-5) from adjustment, written on ASCII file → MICADJ (currently no fission spectrum, no secondary distributions considered),
- posterior variance/covariance data in AMERE format for considered nuclides (based upon Eq. (8)).

MICADJ: Dedicated in-house **ERANOS procedure**
takes ERANOS microscopic cross-section set for each experiment (initially $i = 0$, prior, i.e. from ECCO) and updates this data using the ΔT_is (Eq. (3)). **Enables ERANOS to then assess posterior C-values** (compared to GLLS: *exact, no linear approximation*) **with their uncertainties and also posterior sensitivity coefficients.**

Adjustment formulas (iteration index i = 0, 1, 2, …)

i = 0: Prior values; i = 1: First iteration adjustment (Linear approach), i > 1: Nonlinearity.

G_i : Sensitivity coefficient matrix: (from ERANOS, currently explicit coefficients),

V_E : Experimental error correlation matrix,

V_M : Analytical modeling error correlation matrix,

} iteration independent

M_i : Variance/covariance data matrix (M_0 : Square, symmetric. Prior data extracted from basic variance/covariance library for considered nuclides (GLLS)),

N_i: Corresponding correlation data matrix (diagonal terms equal to 1, else between -1 and +1),

T_i: Cross-section vector $\left(R_C(T_i)\right)_k$: C-value of experiment k by using cross-sections T_i.

$$U_0 = G_0 N_0 G_0^T \quad (1) \quad U_{i+1} = G_i N_{i+1} G_i^T \quad (2)$$

$$\left.\begin{aligned} \Delta T_i &= N_0 G_i^T \left(G_i N_0 G_i^T + V_E + V_M\right)^{-1} CE_i \\ T_{i+1} &= T_i + \delta T_i,\ \delta T_{i,j} = \Delta T_{i,j} . T_{i,j} \end{aligned}\right\} (3) \quad \Delta T_{i,j} = \frac{T_{i+1,j} - T_{i,j}}{T_{i,j}};\ CE_{i,k} = \frac{R_{Ek} - \left(R_C(T_i)\right)_k}{\left(R_C(T_i)\right)_k} \quad (4\text{-}5)$$

j-component of the vector ΔT_i in Eq. (3): relative xs difference from one adjustment to the next (Eq. (4)).

k- component of the vector CE_i in Eq. (3): kth experiment E/C-1 value (Eq. (5)).

$$R_C(T_{i+1}) = R_C(T_i) + \tilde{G}_i\left(T_{i+1} - T_i\right) \quad (6)$$

$\tilde{G}_i = dR_c(T_i)/dT_i$: Jacobian matrix easily deducible from G_i.

$$\Delta\left(R_C(T_i)\right)_k / \left(R_C(T_i)\right)_k = \sqrt{U_{ik,k}} \quad (7)$$

$$N_{i+1} = N_0 - N_0 G_i^T \left(G_i N_0 G_i^T + V_E + V_M\right)^{-1} G_i N_0 \quad (8)$$

Convergence reached when $\boldsymbol{\Delta T_{i,j} \to 0}$
(i = 6 for SG33 benchmark):

1. ERANOS results = GLLS results,
2. sensitivity coefficients do no longer vary.

*C/E*s (JEFF-3.1/COMMARA-2.0)

Configuration	Integral parameter	(a)	Prior	Posterior		Asymptotic posterior		
			ERANOS	ERANOS	GLLS	ERANOS	GLLS with	
							(b)	(c)
Jezebel-Pu239	k_{eff}	0.200	0.993	0.997	0.997	1.000	1.000	1.000
	F28/F25	1.100	0.956	0.991	0.991	1.013	1.013	1.003
	F49/F25	0.900	0.983	0.998	0.998	1.003	1.004	1.001
	F37/F25	1.400	0.990	1.007	1.007	1.011	1.010	1.003
Jezebel-Pu240	k_{eff}	0.200	0.997	1.000	1.001	1.000	1.000	1.000
Flattop-Pu	*F28/F25*	1.100	0.951	0.964	0.980	0.981	0.979	0.993
	F37/F25	1.400	0.993	0.999	1.008	0.999	0.999	1.004
ZPR6-7	k_{eff}	0.251	1.003	1.004	1.002	0.999	1.001	1.001
	F28/F25	3.173	0.965	0.989	0.991	1.009	1.009	1.005
	F49/F25	2.342	1.020	1.027	1.028	1.031	1.032	1.026
	C28/F25	2.614	1.004	1.011	1.011	1.004	1.005	1.006
ZPR6-7 Pu240	k_{eff}	0.241	1.002	1.001	1.001	0.999	0.999	1.000
ZPPR9	k_{eff}	0.153	1.001	1.000	1.000	1.000	1.000	1.000
	F28/F25	2.875	0.962	0.988	0.988	1.009	1.009	1.003
	F49/F25	2.230	0.982	0.989	0.989	0.993	0.993	0.987
	C28/F25	2.141	0.996	1.003	1.003	0.997	0.997	0.998
	Na Void Step 3	4.188	1.059	1.045	1.045	1.031	1.031	1.028
	Na Void Step 5	4.113	1.002	0.990	0.990	0.979	0.978	0.980
JOYO	k_{eff}	0.206	0.997	1.001	1.000	1.000	1.000	1.000

(a) Combination of experimental and calculation uncertainties of the prior *C/E*s (%).
(b) The sensitivity coefficients are taken from the corresponding ERANOS calculations.
(c) The prior sensitivity coefficients are used throughout without further use of ERANOS.

Prior values:
k_{eff}: Over 3σ-underestimation, Jezebel-Pu239 (in line with FLATTOP-Pu);
Spectral indices:
F28/F25 underestimated by 4σ (nuclear data and methods issues). ZPPR9 Na Void Step 3: Overestimated by > 1σ.

First adjustment:
improves *C/E*s. More or less within desired margin.
Exception: k_{eff} Jezebel-Pu239 and *F28/F25* Flattop-Pu.
Somewhat larger differences between ERANOS and GLLS for Flattop-Pu spectral indices.

Asymptotic adjustment:
differs from first adjustment.
Additional improvements for the two deviating parameters and agreement between ERANOS and GLLS as expected.
Simplified adjustment by GLLS: also consistent.

Data uncertainties (JEFF-3.1/COMMARA-2.0)

Configuration	Integral parameter	Prior	Posterior	Asymptotic posterior	
		ERANOS	GLLS	ERANOS	GLLS
Jezebel-Pu239	k_{eff}	0.526	0.159	0.174	0.159
	F28/F25	2.345	0.770	0.622	0.761
	F49/F25	0.715	0.429	0.433	0.429
	F37/F25	1.656	0.629	0.512	0.625
Jezebel-Pu240	k_{eff}	0.587	0.178	0.189	0.177
Flattop-Pu	*F28/F25*	1.842	0.610	0.544	0.607
	F37/F25	1.372	0.598	0.540	0.600
ZPR6-7	k_{eff}	0.972	0.136	0.195	0.138
	F28/F25	6.484	1.609	1.637	1.617
	F49/F25	0.845	0.566	0.580	0.575
	C28/F25	1.496	0.941	0.933	0.953
ZPR6-7 Pu240	k_{eff}	0.973	0.137	0.187	0.137
ZPPR9	k_{eff}	1.203	0.136	0.179	0.136
	F28/F25	8.064	1.901	1.884	1.917
	F49/F25	0.881	0.560	0.571	0.568
	C28/F25	1.530	0.949	0.942	0.964
	Na Void Step 3	7.219	2.445	2.475	2.446
	Na Void Step 5	9.145	2.942	3.010	2.951
JOYO	k_{eff}	0.878	0.198	0.203	0.198

Adjustment:
Smaller uncertainties consistent with other studies.
Significant fraction of this reduction: cross-correlations.
Correspondingly:
Asymptotic posterior *C/E*s within or close within margin of combination of uncorrelated experimental, calculation and nuclear data caused uncertainties.
More important: This margin reduced by adjustment.

Not as for the *C/E*s: Only marginal differences between first adjustment and asymptotic posterior values.

*C/E*s (ENDF/B-VI.8/BOLNA)

Configuration	Integral parameter	(a)	Prior	Posterior		Asymptotic posterior		
			ERANOS	ERANOS	GLLS	ERANOS	GLLS with	
							(b)	(c)
Jezebel-Pu239	k_{eff}	0.200	0.990	0.995	0.996	1.000	1.000	0.999
	F28/F25	1.100	0.935	0.989	0.987	1.026	1.026	1.003
	F49/F25	0.900	0.972	0.997	0.997	1.008	1.008	1.003
	F37/F25	1.400	0.951	0.981	0.980	1.004	1.004	0.988
Jezebel-Pu240	k_{eff}	0.200	0.990	1.000	1.000	1.000	1.000	1.000
Flattop-Pu	*F28/F25*	1.100	0.940	0.967	0.981	0.961	0.968	0.995
	F37/F25	1.400	0.971	0.987	0.993	0.980	0.985	1.000
ZPR6-7	k_{eff}	0.250	1.006	1.001	1.001	1.000	1.000	1.000
	F28/F25	3.173	0.999	0.988	0.987	1.001	1.001	1.000
	F49/F25	2.342	1.029	1.039	1.039	1.036	1.036	1.033
	C28/F25	2.614	1.007	1.019	1.019	1.010	1.010	1.009
ZPR6-7 Pu240	k_{eff}	0.241	1.005	1.001	1.000	0.999	0.999	0.999
ZPPR9	k_{eff}	0.153	1.007	1.001	1.001	1.000	1.000	1.000
	F28/F25	2.875	1.013	0.988	0.987	1.010	1.010	0.999
	F49/F25	2.230	0.992	1.000	1.000	0.997	0.997	0.994
	C28/F25	2.141	0.999	1.012	1.012	1.002	1.002	1.002
	Na Void Step 3	3.843	1.152	1.050	1.048	1.024	1.024	1.024
	Na Void Step 5	3.679	1.134	1.014	1.011	0.986	0.986	0.984
JOYO	k_{eff}	0.206	0.992	1.001	1.000	1.000	1.000	1.000

(a) Combination of experimental and calculation uncertainties of the prior *C/E*s (%).
(b) The sensitivity coefficients are taken from the corresponding ERANOS calculations.
(c) The prior sensitivity coefficients are used throughout without further use of ERANOS.

Comparing with JEFF-3.1/COMMARA-2.0:

Prior, ENDFBVI/8, less accurate than JEFF-3.1: Particularly k_{eff} Jezebel-Pu240 and Na Void Step 5.

However, **asymptotic posterior close:** Difference < calculation+ experimental uncertainty.

This difference decreases from first adjustment to asymptotic.

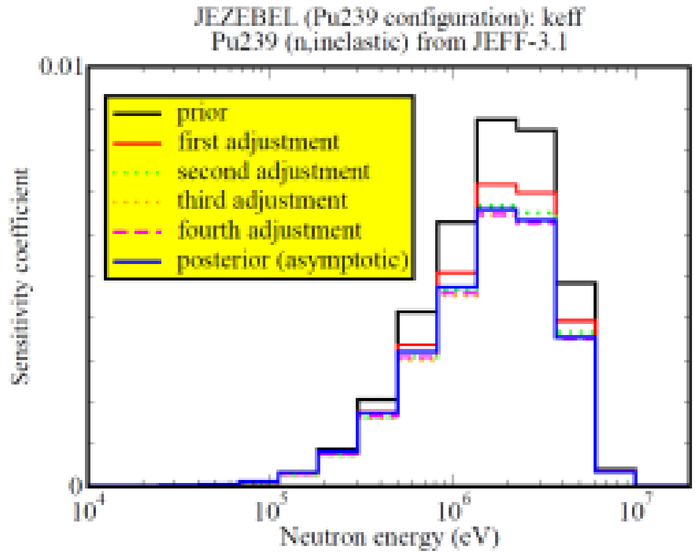
Data uncertainties (ENDF/B-VI.8/BOLNA)

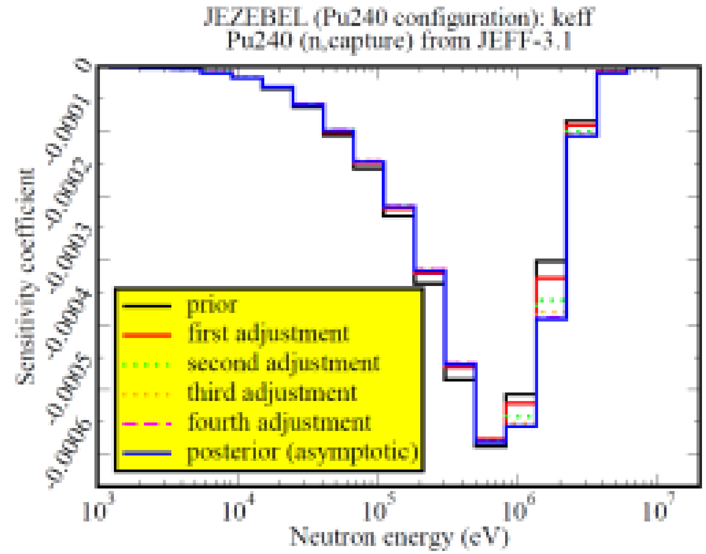
Configuration	Integral parameter	Prior	Posterior	Asymptotic posterior	
		ERANOS	GLLS	ERANOS	GLLS
Jezebel-Pu239	k_{eff}	0.645	0.165	0.178	0.166
	F28/F25	2.814	0.791	0.704	0.725
	F49/F25	0.771	0.451	0.432	0.430
	F37/F25	1.925	0.641	0.511	0.548
Jezebel-Pu240	k_{eff}	0.739	0.185	0.188	0.185
Flattop-Pu	*F28/F25*	2.137	0.624	0.593	0.608
	F37/F25	1.629	0.614	0.516	0.545
ZPR6-7	k_{eff}	1.008	0.137	0.151	0.146
	F28/F25	5.925	1.737	1.805	1.755
	F49/F25	0.826	0.573	0.586	0.585
	C28/F25	2.191	1.095	1.141	1.142
ZPR6-7 Pu240	k_{eff}	1.018	0.148	0.158	0.154
ZPPR9	k_{eff}	1.180	0.137	0.136	0.137
	F28/F25	7.317	1.982	1.977	1.997
	F49/F25	0.877	0.583	0.597	0.597
	C28/F25	2.254	1.118	1.172	1.173
	Na Void Step 3	7.396	2.436	2.453	2.420
	Na Void Step 5	9.283	2.994	3.008	3.007
JOYO	k_{eff}	1.301	0.203	0.212	0.202

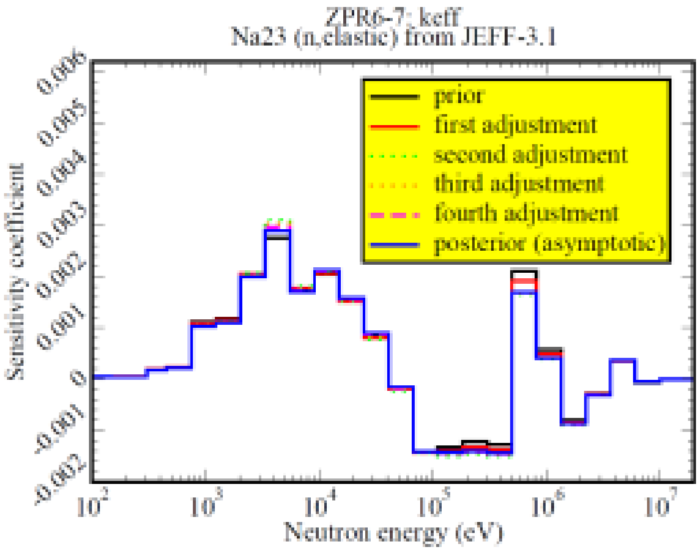
Prior:
Jezebel-Pu239, Jezebel-Pu240, Flattop-Pu, JOYO
> JEFF-3.1/COMMARA-2.0: In line with larger deviations between *C*- and *E*-values. Also for k_{eff} ZPR6-7, ZPR6-7 Pu240, *C28/F25*, and sodium void reactivity. *F28/F25* and *F49/F25* in ZPR6-7 and ZPPR9 reversed trend.

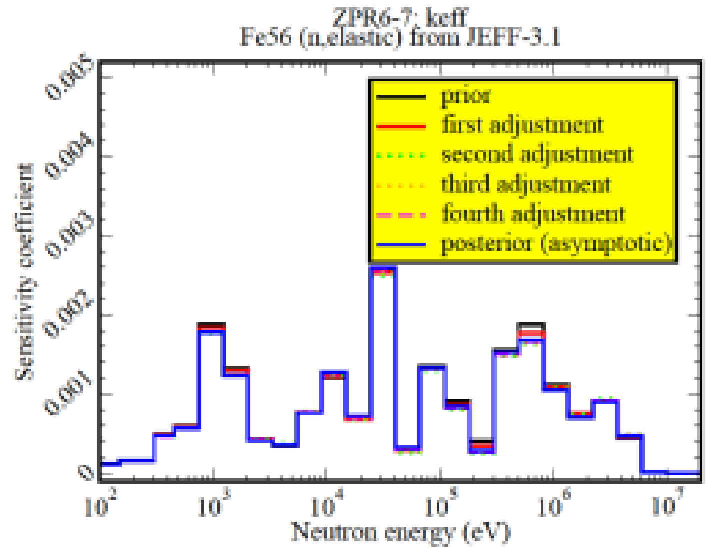
Asymptotic posterior:
Similar to *C/E*s, consistent with JEFF-3.1/COMMARA-2.0, whereas prior values not. **Good !**

Nonlinearity seen in sensitivity coefficient variations

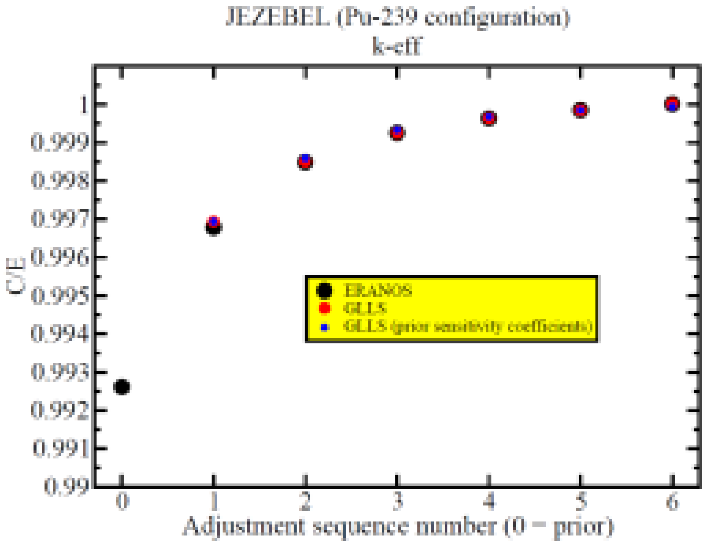


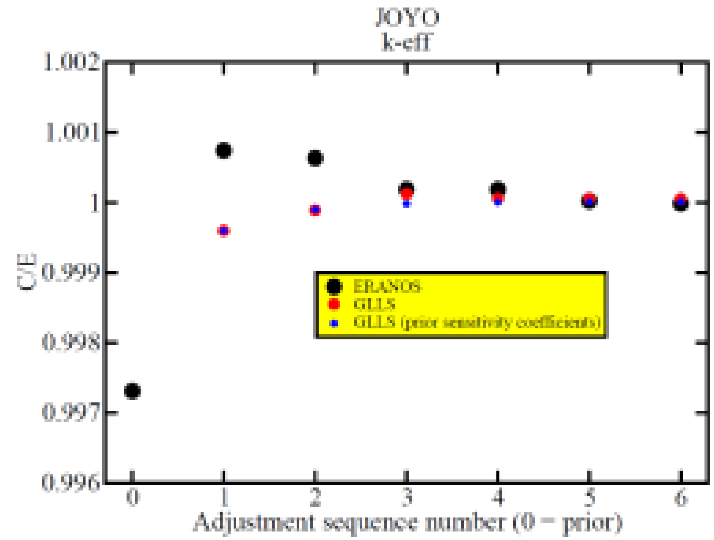


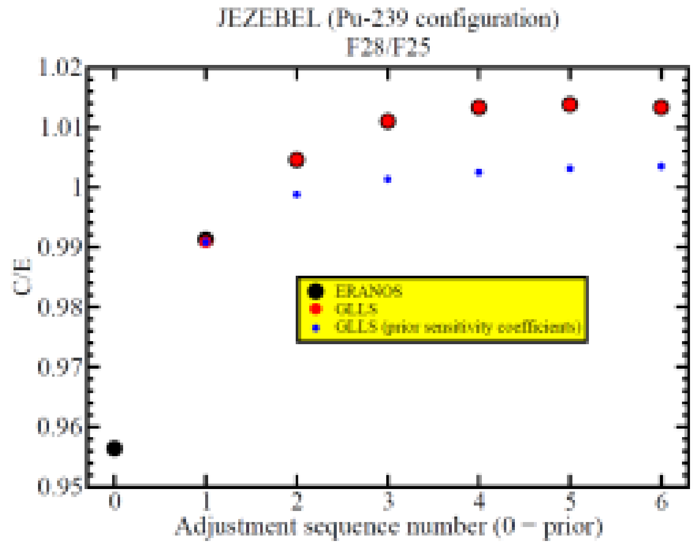


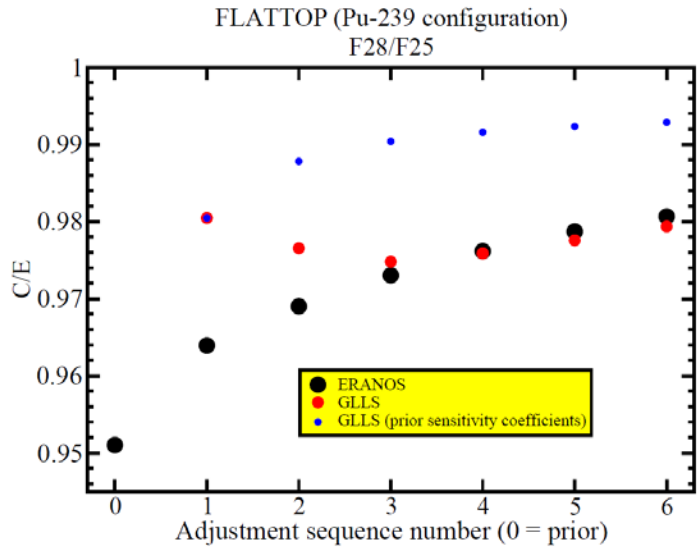


Path to reach adjustment convergence may vary from case to case

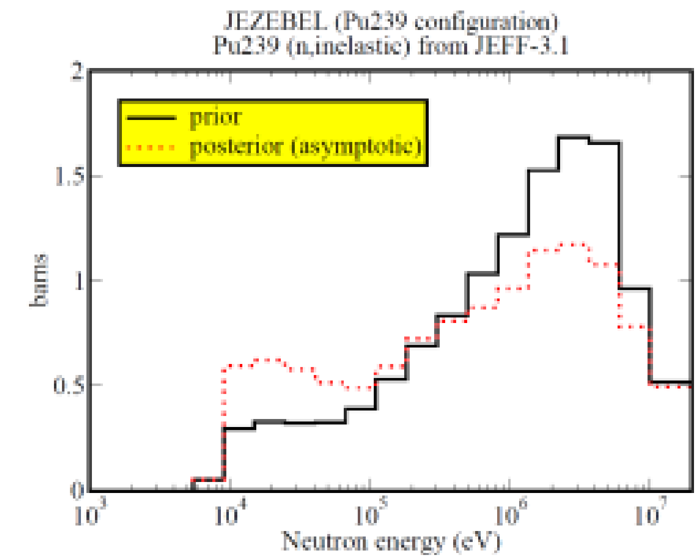


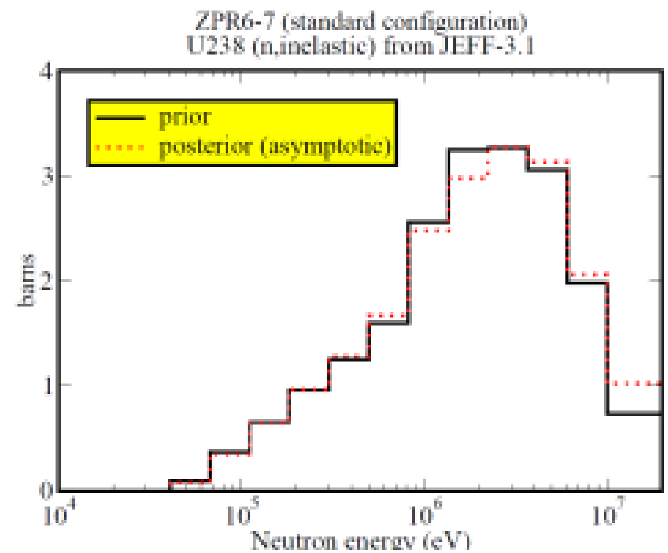




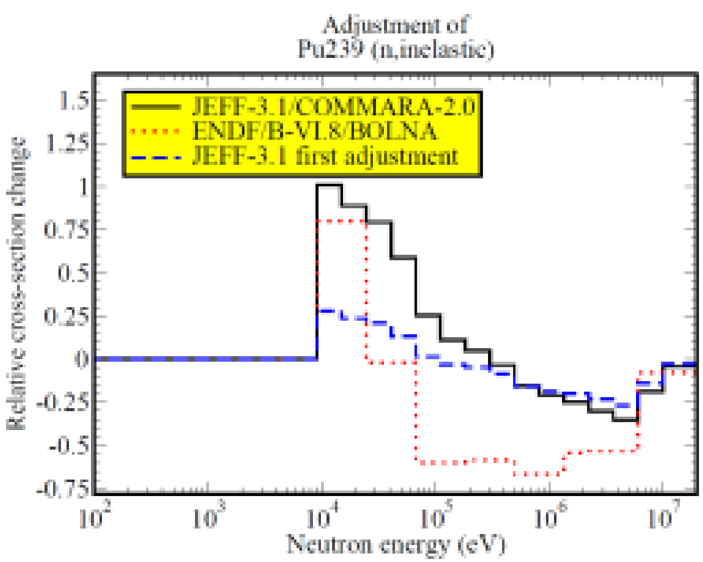


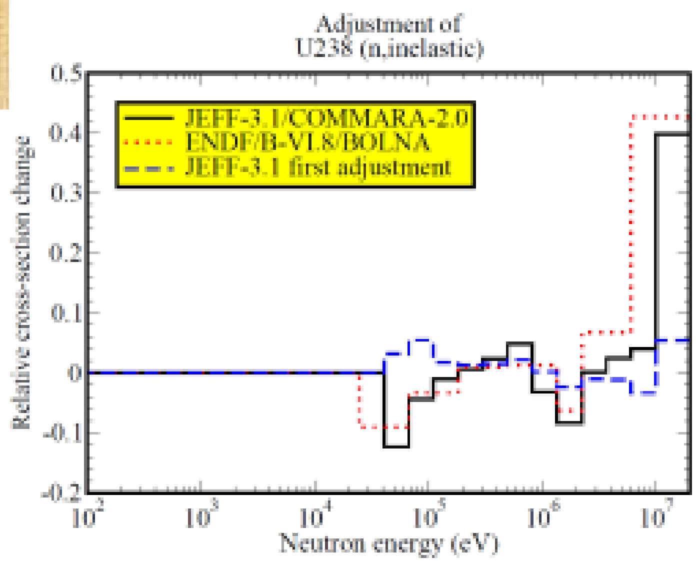
Cross-sections: Asymptotic posterior versus first adjustment





Asymptotic adjustment may be quite different from first adjustment.





Adjusted library (asymptotic) "blindly" used for fast systems not part of the benchmark

Configuration	Integral parameter	Experimental error (%)	Prior C/E	Asymptotic Posterior C/E	Prior uncertainty (%)	Asymptotic posterior uncertainty (%)
Flattop-Pu	k_{eff}	0.300	0.980	1.007	0.904	0.349
Flattop-25	k_{eff}	0.100	0.987	0.991	1.131	0.550
	F28/F25	1.072	0.951	0.971	1.971	1.611
	F49/F25	0.867	0.984	0.998	0.710	0.522
	F37/F25	1.281	0.977	0.975	1.544	1.257
MIX-MET-FAST-001	k_{eff}	0.160	0.987	0.994	0.414	0.227
PU-MET-FAST-010	k_{eff}	0.180	0.982	0.989	1.077	0.345
PU-MET-FAST-009	k_{eff}	0.270	0.971	0.999	0.483	0.153
Godiva	k_{eff}	0.100	0.991	0.993	0.890	0.567
	F28/F25	1.096	0.950	0.972	2.107	1.923
	F49/F25	0.989	0.979	0.995	0.718	0.550
	F37/F25	1.409	0.966	0.966	1.573	1.439

***C/Es* improvement systematic**, particularly k_{eff} : Flattop-Pu and PU-MET-FAST-009.

F37/F25, marginally concerned: ^{237}Np not adjusted.
^{235}U fission cross-section adjustment from k_{eff} JOYO: Rather ineffective in fission source range of interest.

Uncertainty reduction as expected < benchmark particularly *F28/F25*: Low correlation with benchmark.

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.

Possible compensations: Methods deficiencies assimilated into artificial data changes ?

Conclusions

- Improvement by accounting for nonlinearity. However, stronger adjustments required (physical ?).

- Good performance of adjusted library, despite low number of integral parameters and reactions (19 and 6): Also satisfactory for other parameters e.g. Godiva and Flattop
(however, methods and data deficiency mix ?).

- Different data bases (JEFF-3.1/COMMARA-2.0, ENDF/B-VI.8/BOLNA): Different prior results; Similar posterior results only if nonlinearity is accounted for (good !). However, adjusted cross-sections not always consistent.

Recommendations

To include:

- Stress tests: ZPR-9/34 (U/Fe, stainless steel reflector);
  ZPR-3/53 (Pu/C/stainless steel assembly with U-blanket);
  ZPR-3/54 (Pu/C/stainless steel assembly with iron reflector);
  ZPR-6/10 (Pu/C/stainless steel assembly with stainless steel/iron reflectors):

Discrepancy between C- and E-values quite large; possibility of more important non-linear effects. Clearly, ^{12}C and ^{55}Mn additionally to consider.

- Shielding/scattering experiments (secondary neutron distributions included in methodology).

- Target fast-spectrum reactors.

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