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Adjustments at PSI: New benchmark results from the use of

(a) The GLLS methodology and

(b) The combined use of GLLS and the ERANOS code for explicit posterior calculations

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Methodology

Prior results (on the web):
Deterministic ERANOS (Version 2.2-N) in conjunction with JEFF-3.1/COMMARA-2.0.
ERANOS format for COMMARA-2.0: AMERE (generated using an in-house program).

Posterior results:
Generalized Linear Least Squares (GLLS) technique in the framework of the JAEA methodology (Bayesian parameter estimation)→ "Fortran 95" code named GLLS :
The formulas given in Appendix D ("Teaching example of adjustment methods features (Two group example)", by M. Ishikawa) of the SG33 report are the basis, namely

(D.3) for determining relative variations $\Delta T / T$ of the prior cross-sections T through the adjustment,
(D.4) for determining the posterior covariance matrix M',
(D.7) for computing the minimum χ^2, and
(D.8) for the posterior computed values C'.
The matrix inversion routine was taken from the AMARA code (Gandini) available from the NEADB.

GLLS reproduces the detailed output of the corresponding ERANOS module named "SENSITIVITY_ANALYSIS" for each experiment, and generates the corresponding posterior values supplemented by the minimum χ square and the relative cross-section changes which are written on file (ASCII) to be post-processed or used e.g. in ERANOS.
The posterior covariance data (AMERE format) including all the numerous additional cross correlations is also output and this in view of recalculations with ERANOS.

GLLS formulas

(D.3) $\Delta T / T = M G^T D ((E-C) / C)$, $D := (G M G^T + V_e + V_m)^{-1}$

(D.4) $M' = M - M G^T D G M$,

(D.7) $\chi 2_{min} = ((E-C) / C)^T D ((E-C) / C)$,

(D.8) $C' = C + G (\Delta T/T)$

Methodology

For the current SG33 benchmark:
M, the (prior) covariance matrix, is a 2178 by 2178 matrix (2178 = 6*11*33, with 6 reactions, i.e. elastic and inelastic scattering, capture, nxn, fission and v, 11 nuclides to adjust, and 33 groups),
G, the sensitivity coefficient matrix, is a 20 by 2178 matrix, 20 being the number of experiments,
$\mathbf{V_e}$ and $\mathbf{V_m}$, the experimental and analytical modeling error matrices, are 20 by 20 matrices.
Therefore, the (prior) covariance matrix GMG^T of the experiments and the matrix $(GMG^T + V_e + V_m)$ to inverse are also 20 by 20 matrices.
T, the cross-section adjustment vector, is a 2178 by 1 matrix.

Explicit posterior calculations with ERANOS:
Use is made of an in-house ERANOS procedure (ADJMICROS).
The adjustment is thereby made for the individual prior broad group microscopic cross-sections for each experiment which are output of the cell code ECCO, and this in conjunction with the corresponding nuclide-, reaction- and group-wise correction factors obtained in advance by means of GLLS.
Scattering matrix cross-sections (isotropic and anisotropic) are adjusted consistent with the corresponding vector cross-sections by currently using a single correction factor for the out-scattering vector of a given incident group.
E.g. the posterior total cross-section is set equal to the sum of posterior capture, fission, nxn, inelastic and elastic scattering cross-section analogous to the prior total cross-section;
ERANOS specific lumped cross-sections, e.g. disappearance and total scattering matrices, need to be reconstructed in a similar consistent manner according to their definition (NT-SPRC-LEPh-93-252, p. 76-83).

Case II results (prior / posterior GLLS)

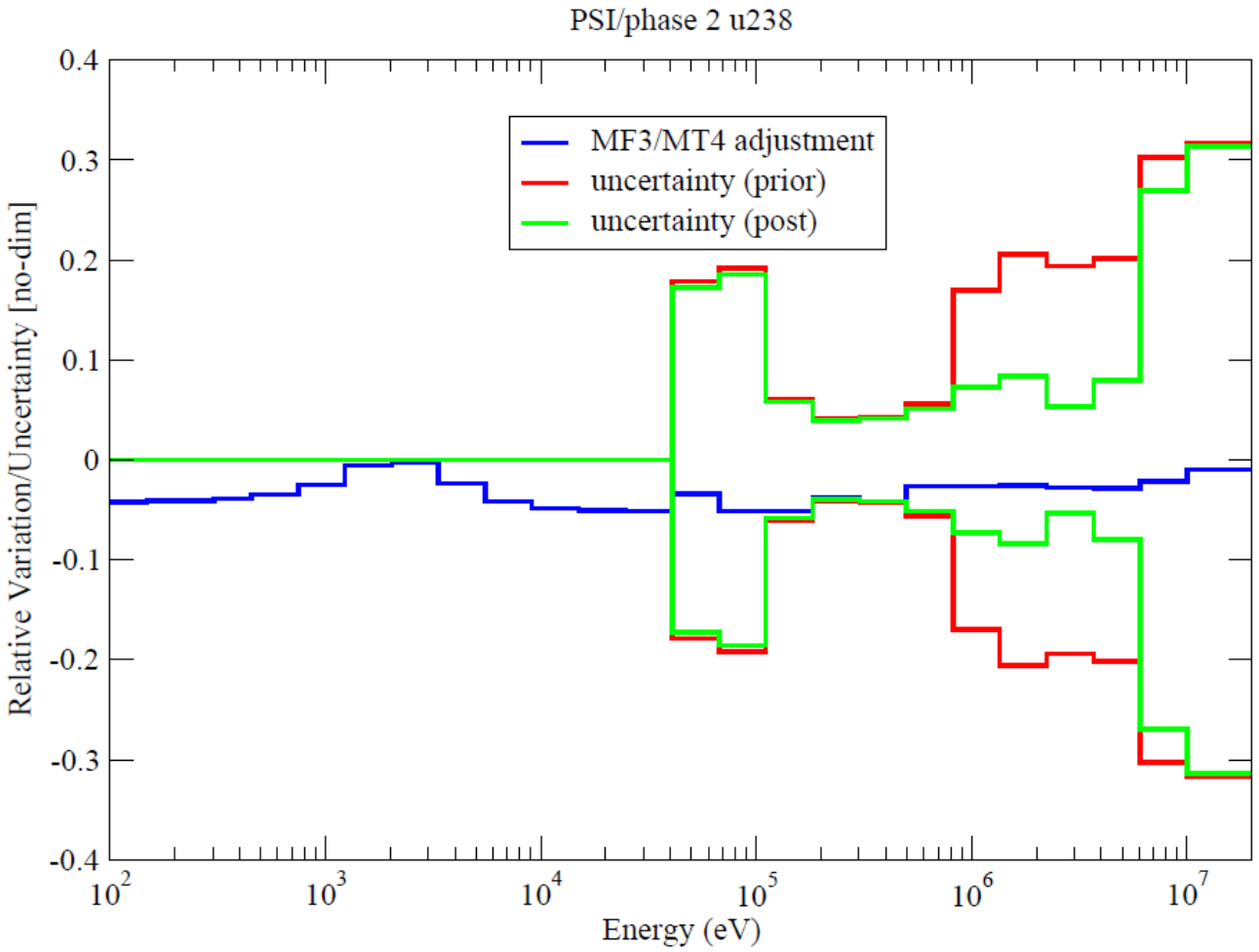
Reactor	Parameter	C/E		Uncertainty (%)	
		prior	posterior GLLS	prior	posterior GLLS
JEZEBEL_Pu239	k_{eff}	0.999413	0.999151	0.511	0.182
JEZEBEL_Pu239	F28/F25	0.982403	0.993123	2.426	1.148
JEZEBEL_Pu239	F49/F25	0.984846	0.989022	0.719	0.512
JEZEBEL_Pu239	F37/F25	1.00013	1.00425	1.604	0.877
JEZEBEL_Pu240	k_{eff}	1.00374	1.00069	0.579	0.198
FLATTOP_Pu239	k_{eff}	0.999291	0.999025	0.829	0.240
FLATTOP_Pu239	F28/F25	0.986328	0.995896	1.948	0.918
FLATTOP_Pu239	F37/F25	1.00702	1.01021	1.421	0.784
ZPR6_7	k_{eff}	1.00144	1.00068	0.972	0.139
ZPR6_7	F28/F25	1.00443	1.02185	6.399	1.600
ZPR6_7	F49/F25	0.959289	0.964713	0.833	0.586
ZPR6_7	C28/F25	1.00469	1.00632	1.493	0.950
ZPR6_7_Pu240	k_{eff}	1.00091	0.999969	0.973	0.140
ZPPR9	k_{eff}	0.999959	0.999975	1.203	0.144
ZPPR9	F28/F25	0.960575	0.978397	7.741	1.792
ZPPR9	F49/F25	0.975799	0.981151	0.846	0.579
ZPPR9	C28/F25	1.00373	1.00569	1.521	0.959
ZPPR9	VOID_STEP3	1.02885	1.03691	7.228	2.867
ZPPR9	VOID_STEP5	0.973152	0.993900	9.157	3.369
JOYO	k_{eff}	0.999443	0.999706	0.878	0.199

$\chi^2_{min} = 15.62$

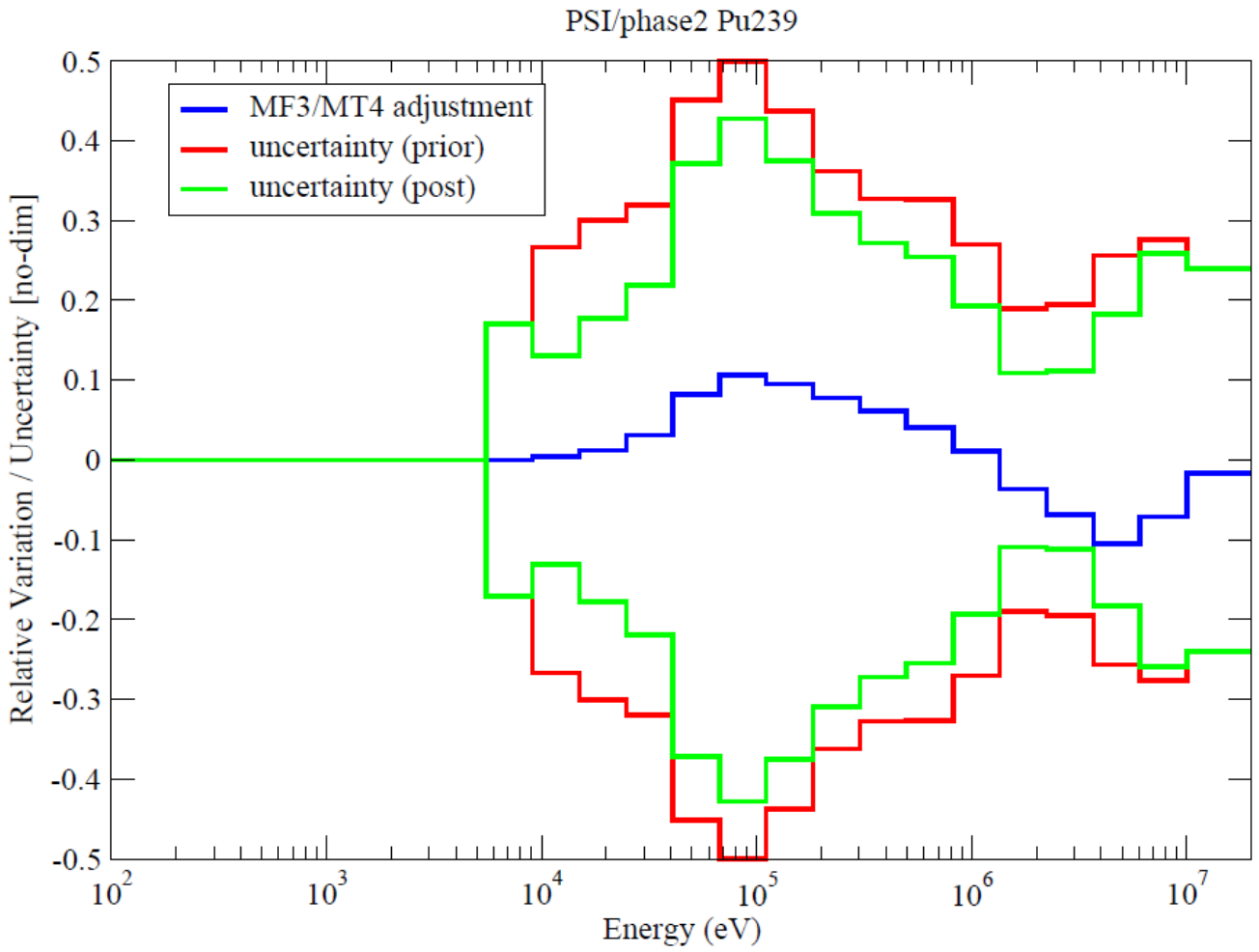
Case II results (posterior: GLLS / GLLS+ERANOS)

Reactor	Parameter	C/E		Uncertainty (%)	
		posterior GLLS	posterior GLLS+ERANOS	posterior GLLS	posterior GLLS+ERANOS
JEZEBEL_Pu239	k_{eff}	0.999151	0.999125	0.182	0.182
JEZEBEL_Pu239	F28/F25	0.993123	0.992846	1.148	1.108
JEZEBEL_Pu239	F49/F25	0.989022	0.989016	0.512	0.514
JEZEBEL_Pu239	F37/F25	1.00425	1.00417	0.877	0.880
JEZEBEL_Pu240	k_{eff}	1.00069	1.00068	0.198	0.195
FLATTOP_Pu239	k_{eff}	0.999025	1.00153	0.240	0.239
FLATTOP_Pu239	F28/F25	0.995896	0.989198	0.918	0.892
FLATTOP_Pu239	F37/F25	1.01021	1.00694	0.784	0.810
ZPR6_7	k_{eff}	1.00068	1.00071	0.139	0.140
ZPR6_7	F28/F25	1.02185	1.02233	1.600	1.594
ZPR6_7	F49/F25	0.964713	0.964836	0.586	0.586
ZPR6_7	C28/F25	1.00632	1.00627	0.950	0.949
ZPR6_7_Pu240	k_{eff}	0.999969	1.00000	0.140	0.141
ZPPR9	k_{eff}	0.999975	1.00002	0.144	0.145
ZPPR9	F28/F25	0.978397	0.979075	1.792	1.777
ZPPR9	F49/F25	0.981151	0.981316	0.579	0.578
ZPPR9	C28/F25	1.00569	1.00572	0.959	0.958
ZPPR9	VOID_STEP3	1.03691	1.03633	2.867	2.862
ZPPR9	VOID_STEP5	0.993900	0.991836	3.369	3.305
JOYO	k_{eff}	0.999706	1.00162	0.199	0.190

Case II selected results (GLLS)



Case II selected results (GLLS)



Case II selected results (GLLS)