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Use of PIA approach. Possible application to neutron propagation experiments

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This study

- Basis: benchmark exercise defined in the framework of SG-33, "Methods and issues for the combined use of integral experiments and covariance data", of the Working Party on Evaluation Cooperation (WPEC) of the OECD Nuclear Energy Agency Nuclear Science Committee (NSC).

- Specifically considered for adjustments in this study:
  - 3 of the 4 experimental configurations having measured spectral indices:
    - ✓ JEZEBEL (^{239}Pu configuration),
    - ✓ ZPR6-7 and ZPPR9: sodium-cooled fast reactor configurations.

    In addition, not part of the benchmark:
    - ✓ GODIVA in view of ^{235}U data.

  - 11 nuclides : ^{10}B, ^{16}O, ^{23}Na, ^{56}Fe, ^{52}Cr, ^{58}Ni, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu.
  - 6 reactions: elastic and inelastic scattering, lumped (n,2n) and (n,3n), capture, fission and $\bar{\nu}$.

This study (continued)

- 14 experiments:
  - ✓ Spectral indices at core center, 12,
  - ✓ ZPPR9: reactivity effects from coolant density reductions i.e. "Na Void Step 3" and "Na Void Step 5", 2:

Configuration	Integral parameter
GODIVA	F28/F25, F49/F25, F37/F25
JEZEBEL-^{239}Pu	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, Na Void Step 5

F28, F25, F49, and F37 are respectively used for ^{238}U, ^{235}U, ^{239}Pu, and ^{237}Np microscopic fission reaction rates per atom; C28 denotes the ^{238}U capture reaction rate per ^{238}U atom.

Data and codes

- Data : JEFF-3.1 cross-sections + COMMARA-2.0 provided in the form of 1-σ standard deviations and correlations in 33 neutron groups.
- Codes :
  - ERANOS: allows computing a priori and a posteriori values for the integral and target parameters and corresponding C/Es.
  - In-house ERANOS procedure MICADJ modifying microscopic multi-group data from the cell code ECCO according to relative adjustment factors.
  - In-house adjustment tool GLLS
    - ✓ producing these factors, giving the most deviating value from 1,
    - ✓ computing χ^2,
    - ✓ predicting a posteriori values for the integral experiments with the assumption of linearity,
    - ✓ generating a priori and a posteriori variance/covariance matrices for the analytical values of the integral experiments.

Methods

- Forward flux, integral parameters, adjoint flux and generalized importance:
  - Finite-difference, discrete-ordinates transport-theory (BISTRO): 1D spherical and 2D (r,z) geometry, P_1S_{16} approximations.
- Sensitivity coefficients:
  - Spectral indices: Generalized Perturbation Theory (GPT).
  - Reactivity effects: Equivalent Generalized Perturbation Theory (EGPT).
- Data adjustment:
  - JAEA approach proposed by Ishikawa: Bayesian theory in conjunction with the Generalized Linear Least-Squares (GLLS) method.

Specific adjustment

Iterative procedure accounting for nonlinearity

- *Iteration parameter i:*

  - $i = 0$: a priori.
  - $i > 0$: a posteriori, i-th adjustment iteration.

- *Iteration dependent data:*

$T_i = \left(T_{i,j}\right)$: central values data vector to adjust (further, if $i > 0$).

$R_C(T_i) = \left((R_c(T_i))_{,k}\right)$: analytical values vector for the set of integral parameters k obtained by means of T_i.

$G_i = \left(G_{i,k,j}\right) = \left(\frac{d\left((R_c(T_i))_{,k}\right)}{(R_c(T_i))_{,k}} \Big/ \frac{dT_{i,j}}{T_{i,j}}\right)$: sensitivity coefficient vector.

Specific adjustment (continued)

- *Iteration independent data:*

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

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

: experimental variance/covariance matrix, relative values.

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

: analytical modeling variance/covariance matrix, relative values. These are not nuclear data based variances/covariances of analytical values $R_C(T)$. The matrix is somewhat arbitrary but would get closer to zero when the number of particles used in stochastic simulations is increased.

Specific adjustment (continued)

For $i = 0, 1, 2, \ldots$ we compute by means of the GLLS code

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

The relative cross-section change ΔT_i allows computing the next iteration vector T_{i+1} from T_i using $(E - C)/C$s, on the basis of its definition:

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

giving

$$T_{i+1} = \ (T_{i+1,j}) = \left(T_{i,j} F_{i,j}\right), \qquad F_i = \left(F_{i,j}\right) = \left(1 + \Delta T_{i,j}\right)$$

F_i is handed over to MICADJ allowing to compute $R_C(T_{i+1})$ by means of ERANOS.

Specific adjustment (continued)

The next iteration variance/covariance data matrix, relative values, is given by

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

$$M_{i+1,j,j'} = cov\left(T_{i+1,j}, T_{i+1,j'}\right) / \left(T_{i+1,j} T_{i+1,j'}\right).$$

- Previous studies: M_0 instead of M_i throughout.
- Overall effect on the results of using M_i instead: small, however faster convergence.

Specific adjustment (continued)

Convergence:

achieved : $F_i \rightarrow 1$.
Up to 10 iterations , sometimes more than 10 needed depending on the case.

- The a posteriori values of the integral experiments predicted with the linear approximation (GLLS) and those computed explicitly become identical.

- Additional iterations would no longer modify these consistent values.
  The variance/covariance data M_i would also not change any more.

Remark:
- $i = 0$, no iterations, was used within SG-33.
- However: adjusted C/Es predicted on the basis of the linear approximation and explicitly computed values are found to be mostly different: nonlinearity.

The current PIA exercise

Progressive Incremental nuclear data Adjustment (PIA) proposed by Palmiotti and Salvatores: demonstrated on the basis of the iterative procedure as follows:

- **Simulation 1**: The 14 experiments comprising 12 spectral indices and 2 coolant density effects are adjusted all simultaneously.
- **Simulation 2** (PIA): Firstly adjusted at the same time with iterations, are the three GODIVA spectral indices, followed by the two ZPPR9 coolant density effects, the tree spectral indices of ZPR6-7, the three of ZPPR9 and last by the three spectral indices of JEZEBEL-^{239}Pu.
- **Simulation 3** (PIA): The reversed adjustment order is used as compared to Simulation 2 i.e. the three JEZEBEL-^{239}Pu spectral indices are adjusted first.

This PIA: correlations between experimental configurations cannot be considered.

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A posteriori C/Es for benchmark configurations

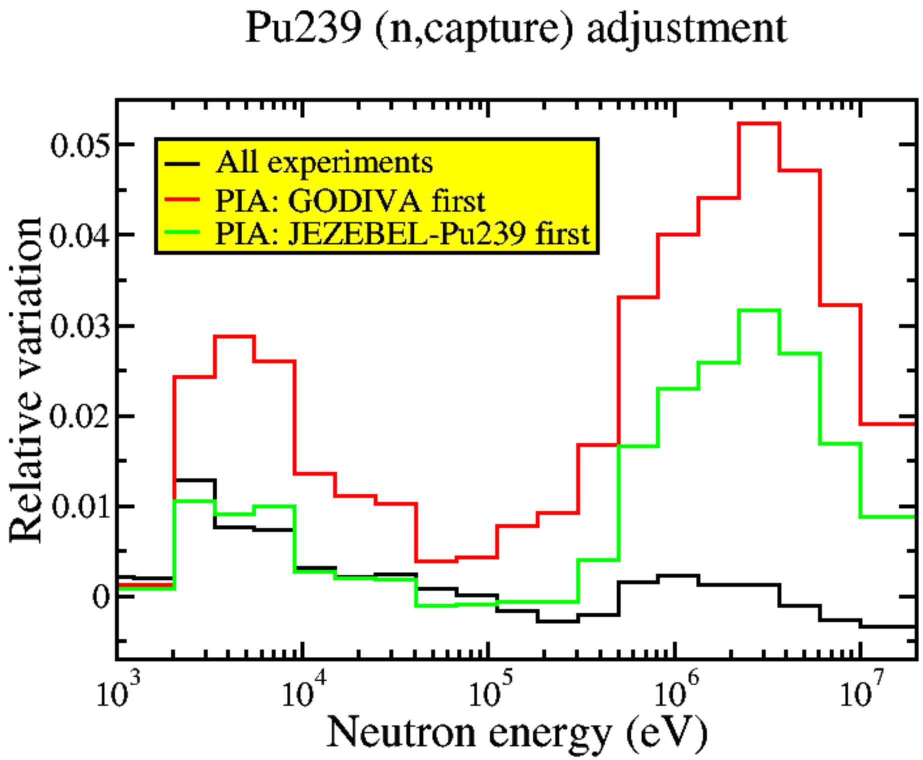
Configuration	Integral parameter	(a)	Simulation 1	Simulation 2	Simulation 3
GODIVA	F28/F25	1.096	0.998	0.999	0.999
	F49/F25	0.989	1.000	1.000	1.000
	F37/F25	1.409	1.000	0.997	0.996
JEZEBEL-^{239}Pu	F28/F25	1.100	0.986	0.996	0.997
	F49/F25	0.900	0.998	0.998	0.999
	F37/F25	1.400	1.007	1.006	1.006
ZPR6-7	F28/F25	3.173	1.034	1.030	1.043
	F49/F25	2.342	0.978	0.974	0.975
	C28/F25	2.614	1.004	1.003	1.004
ZPPR9	F28/F25	2.875	0.977	0.963	0.979
	F49/F25	2.230	0.999	0.994	0.994
	C28/F25	2.141	0.996	0.995	0.996
	Na Void Step 3	4.188	1.028	1.034	1.035
	Na Void Step 5	4.113	0.981	0.977	0.980

(a) Combination of experimental and calculation uncertainties of the a priori C/Es, %

- Adjusted Cs: lie within combined experimental and calculation uncertainty.
- All 3 simulations: quite consistent.

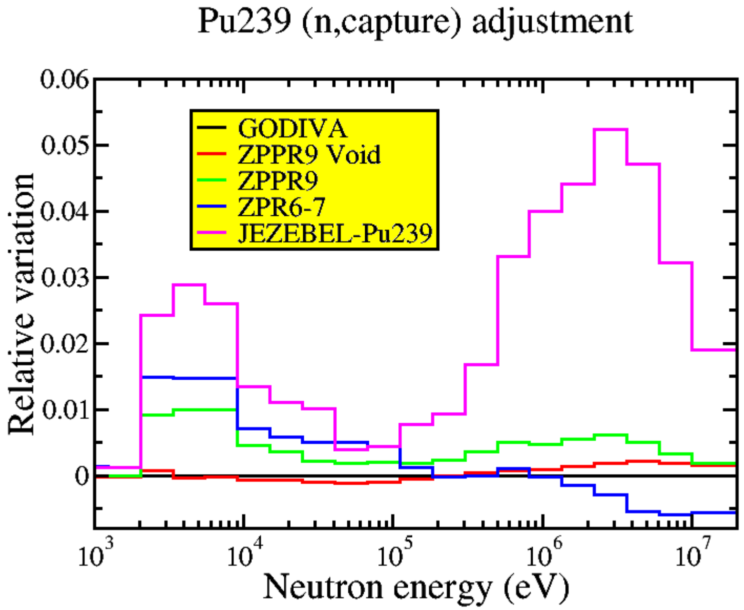
^{239}Pu capture cross-section: representative example for in depth comparison.

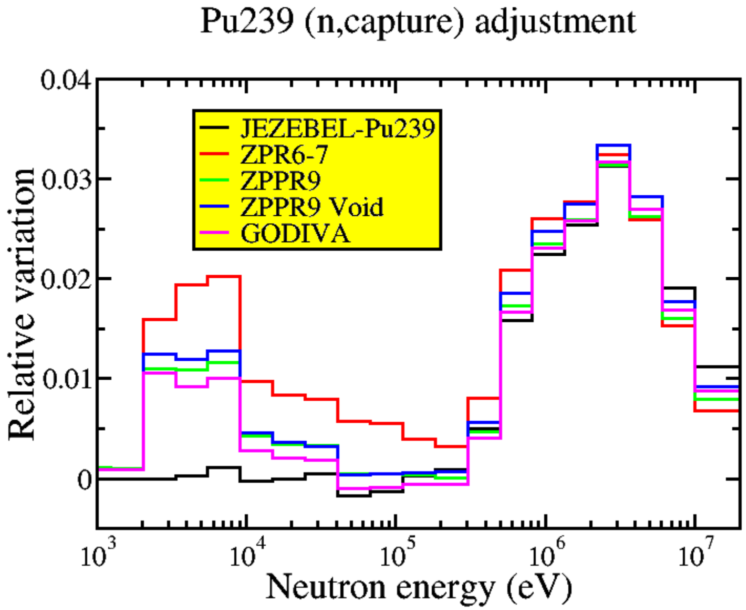
Relative data change with respect to prior data



- PIA simulations 2-3 similar.
- Simulation 1 suffers from larger compensation effects.

PIA: Simulation 2 (left), Simulation 3 (right)





The results from the individual incremental adjustment steps are displayed here with the aim of separating effects, next slide.

PIA results

For ^{239}Pu capture, the progressive incremental adjustment steps indicate:

I. The observed increase of the cross-section in the fission source range is primarily the result of assimilating the JEZEBEL experimental data.

II. While at energies not far from those of the Na elastic scattering resonance, ZPR6-7 plays the major role.

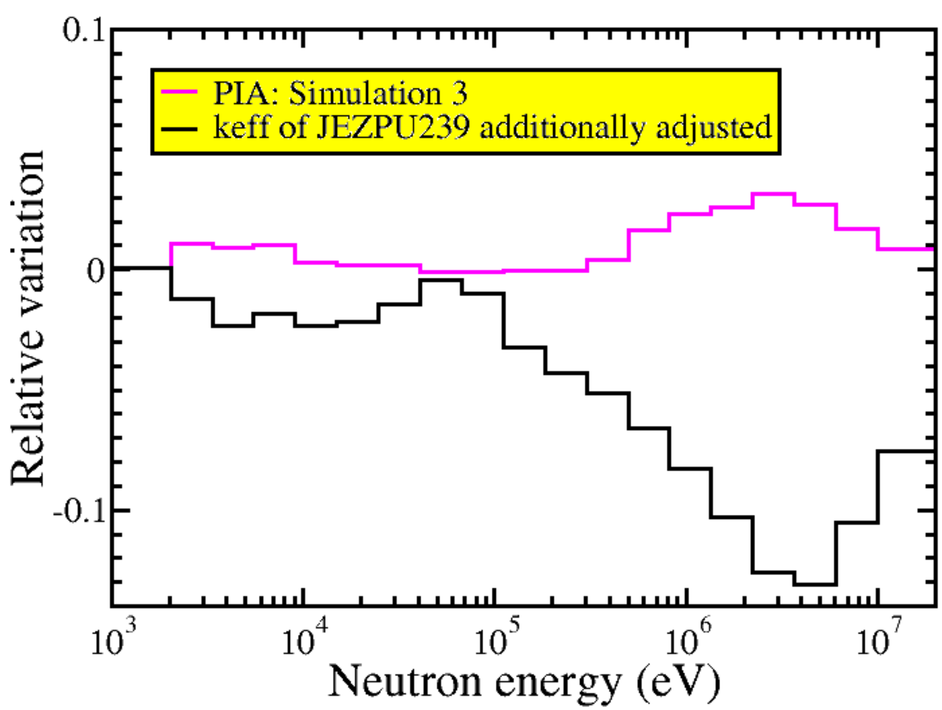
III. ZPPR9 is rather unimportant, i.e. it is redundant in this case.

IV. That in Simulation 3 GODIVA has a small impact although ^{239}Pu is not directly involved, is due to cross correlations originating in the course of the adjustment.

PIA results (continued)

Additionally adjusting the effective multiplication factor:

Pu239 (n,capture) adjustment



- C/Es almost unchanged, good.
- Compensation effects evident, bad: “Tsunami” effect on this and other cross-sections.
- However: could be useful, if limited to specific data not adjustable elsewhere with negligible impact on the bulk of cross-sections, e.g. $\bar{\nu}$.

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PIA results (continued)

Additionally adjusting the $k_{eff}s$ limited to $\bar{\nu}$:

- C/Es almost unchanged: good.

- A posteriori values for target k_{eff}-values also quite consistent:

GODIVA	JEZEBEL-^{239}Pu	ZPR6-7	ZPPR9
0.997	0.998	1.002	1.000

Conclusions

- Adjusted cross-sections and also associated variance/covariances are largely independent of a PIA sequence, provided that
  - multiplication factors are not considered and
  - non-linearity is accounted for in the adjustment for each incremental step.

- Multiplication factors as target parameters are a good check for the adjustment. However, they could also be beneficial in the adjustment , if this is done at the end. In addition the k_{eff}-adjustment should be limited to specific data which is not adjustable elsewhere and which adjustment has negligible impact on the bulk of cross-sections.

- The proposed incremental approach allowing separating effects therefore provides an automatic criterion how to exclude experiments. The role of transmission experiments within this approach is recognized.

We propose considering spatial reaction rates and reactivity effects. Individual PIA steps include groups of well documented experiments carried out in the same configuration. Individual experiments or configurations without effects on the adjustment are excluded.

Experiments leading to a contradictory trend need separate investigations.

Multiplication factors are excluded except for adjusting at the end χ, $\bar{\nu}$ and $\bar{\mu}$.