SG44 Computational Inter-comparison Study Revised

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Original Hypothesis

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WPEC/SG44
Inter-comparison Study

WPEC/SG44 inter-comparison study

"*The goal of this inter-comparison study is to* ***identify "stable" correlations*** *which come from the immutable nature of the reactor physics in the integral benchmarks and can be estimated almost independently of the choice of nuclear data library, integral experiments or methodology. Of primary focus for us will be comparing* ***correlations between fission, capture and nu-bar*** *for the three actinides.*"

[Vladimir Sobes by email October 23, 2019]

- Use whatever nuclear data library you are familiar working with
- Use a set of integral benchmarks representative of the testing suit
- Use whatever integral experiment assimilation technique you are familiar with
- Estimate the correlation coefficients which arise due to the application of your assimilation technique to your set of integral benchmarks with your nuclear data library
- Group structure to be fast (group 1), 20 MeV - 50 keV, intermediate (group 2), 50 keV - 0.625 eV, and thermal (group 3), 0.625 eV - 1e-5 eV.
- Report the results for the cross-reaction correlations

Updated Hypothesis

1. The hypothesis was revised to remove the assumption that the correlations will be stable independent of the integral system(s) used.

2. Demonstration is provided here for PU-MET-FAST system using different:
   1. Initial cross section library
   2. Assimilation methodology
   3. Energy group structure

3. The original goal was to establish a “soft” hypothesis which would be useful.

Concluding Remarks

- In response to the proposal of the inter-comparison study, 3-group correlation coefficients were computed with:
  - Cross-section adjustment method used in JAEA
  - Covariance data of JENDL-4.0
  - JAEA’s integral experimental database for fast reactors
- Correlation coefficients which arise due to the adjustment method were estimated for three use cases of integral experiments:
  - Case 1 (ZPPR-9 KEFF)
  - Case 2 (JEZEBEL KEFF)
  - Case 3 (ADJ2017)
- The results show that the correlation coefficients depend on the choice of integral experiments

  → Need to find another hypothesis or solution

- Details of the estimated correlation coefficients are stored in the spread sheets

Yokoyama Methodology

Tools and Data for Analyses

- Sensitivity coefficients:
  - MARBLE/SAGEP code system based on GPT (generalized perturbation theory) [1-3] for static integral parameters
  - MARBLE/PSAGEP code system based on DPT (depletion perturbation theory) [4-6] for time-dependent integral parameters
- Covariance of nuclear data:
  - JENDL-4.0 [7]
  - Processed by NJOY99.396
- Energy group structure:
  - Equivalent to the 3-group structure proposed in SG44*

Table 3-energy group structure

Group	SG44 proposed	This analysis
1	20MeV	←
2	50keV	52.5keV
3	0.625eV	0.683eV
	1e-5eV	←

[1] L. N. Usachev, J. Nucl. Energy A/B 18, 571-583 (1964)
[2] A. Gandini, J. Nucl. Energy 21, 755-765 (1967)
[3] W. M. Stacey Jr., J. Math. Phys. 13, 1119-1125 (1972)
[4] A. Gandini, et al., NSE 62, 339-345 (1977)
[5] M. L. Williams, NSE 70, 20-36 (1979)
[6] T. Takeda, et al., NSE 91, 1-10 (1985)
[7] K. Shibata, et al., J. Nucl. Sci. Technol. 48[1], 1-30 (2011)

Methodology

- Cross-section adjustment method used in JAEA*

$$\boldsymbol{T}' = \boldsymbol{T}_0 - \mathbf{M}\mathbf{G}^{\mathrm{T}}\left(\mathbf{G}\mathbf{M}\mathbf{G}^{\mathrm{T}} + \mathbf{V}_e^{(1)} + \mathbf{V}_m^{(1)}\right)^{-1}\left(\boldsymbol{R}_e - \boldsymbol{R}_c(\boldsymbol{T}_0)\right)$$

$$\mathbf{M}' = \boldsymbol{T}_0 - \mathbf{M}\mathbf{G}^{\mathrm{T}}\left(\mathbf{G}\mathbf{M}\mathbf{G}^{\mathrm{T}} + \mathbf{V}_e^{(1)} + \mathbf{V}_m^{(1)}\right)^{-1}\mathbf{G}\mathbf{M}$$

where

- $\boldsymbol{T}'$: adjusted cross sections (= $\boldsymbol{\sigma}'$ in SG39's nomenclature)
- $\boldsymbol{T}_0$: unadjusted cross sections (= $\boldsymbol{\sigma}$)
- $\mathbf{M}'$: covariance matrix of adjusted cross sections (= $\mathbf{M}'_{\sigma}$)
- $\mathbf{M}$: covariance matrix of unadjusted cross sections (= $\mathbf{M}_{\sigma}$)
- $\boldsymbol{R}_e$: measured value of integral experiments (= $\boldsymbol{E}$)
- $\boldsymbol{R}_c(\boldsymbol{T}_0)$: calculation value of integral experiments (= $\boldsymbol{C}$)
- $\mathbf{G}$: sensitivity matrix of integral experiments (= $\boldsymbol{S}$)
- $\mathbf{V}_e$: covariance matrix of experimental error (= $\mathbf{M}_{E}$)
- $\mathbf{V}_c$: covariance matrix of analysis method error (= $\mathbf{M}_{C}$)

*: Appendix A5 "JAEA methodology" in the SG33 Intermediate Reports, "Assessment of Existing Nuclear Data Adjustment Methodologies," NEA/NSC/WPEC/DOC(2010)429 (2011)

Yokoyama Results

Pu-239 vs Pu-239: Case 2 (JEZEBEL KEFF)

Table: Correlation coefficients generated by adjustment (in %)

		MAT	Pu-239																	
		MT	2			4			16			18			102			452		
MAT	MT	Group	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
Pu-239	2	1	J40	J40	0	-4	0													
		2		J40	J40	-1	0													
		3	0		J40	0	0													
	4	1				J40	J40	J40												
		2					J40	J40												
		3						J40												
	16	1	0	0	0	0	0		J40	J40	J40									
		2								J40	J40									
		3									J40									
	18	1	-8	-1	0	-27	0		0			J40	J40	0				-58	-2	0
		2	-2	J40	J40	-8	0		0				J40	J40				-17	0	0
		3	0	J40	J40	0	0		0			0		J40				0	0	0
	102	1	4	1	0	13	0		0			26	8	0	J40	J40	0	28	1	0
		2	0	J40	J40	1	0		0			2	J40	J40		J40	J40	2	0	0
		3	0	J40	J40	0	0		0			0	J40	J40	0		J40	0	0	0
	452	1	-9	-1	0	-29	0		0									J40	J40	J40
		2	0	0	0	-1	0		0										J40	J40
		3	0	0	0	0	0		0											J40

	Pu-239 nu-bar		
Pu-239 fission	-58	-2	0
	-17	0	0
	0	0	0

2: elastic, 4: inelastic, 16: (n,2n), 18: fission, 102: (n,γ), 452: nu-bar

- Correlations between Pu-239 fission and nu-bar are large

→ Large correlations can be generated by one integral experiment

Rochman Methodology

PAUL SCHERRER INSTITUT PSI BMC/BFMC + differential/integral data

- Step 1 - Preliminary work: in-depth cross section evaluation (traditional method of parameters/models adjustment)

- Step 2 - BMC: Based on step 1,
  – Generate n=100 000 (or 1000) random files (TMC-way)
  – Calculate n times the benchmarks
  – Assign weights to all realizations *i* with a chi2 and update the parameter distributions

For a random file i and a set of p benchmarks:

$$\chi_i = \sum_j^p \left(\frac{k^{(j)}_{eff,i} - k^{(j)}_{exp}}{\Delta k^{(j)}} \right)^2 \quad (1)$$

$$w_i = \exp(-\frac{\chi_i}{2}) \quad (2)$$

$$\begin{cases} \omega = \sum_i^n w_i \\ \omega_\sigma = \sum_i^n w_i \cdot \sigma_i / \omega \end{cases}$$

  – Update the cross sections with the weights.

- BFMC variation compared to BMC:

(EPJ/ N 4 (2018) 35,
J. Kor. Phys. Soc. 59, 1218 (2011).)

$$w_i = \exp\left[- \left(\frac{\chi_i^2}{\chi_{min}^2} \right)^2 \right].$$

Rochman Results

PAUL SCHERRER INSTITUT PSI

BMC/BFMC + 1 fast benchmark (pmf1)

- Based on pmf1 : ^{239}Pu (EPJ/N 3 (2017) 14)

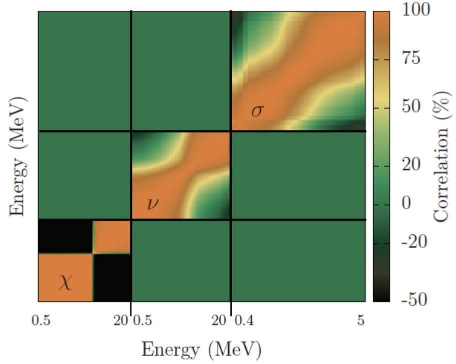
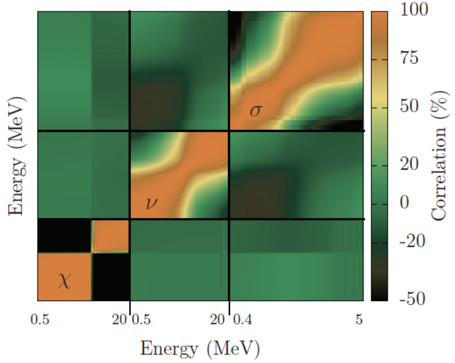


Fig. 2. Prior correlation matrix for ^{239}Pu ν, σ and χ (for the incident neutron energy of 750 keV). The energy axis is for the incident neutrons for ν and σ, and for the outgoing neutron for χ. The X- and Y-axis are in linear scale.



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Cabellos Methodology

2. Methodology based on "1D one-group transport equation"

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- A general **1D one-group simplified transport equation**:

$$k_{eff} = \frac{\bar{\nu} \cdot \sigma_f}{\sigma_f + \sigma_\gamma + L} \qquad \textbf{(Eq. 1)}$$

- Assuming that the above equation is universally valid and that the **typical uncertainty reachable in critical experiments is ~300 pcm**, then we can derive strong anti-correlations between $\bar{\nu}$ and $\sigma_{fission}$.
- **Methodology:**
  - **Spectrum-averaged** for $\bar{\nu}$, σ_f and σ_γ values according Vlad's proposal:
    - fast (group 1): 20 MeV - 50 keV
    - intermediate (group 2): 50 keV - 0.625 eV
    - thermal (group 3): 0.625 eV - 1e-5 eV
  - In this work, **NJOY iwt=4 option is used**. This weight function combines a thermal Maxwellian at low energies, a 1/E function at intermediate energies, and a fission spectrum at high energies
  - **Here, the constrain** that the uncertainty of critical experiments is **100 pcm (Δk_0).**
  - Simple generic correlation coefficients are derived, focusing mainly on $\bar{\nu}$-σ_f .
  - The **UMC-B approach** is compared to results of a **GLSQ procedure**.

Cabellos Results

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3. Inter-comparison of Results

Results: Pu-239

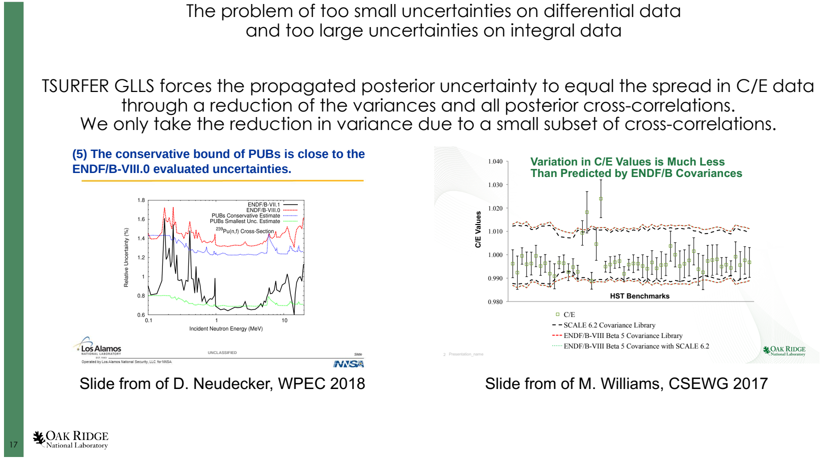
Table 5. Pu-239 Vlad' correlations versus "1D one-group simplified transport equation constraint". Both methods, UMC-B and GLLS provide similar values.

		MAT	Vlad's correlations			1-D one group keff constarint					
						ENDF/B-VIII.0			JEFF-3.3		
		MT	452			452			452		
MAT	MT	Group	1	2	3	1	2	3	1	2	3
Pu-239	18	1	-57	-37		-33			-49		
		2		-9	-87		-8			-26	
		3		-38	-40			-20			-39
	102	1	14	11		27			37		
		2		4	3		9			31	
		3		28	31			17			1

Fast (group 1): 20 MeV - 50 keV
Intermediate (group 2): 50 keV - 0.625 eV
Thermal (group 3): 0.625 eV - 1e-5 eV

Sobes Methodology

1. Start with ENDF/B-VIII.0
2. Use TSURFER GLLS based on PMF-1
3. Extract only the posterior correlations for Pu-239



Sobes Results

		MAT	Pu-239		
		MT	452		
MAT	MT	Group	1	2	3
Pu-239	18	1	-48	-26	-25
		2			
		3			
	102	1	10		
		2		3	13
		3		14	20

1. For a PMF system only, I would consider only the fast / fast correlations to be estimated in a reliable manner.

2. The fission / nu-bar correlation coefficient is very consistent with other findings.

3. The capture / nu-bar correlation is not very consistent with Yokoyama and Cabellos.

Comparison of Results

Pu-239 vs Pu-239: Case 2 (JEZEBEL KEFF)

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		2								J40	J40									
		3									J40									
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		3	0	J40	J40	0	0		0			0		J40				0	0	0
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		2	0	J40	J40	1	0		0			2	J40	J40		J40	J40	2	0	0
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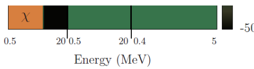
: benchmark (pmf1)



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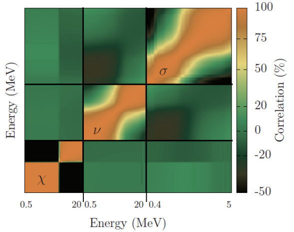

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Rochman

http://www.psi.ch/stars 2019.11.26/STARS/RD41 - (7 / 18)

Sobes Results

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MAT	MT	Group	1	2	3
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		2			
		3			
	102	1	10		
		2		3	
		3		14	

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Cabellos

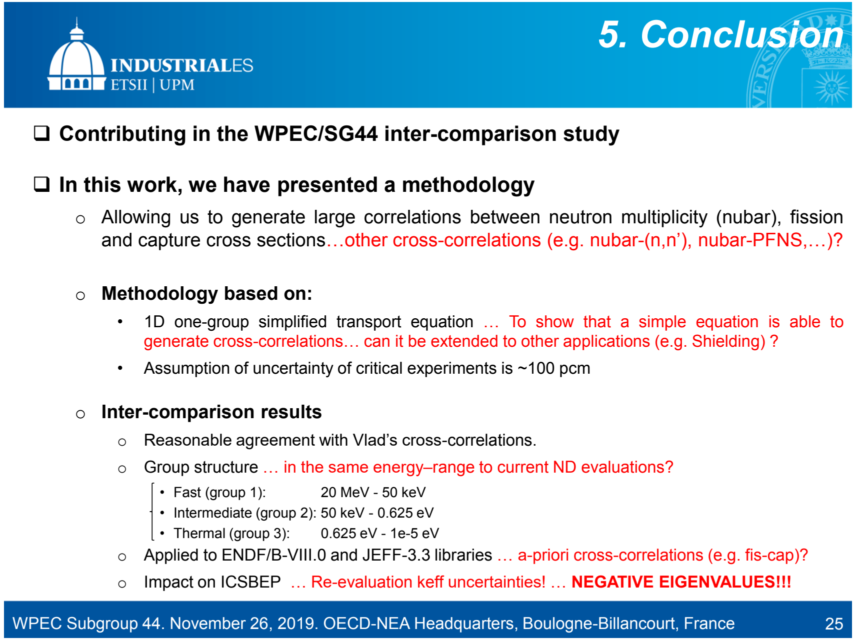
Parting Thoughts

Thank you all for your participation!

1. Fission / nu-bar correlations show stability in estimation under the new hypothesis.

2. There needs to be a balance between the formulation of a “soft” hypothesis and it’s utility in practice.

3. Negative eigenvalues remain an issue to be investigated.



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