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Preliminary results on SG44 covariance inter-comparison study using JENDL-4.0 and JAEA's integral database

Kenji Yokoyama
Research Group for Reactor Physics and
Standard Nuclear Code System
Japan Atomic Energy Agency (JAEA)

Background & Abstract

- Background
  - Nuclear data community has a common problem that the nuclear data covariance usually overestimates the uncertainty of integral quantities such as Keff
  - Considerations to integral data are essential during the nuclear data evaluation process but this consideration is usually not reflected to the covariances
  - A recommended methodology to overcome this problem is to adjust the covariance (or correlation coefficients) by adding information of integral data used in the nuclear data evaluation
  - In an e-mail on Oct. 23, 2019, Dr. V. Sobes proposed a computational inter-comparison study based on a hypothesis that the correlation coefficients are independent from the choice of nuclear data library, integral experiments or methodology
- Abstract
  - According to his proposal, we tried to verify the hypothesis by using our familiar nuclear data library, integral experiments and methodology
  - Our preliminary results denied the hypothesis
    - Correlation coefficients depend on the choice of integral experiments

Inter-comparison study proposed by Dr. V. Sobes*

- The computational inter-comparison study proposes to estimate correlation coefficients which are absent from the present covariance libraries but would come up as a result of "some use" of integral experiments in the evaluation of the mean values. The prosed study is centered on the hypothesis that correlation between certain differential quantities can be reliably estimated without exact knowledge of the integral experiments used or the methodology which was used for the assimilation (whether systematic or non-systematic). A simple example is that fission and nu-bar will have a negative correlation coefficient regardless of what integral experiment or what methodology is used. The details of the inter-comparison study are below.
  - Please use whatever nuclear data library you are familiar working with
  - Use a set of integral benchmarks representative of the testing suit that your organization uses
  - Use whatever integral experiment assimilation technique you are familiar with. E.g. GLLS, PIA, Bayesian Monte Carlo, rejection of poor performing evaluations, etc...
  - 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

*: V. Sobes, "WPEC November 2019 Subgroup 44 Meeting", SG44 mailing list, Oct. 23, 2019

Inter-comparison study proposed by Dr. V. Sobes*

- **Please report the results for the quantities given in the attached spreadsheet.**
- **In my methodology, I have defined the 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. Feel free to define your own 3-group boundaries within reasonable nuclear engineering limits.**
- **I have also filled in the spread sheet with cross-isotope and cross-reaction correlations already existing in the current ENDF/B-VIII.0 library. You may do the same for the library that you will be working with.**

- **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. Of secondary focus is finding "stable" correlations else-where in the matrix of isotopes, reactions and energies in the attached spread sheet. The benefit of this computational inter-comparison study will be the reproducibility and reliability of the estimated correlation values.**

*: V. Sobes, "WPEC November 2019 Subgroup 44 Meeting", SG44 mailing list, Oct. 23, 2019

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*

$$\boldsymbol{T}' = \boldsymbol{T}_0 - \mathbf{M}\mathbf{G}^{\mathrm{T}} \left(\mathbf{G}\mathbf{M}\mathbf{G}^{\mathrm{T}} + \mathbf{V}_e^{(1)} + \mathbf{V}_m^{(1)}\right)^{-1} \left(\boldsymbol{R}_e - \boldsymbol{R}_c(\boldsymbol{T}_\mathbf{0})\right)$$

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

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 (= $\mathbf{M}'_{\boldsymbol{\sigma}}$)
- $\mathbf{M}$: covariance matrix of unadjusted cross sections (= $\mathbf{M}_{\boldsymbol{\sigma}}$)
- $\boldsymbol{R}_e$: measured value of integral experiments (= $\boldsymbol{E}$)
- $\boldsymbol{R}_c(\boldsymbol{T}_\mathbf{0})$: calculation value of integral experiments (= $\boldsymbol{C}$)
- $\mathbf{G}$: sensitivity matrix of integral experiments (= $\boldsymbol{S}$)
- $\mathbf{V}_e$: covariance matrix of experimental error (= $\mathbf{M}_{\boldsymbol{E}}$)
- $\mathbf{V}_c$: covariance matrix of analysis method error (= $\mathbf{M}_{\boldsymbol{C}}$)

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

Integral Benchmarks

- A new version of unified (adjusted) cross-section set ADJ2017 for fast reactors based on JENDL-4.0 was recently developed*
- 620 Integral experiments are available for the inter-comparison study using JENDL-4.0
  - Various types of integral experiments with fast spectrum
    - ZPPR, FCA, BFS, MASRUCA, LANL, ZEBRA, JOYO, MONJU, SEFOR, PFR, YAYOI
    - criticality, reaction rate ratio/distribution, control rod worth, sodium void reactivity, Doppler reactivity, burnup reactivity coefficients, …
    - Addition of 132 integral experiments relating to minor actinides and degraded plutonium in comparison of the previous version ADJ2010[1][2]
  - 70-group sensitivity coefficients evaluated with JENDL-4.0 and uncertainties due to experiments and analytical models including correlations

*: K. Yokoyama, K. Sugino, M. Ishikawa, S. Maruyama, Y. Nagaya, K. Numata, T. Jin, "Development of the Unified Cross-section Set ADJ2017," JAEA-Research 2018-010 [in Japanese]

References on the previous version ADJ2010 are written in English:

[1] J. Korean Physical Society, Vol. 50, No. 2, pp. 1357-1360 (2011)
[2] Nuclear Data Sheets, Vol. 123, pp. 97-103 (2015)

Three Use Cases of Integral Experiments

- Case1 (ZPPR-9 KEFF)
  - Single integral experiment: Criticality of ZPPR-9
    - 600MWe-class, 2-region homogeneous MOX core
    - Pu enrichment: inner core = ~11wt%, outer core = ~16wt%
    - Pu-239/Pu = 87%
- Case 2 (JEZEBELL KEFF)
  - Single integral experiment: Criticality of JEZEBEL
    - Bare sphere of Pu-239
    - Pu enrichment: 100wt%
    - Pu-239/Pu = 95%
- Case 3 (ADJ2017)
  - Full set of 620 integral experiments used for ADJ2017
    - ZPPR, FCA, BFS, MASRUCA, LANL, ZEBRA, JOYO, MONJU, SEFOR, PFR, YAYOI
    - criticality, reaction rate ratio/distribution, control rod worth, sodium void reactivity, Doppler reactivity, burnup reactivity coefficients, …

Pu-239 vs Pu-239: Case 1 (ZPPR-9 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	0	0													
		2		J40	J40	0	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	0	0	0	0	0		0			J40	J40	0				-2	-1	0
		2	0	J40	J40	0	0		0				J40	J40				-1	0	0
		3	0	J40	J40	0	0		0			0		J40				0	0	0
	102	1	0	0	0	0	0		0			3	2	0	J40	J40	0	2	1	0
		2	0	J40	J40	0	0		0			2	J40	J40		J40	J40	1	1	0
		3	0	J40	J40	0	0		0			0	J40	J40	0		J40	0	0	0
	452	1	0	0	0	0	0		0									J40	J40	J40
		2	0	0	0	0	0		0										J40	J40
		3	0	0	0	0	0		0											J40

Pu-239 nu-bar

Pu-239 fission			
	-2	-1	0
	-1	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 small

→ Large correlations are not generated by only one integral experiment ?

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

Pu-239 vs Pu-239: Case 3 (ADJ2017)

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	-15	0													
		2		J40	J40	-3	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	-26	1		0			J40	J40	-1				-59	-1	0
		2	0	J40	J40	2	1		0				J40	J40				-4	-7	0
		3	0	J40	J40	0	0		0			-1		J40				0	0	0
	102	1	-8	-1	0	-25	0		0			8	10	0	J40	J40	0	52	9	0
		2	2	J40	J40	9	4		0			-10	J40	J40		J40	J40	-13	35	0
		3	0	J40	J40	0	0		0			0	J40	J40	0		J40	0	0	0
	452	1	-12	-1	0	-37	-1		0									J40	J40	J40
		2	0	-1	0	4	0		0										J40	J40
		3	0	0	0	0	0		0											J40

	Pu-239 nu-bar		
Pu-239 fission	-59	-1	0
	-4	-7	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 similar to those of Case 2 (JEZEBEL KEFF)

→ Coincidence? JEZEBEL KEFF determines the correlations?

U-238 vs Pu-239: Case 1 (ZPPR-9 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
U-238	2	1	0	0	0	0	0		0			0	0	0	0	0	0	0	0	0
		2	0	0	0	0	0		0			0	0	0	0	0	0	0	0	0
		3	0	0	0	0	0		0			0	0	0	0	0	0	0	0	0
	4	1	0	0	0	0	0		0			2	2	0	-3	-2	0	2	1	0
		2	0	0	0	0	0		[illegible]			[illegible]	-1	0	1	1	0	-1	0	0
		3																		
	16	1	0	0	0	[illegible]	[illegible]		[illegible]			[illegible]	0	0	0	0	0	0	0	0
		2																		
		3																		
	18	1	0	0	0	0	0		[illegible]			0	J40	0	2	1	0	-1	0	0
		2	0	0	0	0	0		0			-1	[illegible]	0	1	1	0	-1	0	0
		3	0	0	0	0	0		0			0	0	0	0	0	0	0	0	0
	102	1	0	0	0	-2	0		0			29	21	0	-42	-27	0	24	9	0
		2	0	0	0	0	0		0			2	2	0	-3	-2	0	2	1	0
		3	0	0	0	0	0		0			0	0	0	-1	0	0	0	0	0
	452	1	0	0	0	0	0		0			-1	-1	0	1	1	0	-1	0	0
		2	0	0	0	0	0		0			0	0	0	0	0	0	0	0	0
		3	0	0	0	0	0		0			0	0	0	0	0	0	0	0	0

U-238 capture / Pu-239 capture

-42	-27	0
-3	-2	0
-1	0	0

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

- Correlations between U-238 capture and Pu-239 capture are large

→ ZPPR-9 KEFF and JEZEBEL KEFF generates different correlations

U-238 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
U-238	2	1																		
		2																		
		3																		
	4	1																		
		2																		
		3																		
	16	1																		
		2																		
		3																		
	18	1	-2	0	0	-6	0						J40	0	6	1	0	-14	0	0
		2										J40		J40						
		3																		
	102	1																		
		2																		
		3																		
	452	1																		
		2																		
		3																		

Pu-239 capture

U-238 capture

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

- Correlations between U-238 capture and Pu-239 capture are not generated

→ JEZEBEL has no sensitivity of U-238 since its core consists of only Pu-239

U-238 vs Pu-239: Case 3 (ADJ2017)

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
U-238	2	1	3	0	0	11	0		0			-7	-2	0	18	-1	0	3	-1	0
		2	0	-2	0	3	0		0			-3	-5	0	8	8	0	4	-2	0
		3	0	0	0	0	0		0			0	-1	0	0	1	0	0	0	0
	4	1	0	1	0	-14	1		0			2	3	0	-13	8	0	2	4	0
		2	0	0	0	1	0		[illegible]			[illegible]	0	0	1	-1	0	0	0	0
		3																		
	16	1	0	0	0	[illegible]	[illegible]		[illegible]			[illegible]	0	0	0	0	0	0	0	0
		2																		
		3																		
	18	1	-1	1	0	0	1		[illegible]			[illegible]	J40	0	-9	-7	0	-17	0	0
		2	2	1	0	9	0		0			-14	[illegible]	0	-8	-4	0	1	-1	0
		3	0	0	0	0	0		0			0	0	0	0	0	0	0	0	0
	102	1	-2	1	0	-14	3		0			18	5	0	-12	21	0	-9	0	0
		2	-2	-3	0	-2	-1		0			10	18	0	13	-26	0	-1	2	0
		3	0	0	0	0	0		0			1	2	0	1	-2	0	0	0	0
	452	1	2	1	0	5	1		0			5	0	0	17	-4	0	-3	-2	0
		2	-1	-1	0	-2	0		0			-2	0	0	-6	2	0	1	1	0
		3	-1	-1	0	-2	0		0			-2	0	0	-6	2	0	1	1	0

U-238 capture vs Pu-239 capture:

-12	21	0
13	-26	0
1	-2	0

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

- Correlations between U-238 capture and Pu-239 capture are different from those of Case 1 (ZPPR-9 KEFF)

→ The correlations depend on the choice of integral experiments

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