SG44 Report

Vladimir Sobes

THE UNIVERSITY OF
TENNESSEE
KNOXVILLE

Meeting Agenda

Duration	PDT (CA, USA)	CEST (Paris)	JST (Tokyo)	Topic	
00:15	05:00	**14:00**	21:00	Welcome	V. Sobes, C. de Saint Jean
00:25	05:15	**14:15**	21:15	Multivariate statistical reduction of cross section uncertainties in neutron reactions	C. Opera
00:25	05:40	**14:40**	21:40	TBC	A. Sonzogni
00:30	06:05	**15:05**	22:05	An update on the SG44 computational inter-comparison study	V. Sobes
00:20	06:35	**15:35**	22:35	Short break	
01:00	06:55	**15:55**	22:55	Discussion on draft report	V. Sobes
00:10	07:55	**16:55**	23:55	AOB	
	08:05	**17:05**	00:05	Close	

OECD / NEA Nuclear Science Committee

Working Party on International Nuclear Data Cooperation (WPEC) 32nd

Meeting of the WPEC Subgroup 44 on the Investigation of Covariance Data in General Purpose Nuclear Data Libraries

May 11 - 15 2020,

Boulogne - Billancourt France

Multivariate Statistical Reduction of Cross Section Uncertainties in Neutron Reactions

Introductive study

Cristiana Oprea, Ioan Alexandru Oprea

Joint Institute for Nuclear Research, Frank Laboratory of Neutron Physics, Department of Experimental Nuclear Physics, Joliot-Curie 6, 141980 Dubna, Russian Federation, E-mail: istina@nf.jinr.ru

1. Introduction

Fast neutron reactions - investigated for a long time at LNF facilities

Fundamental research – new data on nuclear reaction mechanisms and structure of nuclei

Applicative researches – precise nuclear data for nuclear fission and fusion reactors; reprocessing of *U* and *Th* for transmutation and energy projects and ADS; Fast Neutron Activation Analysis

Neodymium Nucleus – 5 stable isotopes, $^{142, 143, 145, 146, 148}$Nd (Z=60)
- of interest in many applications – permanent powerful magnets; Samarium – Neodymium dating -> age relationship of rocks and meteorites

^{143}Nd reactions with fast neutrons – alpha channels very low cross section

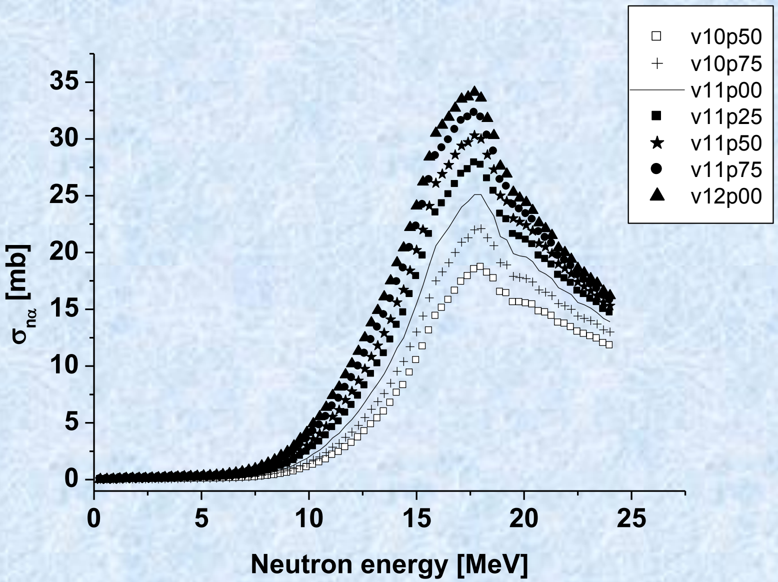
Investigated process – ^{143}Nd(n,α)^{143}Ce with FN from 0.5 MeV up to 25 MeV

4. Multivariate Analysis. Cross Section Data

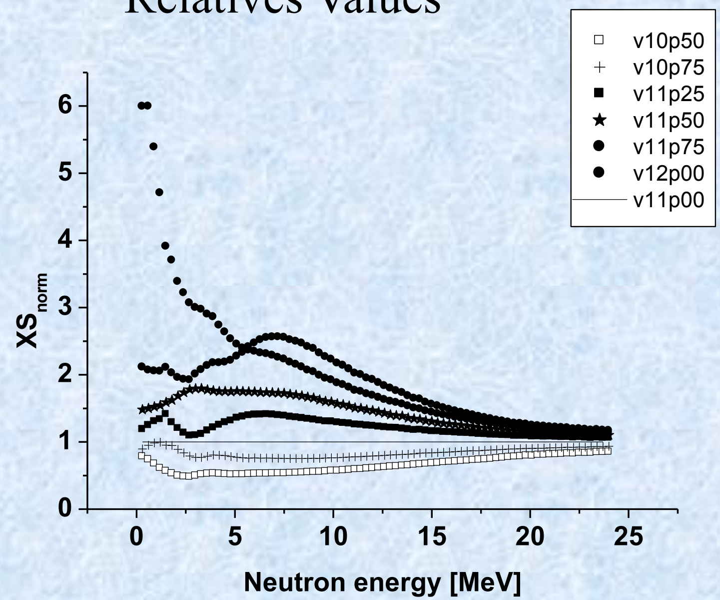
Emergent Alpha Channel – Volume Parameters Variation - Real Part

$P_0 = V_{V0} = 172$ MeV, $P = V_V \in \{0.5, 0.75, 1.00, 1.25, 1.50, 1.75, 2.00\} \times V_{V0}$

Absolute Values



Relatives Values



$Xs_{norm} = \sigma_{n\alpha}(P)/\sigma_{n\alpha}(P_0)$

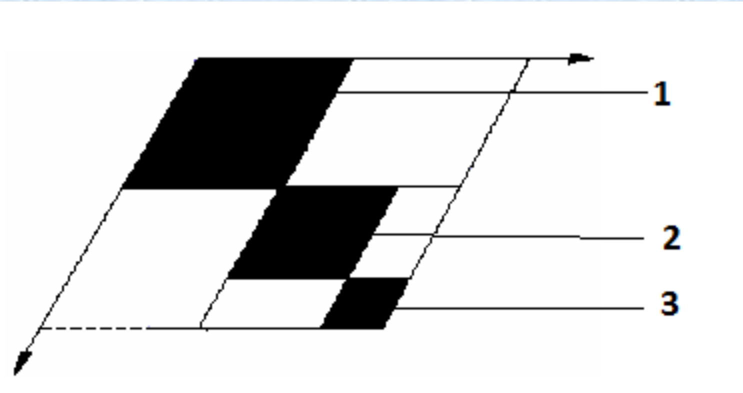
Alpha Volume Real Part V_V – very sensible in 10 – 20 MeV range

Relative values - at low energy up to 5 MeV – are changing by 3 – 6 times

4. Factor Analysis – Principal Components (Data Reduction)

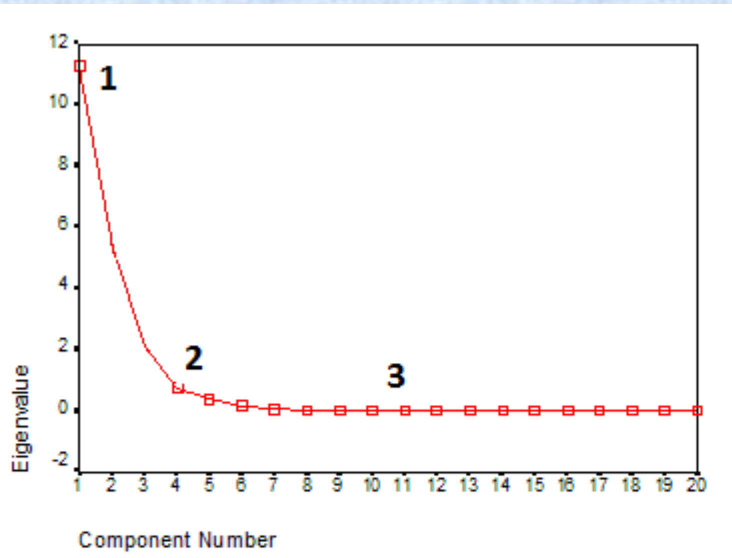
Solving eigenvalues problem

$$(\mathbf{R} - \lambda_l \mathbf{I})\boldsymbol{\alpha}_1 = \mathbf{0}$$



Structure of **R** matrix

- 2 factors are obtained λ_1, λ_2
  - 1 – with a weight larger than 90%
  - 2 – weight about few percents
  - 3 – neglected part (< 1 %)



- The most important factor (1) is given by Real part of Volume WS potential (V_V) of alpha channel
- The second factor (2) most probably comes from Imaginary part of Surface component (W_D) of alpha channel
- Region (3) – influence of other variables statistically can be neglected

Low energy part and Giant Resonance are most sensible for variables changes

SG44 Computational Inter-comparison Study Revised

Vladimir Sobes

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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

Comparison of 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

Yokoyama

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

benchmark (pmf1)

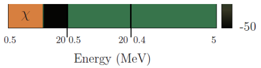

Fig. 2. Prior correlation matrix for [239]Pu ν, σ and χ (for the incident neutron energy of 750 keV). The energy axis is for the incident neutrons for ν and σ, and for the outgoing neutron for χ. The X- and Y-axis are in linear scale.

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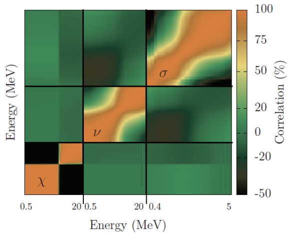

Fig. 5. Posterior correlation matrix for [239]Pu ν, σ and χ (for the incident neutron energy of 750 keV). The energy axis is for the incident neutrons for ν and σ, and for the outgoing neutron for χ. The X- and Y-axis are in linear scale.

Rochman

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	
		3		14	

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

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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

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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5. Conclusion

- **Contributing in the WPEC/SG44 inter-comparison study**
- **In this work, we have presented a methodology**
  - Allowing us to generate large correlations between neutron multiplicity (nubar), fission and capture cross sections…other cross-correlations (e.g. nubar-(n,n’), nubar-PFNS,…)?
  - **Methodology based on:**
    - 1D one-group simplified transport equation … To show that a simple equation is able to generate cross-correlations… can it be extended to other applications (e.g. Shielding) ?
    - Assumption of uncertainty of critical experiments is ~100 pcm
  - **Inter-comparison results**
    - Reasonable agreement with Vlad’s cross-correlations.
    - Group structure … in the same energy–range to current ND evaluations?
      - Fast (group 1): 20 MeV - 50 keV
      - Intermediate (group 2): 50 keV - 0.625 eV
      - Thermal (group 3): 0.625 eV - 1e-5 eV
    - Applied to ENDF/B-VIII.0 and JEFF-3.3 libraries … a-priori cross-correlations (e.g. fis-cap)?
    - Impact on ICSBEP … Re-evaluation keff uncertainties! … **NEGATIVE EIGENVALUES!!!**

Draft of SG44 Final Report

Section	Responsible	Status	Topic
1*	V. Sobes	Complete	Introduction
2.a	C. de Saint Jean	Committed	Summary of main evaluation tecniques used, Bayesian Monte-Carlo
2.b	D. Neudecker	Complete	Summary of known problems due to defects, biases, resonance range
3.b	H. Sjöstrand	Committed	Methods for autonomous interpretation of experimental data
3.c	H. Sjöstrand	Committed	Methods to address discrepant data sets
4.a	V. Sobes	Complete	Use of integral experiments in evaluations
4.b.i	V. Sobes	Complete	Other probability distributions for uncertainties
4.b.ii	C. Mattoon	Complete	Additional contribution with GNDS comments
4.c	V. Sobes	Complete	Analysis of consistency of covariance data
4.d	I. Hill	Complete	Integral experiment cross-correlation
5.a	V. Sobes	Complete	Cross-isotope correlations
5.a+	D. Rochman	Complete	Additional contribution from PSI on cross-isotope data
5.a++	C. de Saint Jean, R. Capote	Committed	Impact of prior covariance matrices on correlation coefficient estimation
6*	V. Sobes	Committed	Intercomparison study
7.a	D. Neudecker	Complete	Documentation of covariance evaluatino techniques
7.b	L. Fiorito	TBC	Comments on angular distribution covariance format and use
7.c	C. Mattoon	Complete	Verification of eigenvalues and decompositions
7.d	V. Sobes	Committed	TSL covariances
8.a	D. Neudecker	Complete	PFNS covariances
8.b	A. Trkov	Committed	Legendre coefficient covariances and processing
8.c	A. Koning	Committed	MF: 36, 37, 42, 45. Where we have mean values and will "never" have covariance.
8.d	H. Sjöstrand	Committed	Random files

Parting Thoughts

Future Subgroups

Closing of SG44

Thank you for your participation!

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