Results of Nuclear Data S&U Analysis for Benchmark Exercises Using DANTSYS/SUSD3D with COMMARA-2.0

S.J. KIM, D.H. KIM, C.S. GIL

Korea Atomic Energy Research Institute

7th Meeting of WPEC Subgroup 33 on “Methods and Issues for the Combined Use of Integral Experiments and Covariance Data”

May 22 - 23, 2012

NEA, Issy-les-Moulineaux, FRANCE

KAERI 한국원자력연구원 Korea Atomic Energy Research Institute

CONTENTS

- Introduction
- Results for Benchmark Exercises
- Status of V&V Activity
- Summary

I. Introduction

Preparation of Cross Section Data

- Source ENDF
  - ENDF/B-VII.0
- NJOY99 Code Processing
  - Same NJOY processing options as KAFAX-libraries (NEA-1815, -1816, -1817) except for energy group structure (150 groups)
  - MATXS-format
  - Energy group structure: 33 groups of SG33 standard
  - Weighting function: KALIMER-150 core spectrum

Preparation of JENDL-4.0 Covariance Data

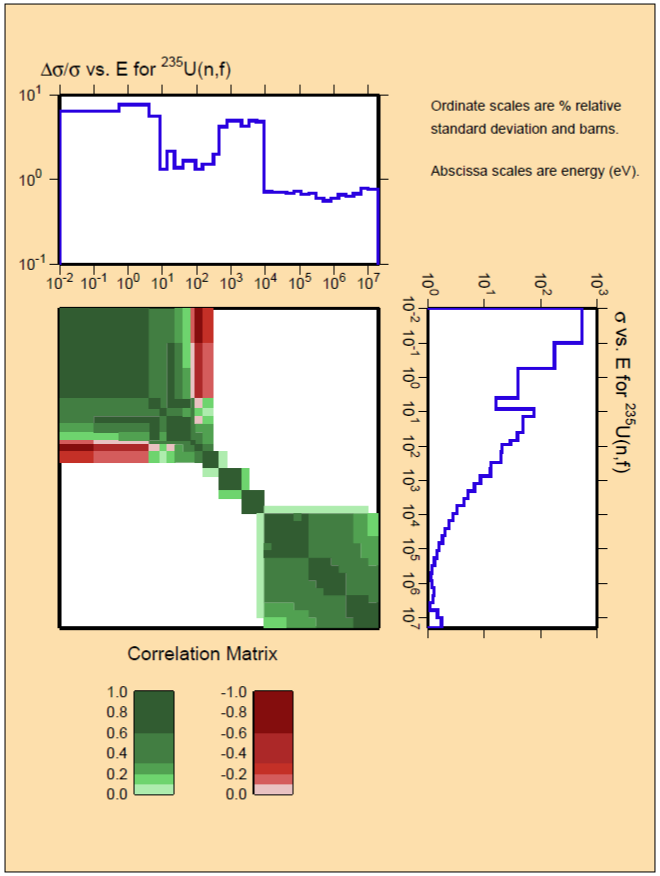
- Source Covariance Data
  - JENDL-4.0
- NJOY99 (ERRORR) Code Processing
  - COVFIL-format
  - Energy group structure: 33 groups of SG33 standard
- Nuclides included
  - Non-Actinides: B-10, B-11, O-16, Na-23, Mn-55, Fe-56, Co-59, Ni-58, Ni-60
  - Actinides: U-234, U-235, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241

Preparation of COMMARA-2.0 Covariance Data

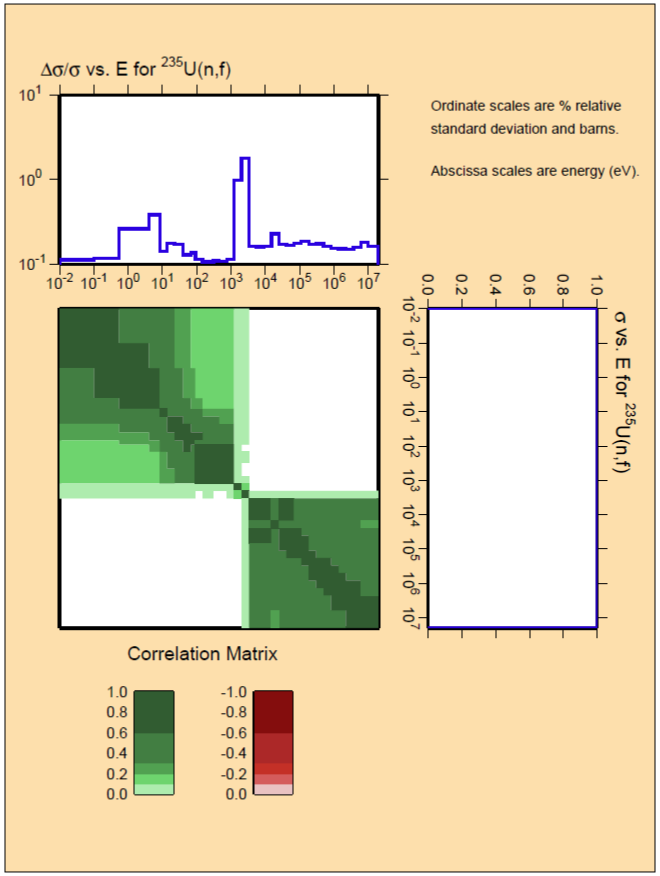
- Source Covariance Data
  - COMMARA-2.0
- Modified ANGELO Code from I. Kodeli
  - Data conversion of COMMARA-2.0 to COVFIL-format
  - Verification of covariance matrices by LAMBDA code
  - Energy group structure: 33 groups of SG33 standard
- Nuclides included
  - Non-Actinides: B-10, B-11, O-16, Na-23, Mn-55, Fe-56, Co-59, Ni-58, Ni-60
  - Actinides: U-234, U-235, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241

Comparison of U-235 Fission Covariance Data

< JENDL-4.0 >

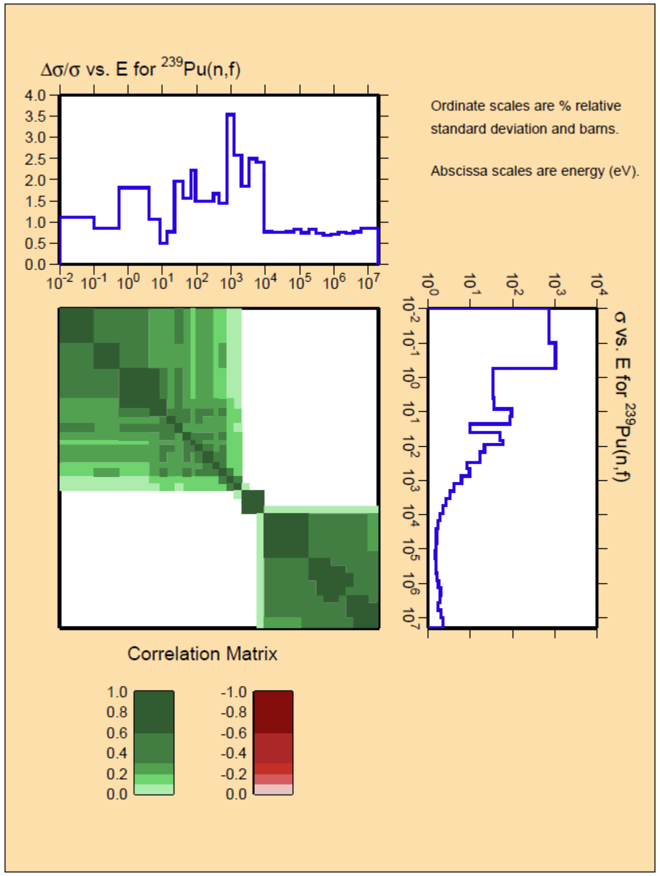


< COMMARA-2.0 >

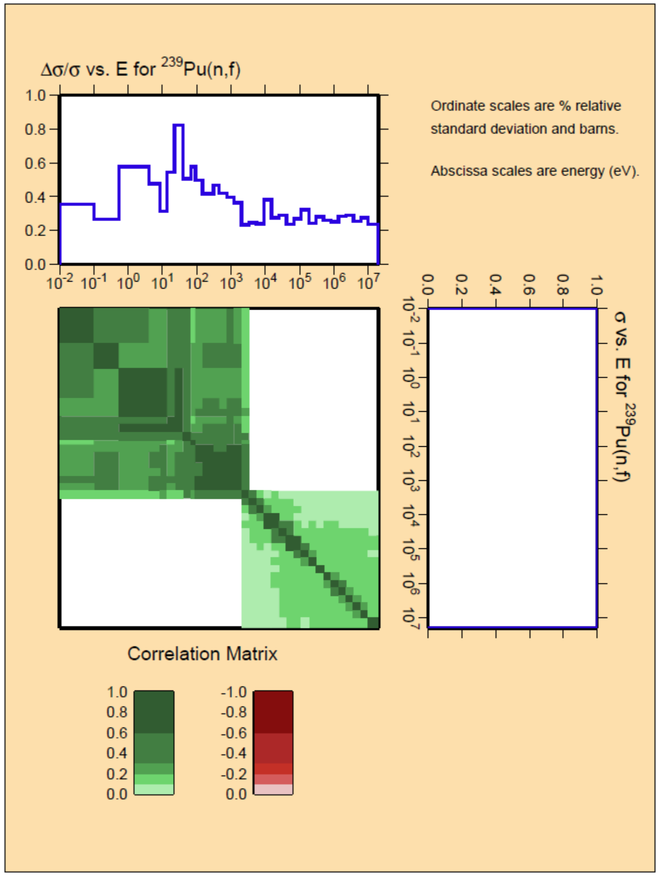


Comparison of Pu-239 Fission Covariance Data

< JENDL-4.0 >

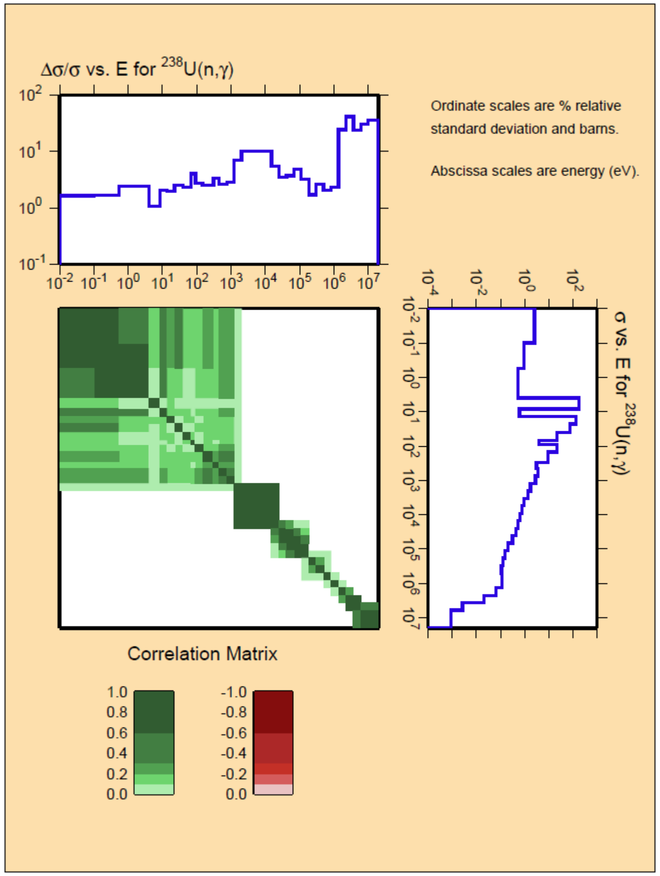


< COMMARA-2.0 >

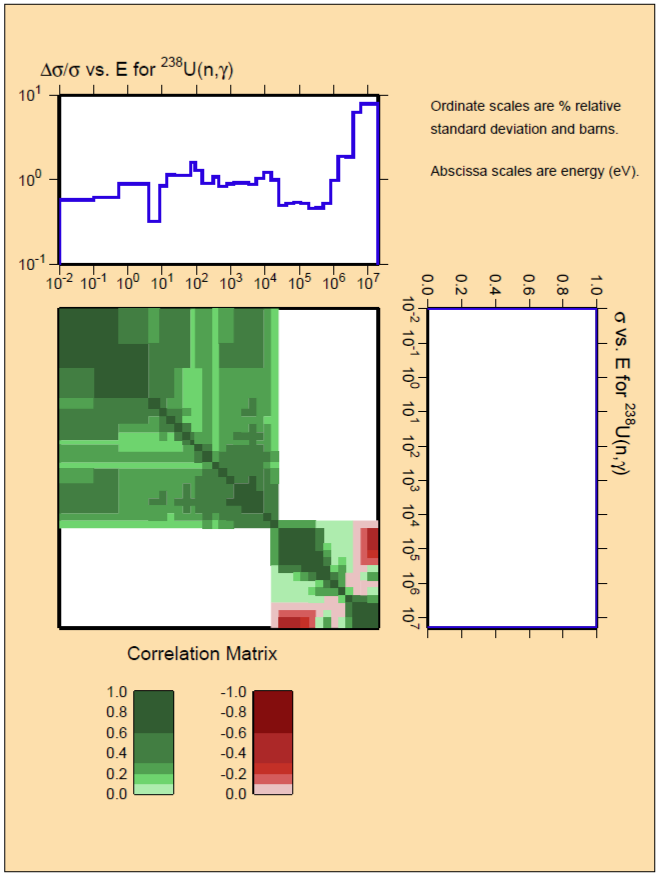


Comparison of U-238 Capture Covariance Data

< JENDL-4.0 >



< COMMARA-2.0 >

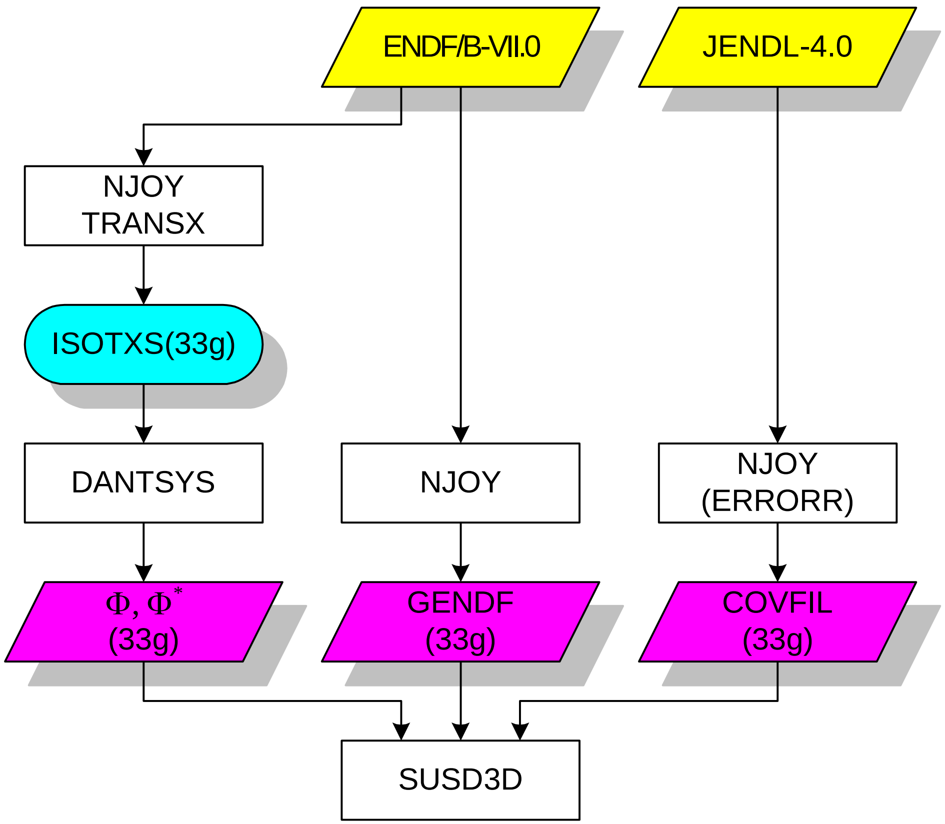


Sn Transport Calculation by DANTSYS

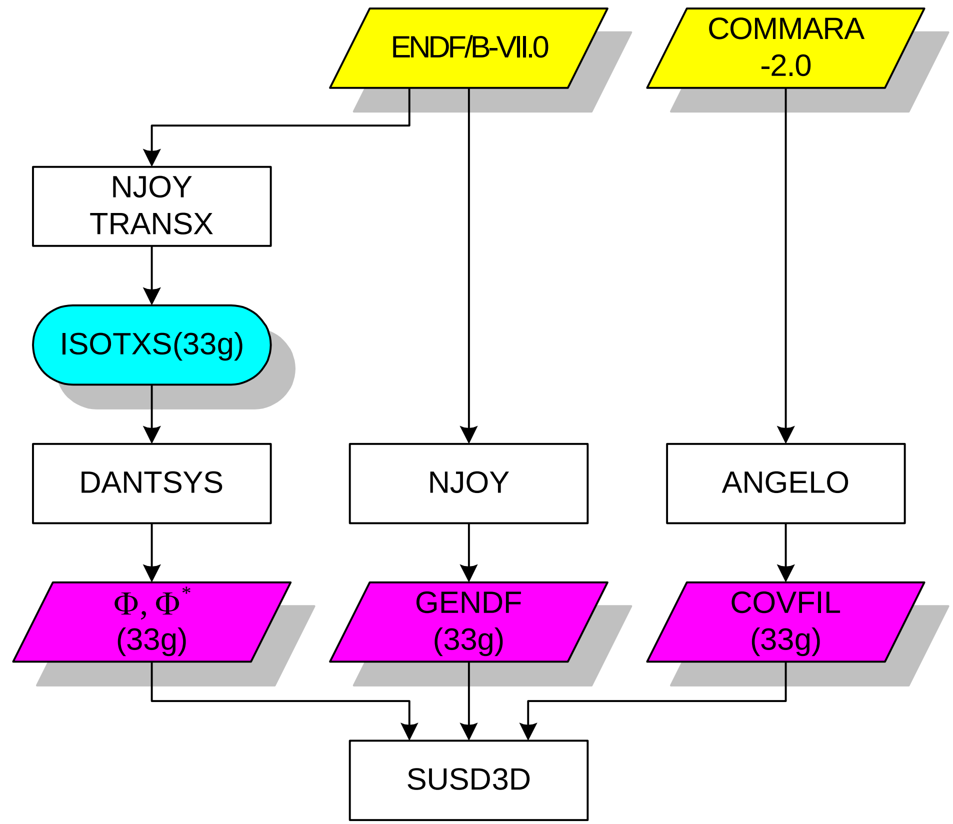
- Geometry
  - 1-D Sphere model: JEZEBEL-Pu239, JEZEBEL-Pu240, FLATTOP-Pu
  - 2-D Cylinder (R-Z) model: ZPR-6/7, ZPR-6/7 High-Pu240, JOYO Mk-I
- Angular Quadrature Sets
  - S16, S8, S4: Traditional built-in Pn constants given by DANTSYS (IQUAD=1)

S&U Analysis by SUSD3D

< JENDL-4.0 >



< COMMARA-2.0 >



II. Results for Benchmark Exercises

This Study

- Benchmark calculations have been carried out for 7 benchmark exercises of WPEC SG33.
- Validation of Integral Parameters
  - k-eff, spectral indices, Na void reactivities (ZPPR-9)
  - DANTSYS calculations
    - ENDF/B-VII.0-based MATXS-format libraries
    - Options: P1-S4, P1-S8 (JEZEBEL-Pu239, ZPR-6/7), P3-S16
    - Same meshing and isotopic compositions as SG33 standard
    - Different angular quadrature sets (S4) from SG33 standard
  - Corrective Factors for homogeneous deterministic calculations (P1-S4, 33 groups)

This Study

- Calculation of Nuclear Data Uncertainties to k-eff
  - Forward & Adjoint Fluxes: ENDF/B-VII.0
  - Covariance Data: JENDL-4.0 vs. COMMARA-2.0
  - Considering
    - most of nuclides with covariance data
    - most of nuclear reactions of covariance file
    - inelastic scattering reactions (MT=4)
    - normalized to sum of total nu sensitivities (MT=452) for all actinides
- Comparison of Uncertainty Contributions
  - by nuclides & by dominant reactions of major nuclides
  - for JENDL-4.0 vs. COMMARA-2.0 covariance data

Summary of DANTSYS/SUSD3D S&U Results

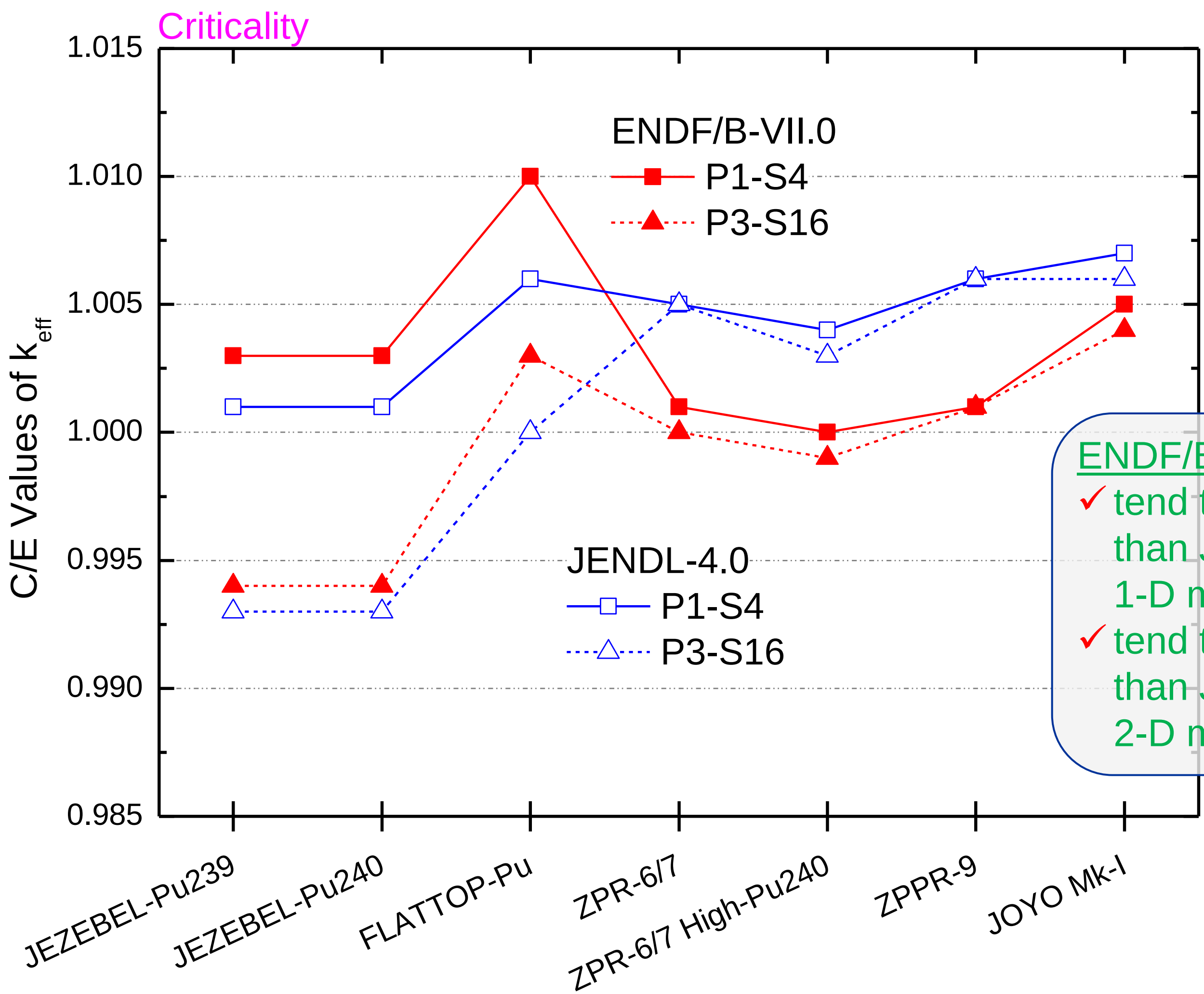
No.	Core	Parameter	Experiment	DANTSYS w/ ENDF/B-VII.0 (P1-S4) C/E	SUSD3D w/ COMMARA-2.0 Cov. Uncertainty (%)	SUSD3D w/ JENDL-4.0 Cov. Uncertainty (%)
1	JEZEBEL-Pu239	keff	**1.00000**	**1.003**	**0.117**	**0.484**
2		F28/F25	**0.2133**	**0.984**		
3		F49/F25	**1.4609**	**0.980**		
4		F37/F25	**0.9835**	**0.974**		
5	JEZEBEL-Pu240	keff	**1.00000**	**1.003**	**0.123**	**0.419**
6	FLATTOP-Pu	keff	**1.00000**	**1.010**	**0.123**	**0.471**
7		F28/F25	**0.1799**	**0.987**		
8		F37/F25	**0.8561**	**0.986**		
9	ZPR-6/7	keff	**1.00051**	**1.001**	**0.313**	**1.177**
10		F28/F25	**0.0223**	**0.988**		
11		F49/F25	**0.9435**	**1.013**		
12		C28/F25	**0.1323**	**1.024**		
13	ZPR-6/7 High-Pu240	keff	**1.00080**	**1.000**	**0.311**	**1.152**
14	ZPPR-9	keff	**1.00080**	**1.001**	**0.384**	**1.290**
15		F28/F25	**0.0207**	**0.991**		
16		F49/F25	**0.9225**	**0.989**		
17		C28/F25	**0.1296**	**1.027**		
18		Na void (Step 3), pcm	**106.0000**	**1.048**		
19		Na void (Step 5), pcm	**109.0000**	**1.075**		
20	JOYO Mk-I	keff	**1.00105**	**1.005**	**0.348**	**0.852**

COMMARA-2.0

- ✓ produce smaller k-eff uncertainties than JENDL-4.0 covariance data
- ✓ due to smaller ND uncertainties for dominant reaction covariances

Comparison of Criticality Results

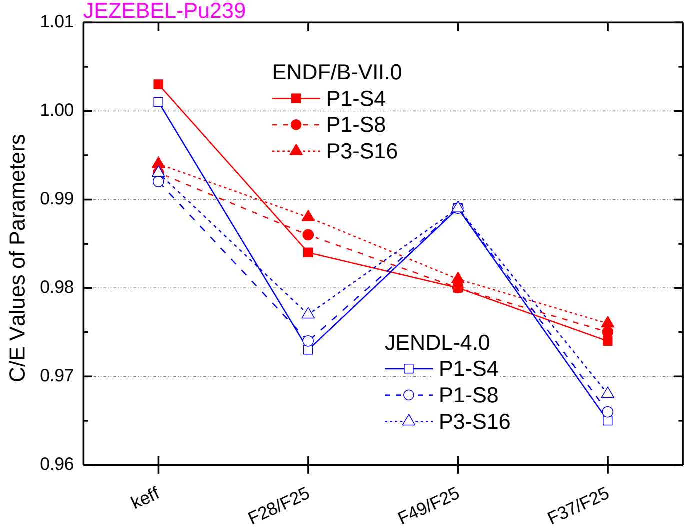
ENDF/B-VII.0 vs. JENDL-4.0

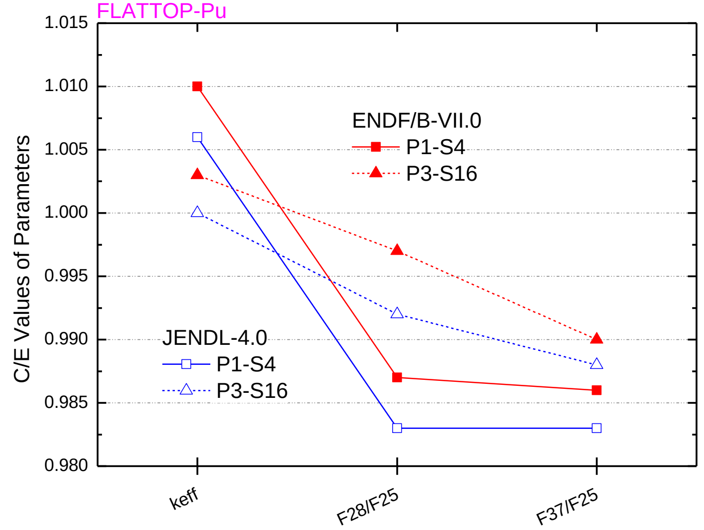


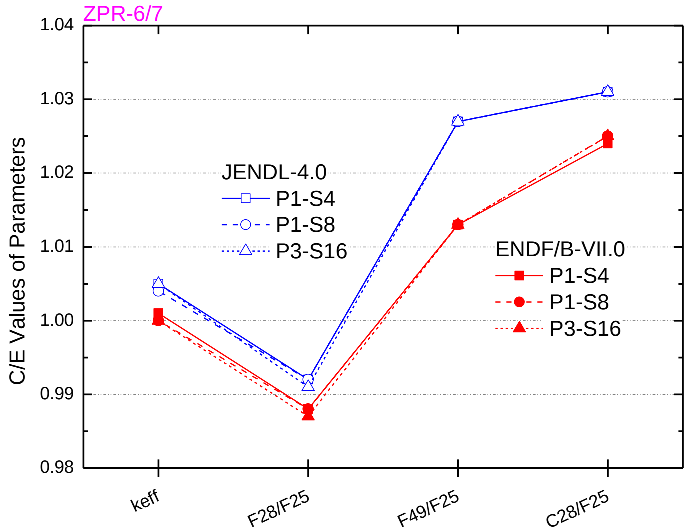
ENDF/B-VII.0
- ✓ tend to be larger than JENDL-4.0 for 1-D models
- ✓ tend to be smaller than JENDL-4.0 for 2-D models

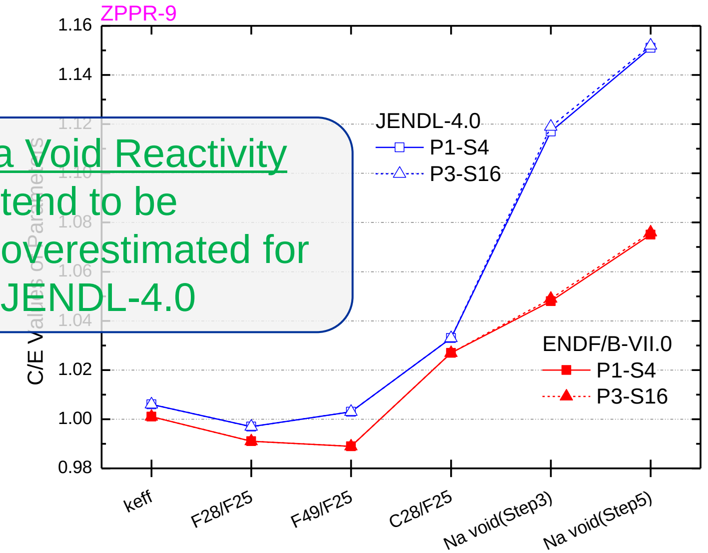
Comparison of Integral Parameters

ENDF/B-VII.0 vs. JENDL-4.0





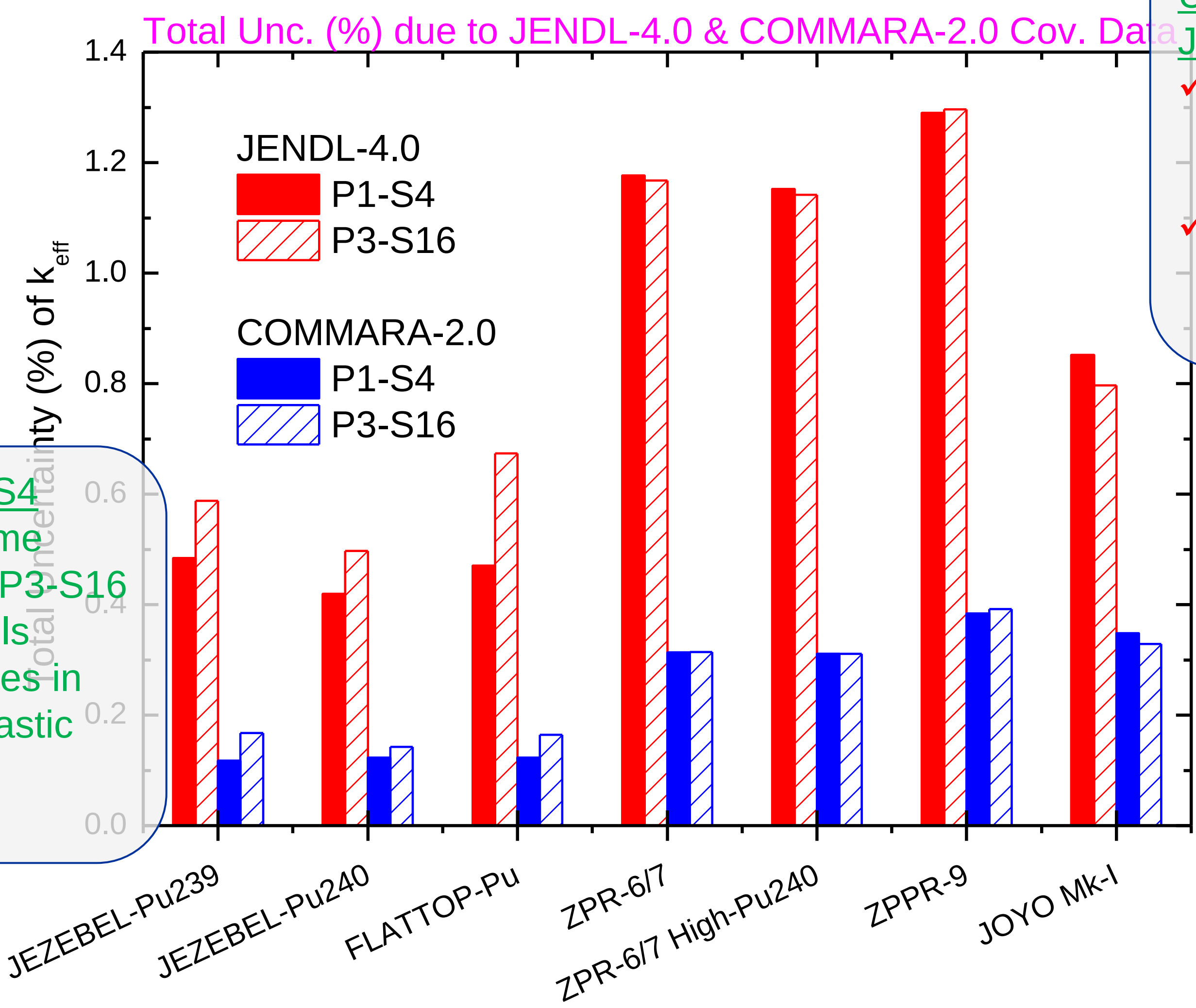




Na Void Reactivity
✓ tend to be overestimated for JENDL-4.0

Comparison of Total Uncertainty

JENDL-4.0 vs. COMMARA-2.0



Total k-eff Uncertainties due to JENDL-4.0
- ✓ over 3 ~ 4 times larger than COMMARA-2.0
- ✓ except JOYO Mk-I with 2.5 times larger unc.)

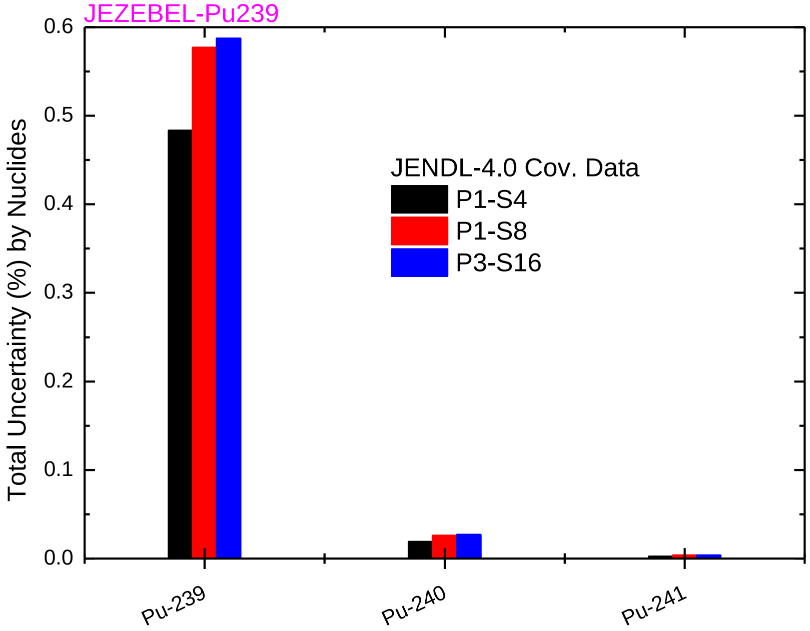
Uncert. for P1-S4
- ✓ tend to become smaller than P3-S16 for 1-D models
- ✓ due to changes in elastic & inelastic scattering contributions

Uncertainty Contribution by Nuclides & Reactions

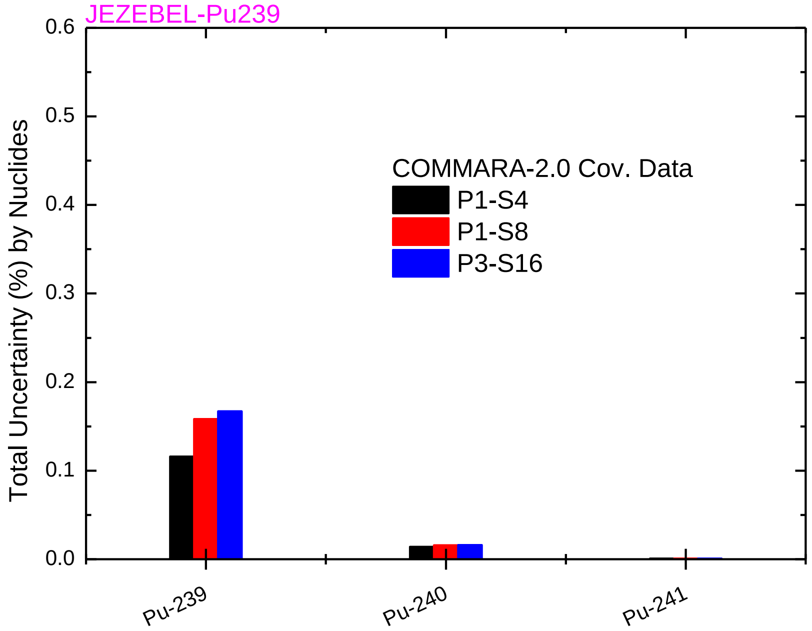
JEZEBEL-Pu239

< by Nuclides >

JENDL-4.0



COMMARA-2.0



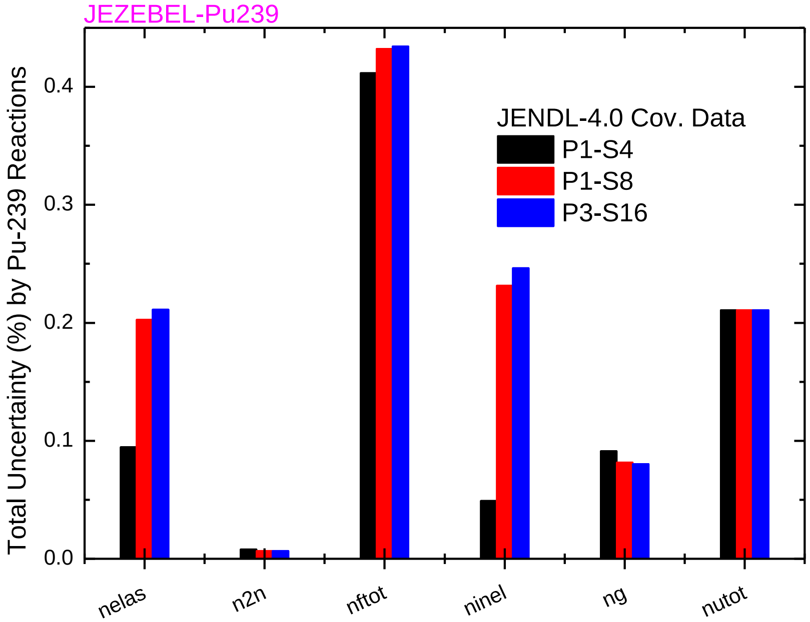
JENDL-4.0 vs. COMMARA-2.0

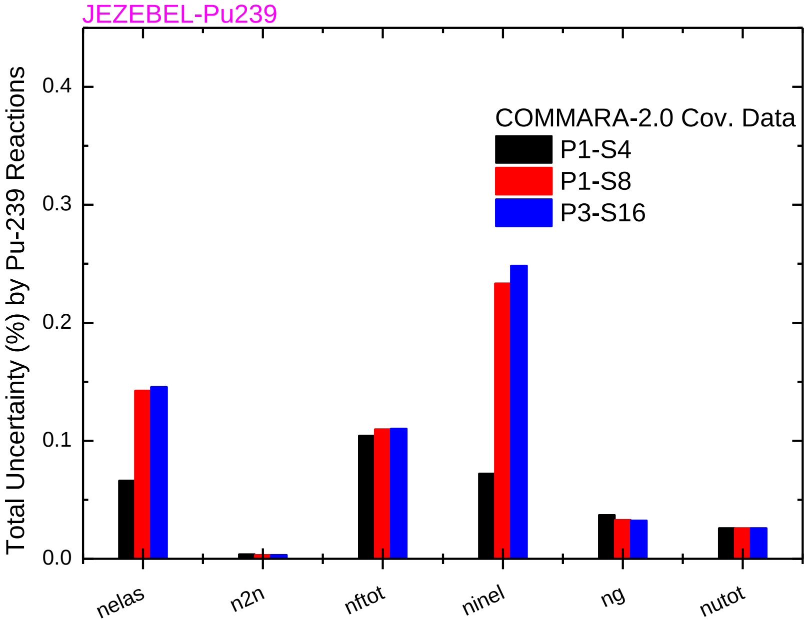
✓mainly brought about by contribution of Pu-239

< by Reactions of Pu-239 >

JENDL-4.0

COMMARA-2.0





JENDL-4.0 vs. COMMARA-2.0

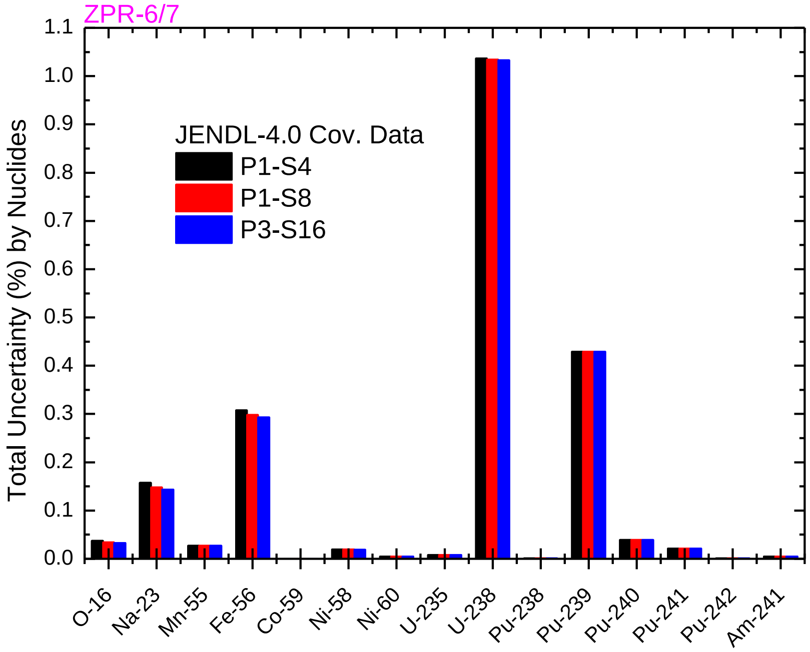
✓larger differences in fission & nutot contributions

✓significant changes in elastic & inelastic scattering contributions of S8 & S16 results against S4 results

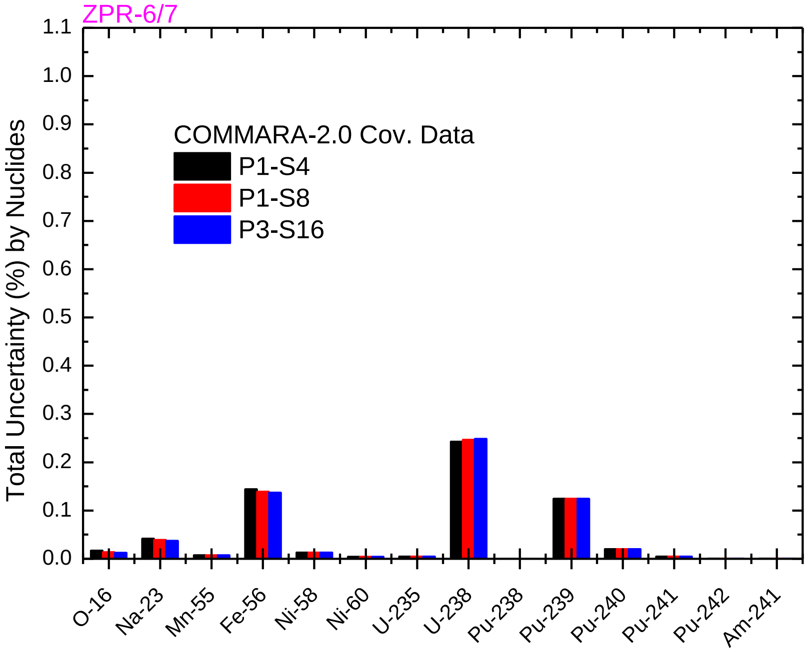
ZPR-6/7

< by Nuclides >

JENDL-4.0



COMMARA-2.0

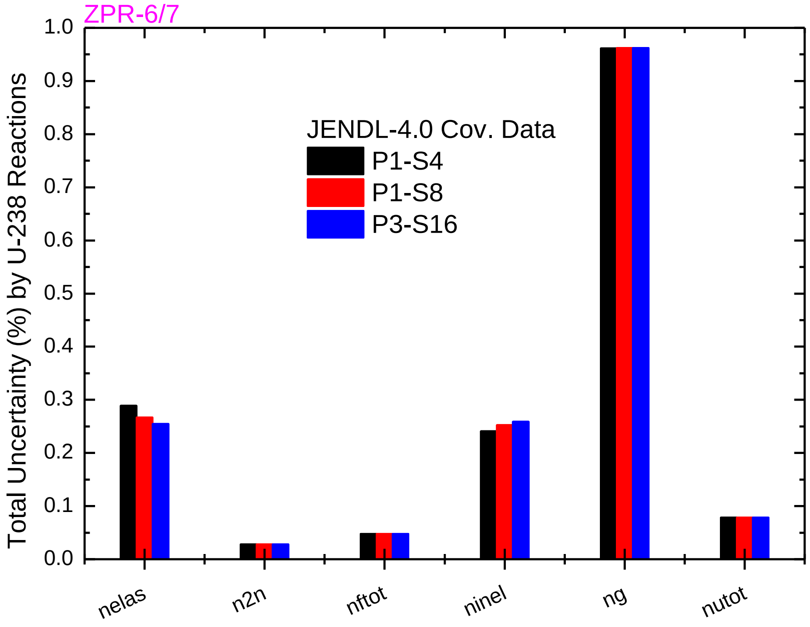


JENDL-4.0 vs. COMMARA-2.0

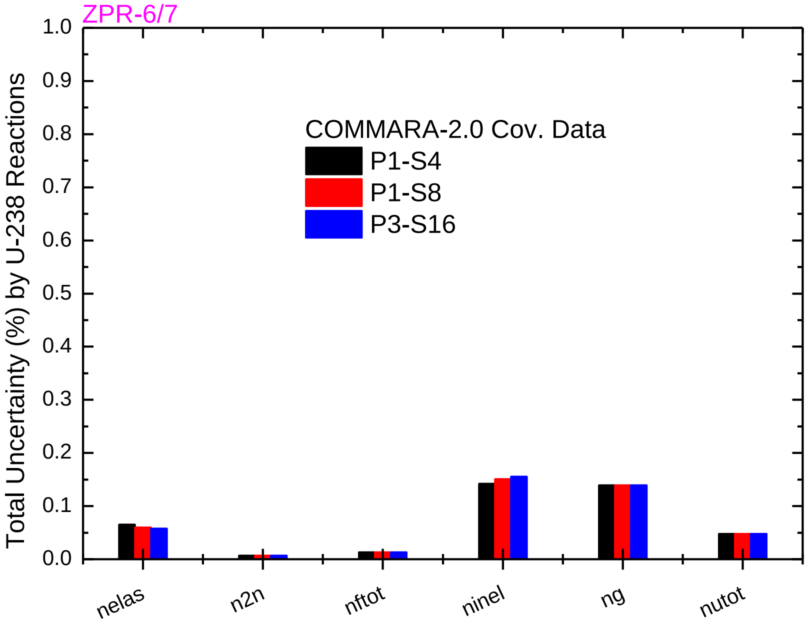
✓mainly brought about by contribution of U-238, Pu-239, Fe-56, and Na-23

< by Reactions of U-238 >

JENDL-4.0



COMMARA-2.0



JENDL-4.0 vs. COMMARA-2.0

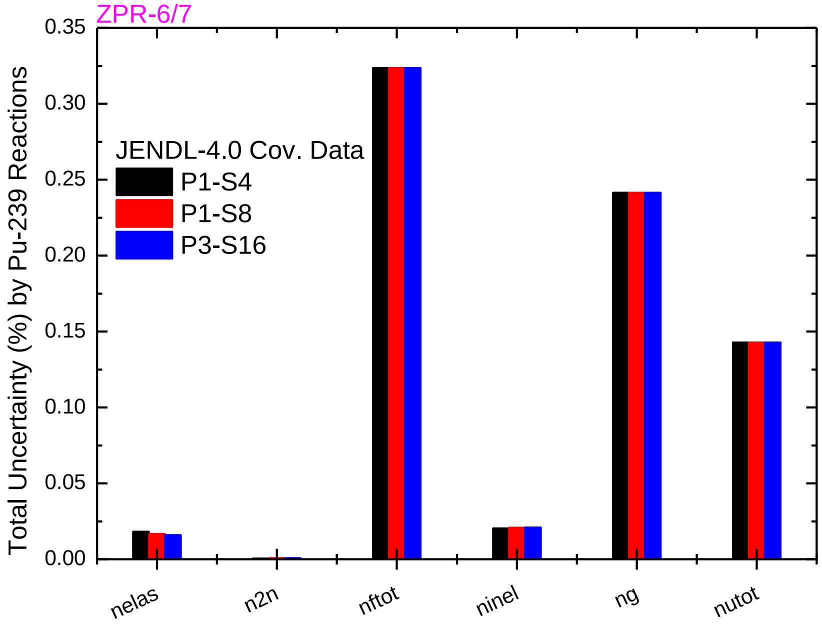
✓extremely large U-238 capture contributions for JENDL-4.0

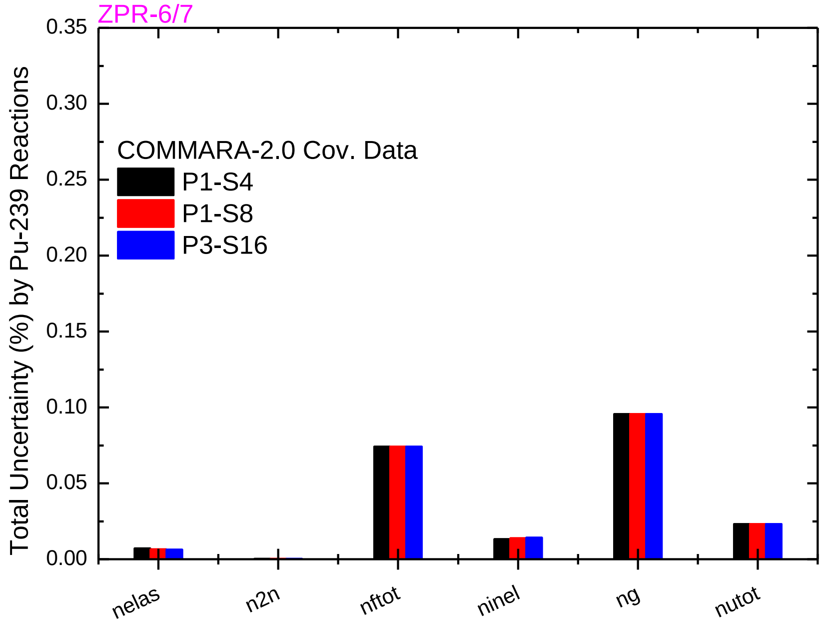
✓slight changes in elastic & inelastic scattering contributions among S4, S8, & S16 results

< by Reactions of Pu-239 >

JENDL-4.0

COMMARA-2.0



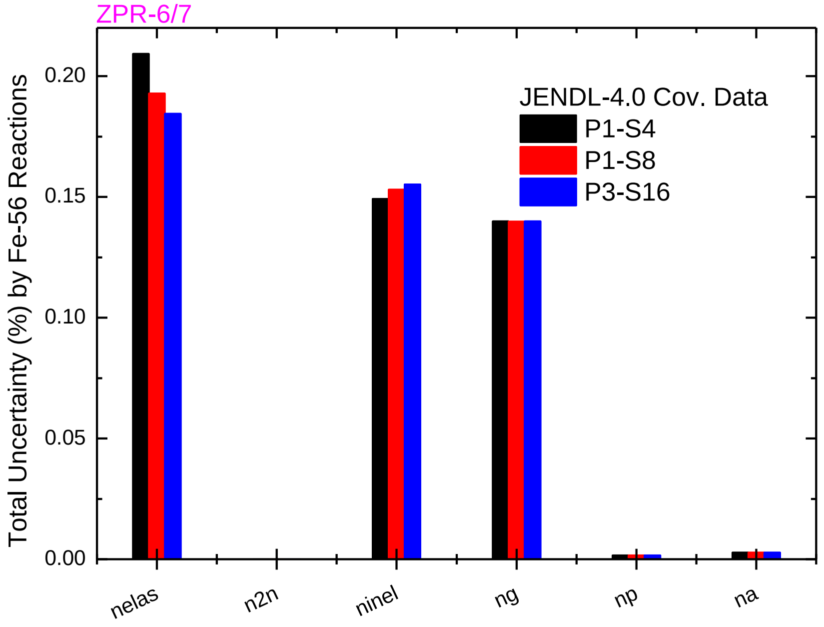


JENDL-4.0 vs. COMMARA-2.0

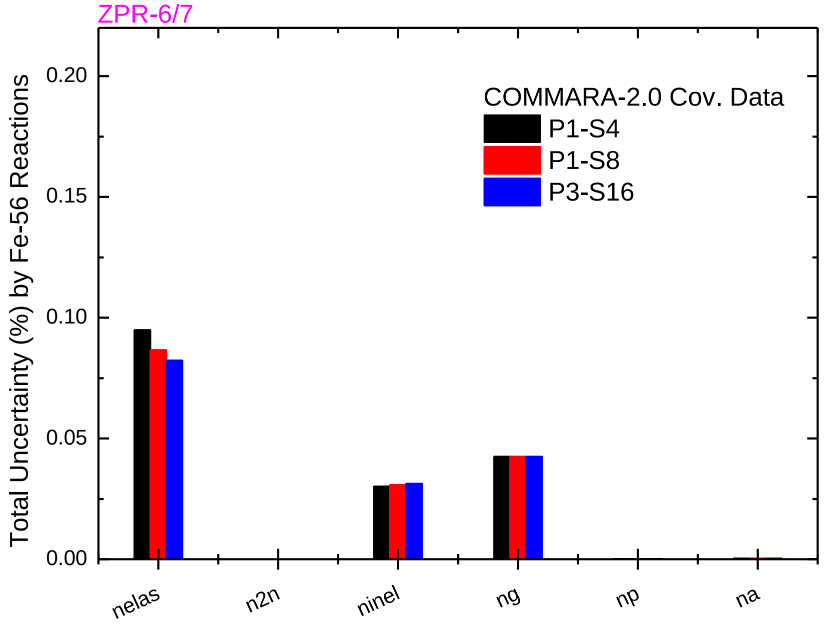
✓larger differences in Pu-239 fission, capture, & nutot contributions

< by Reactions of Fe-56 >

JENDL-4.0



COMMARA-2.0

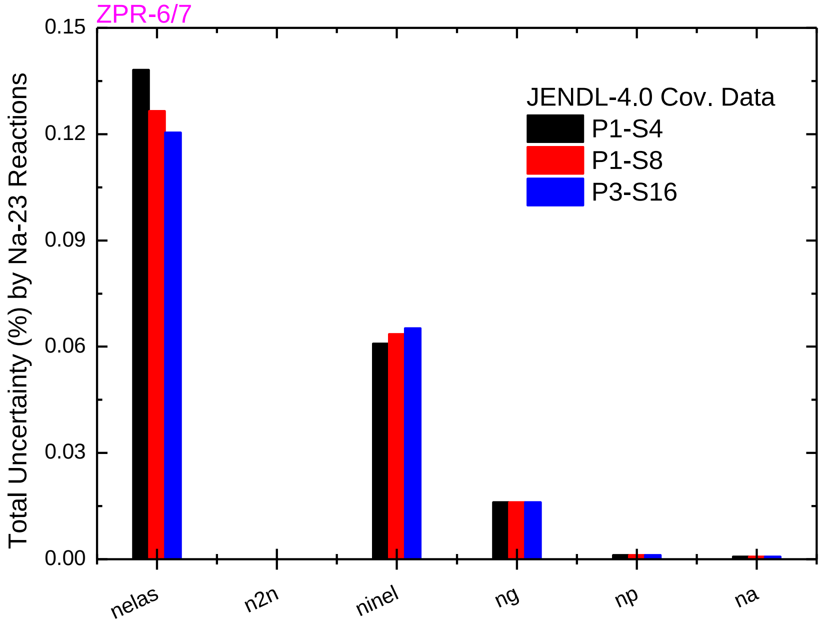


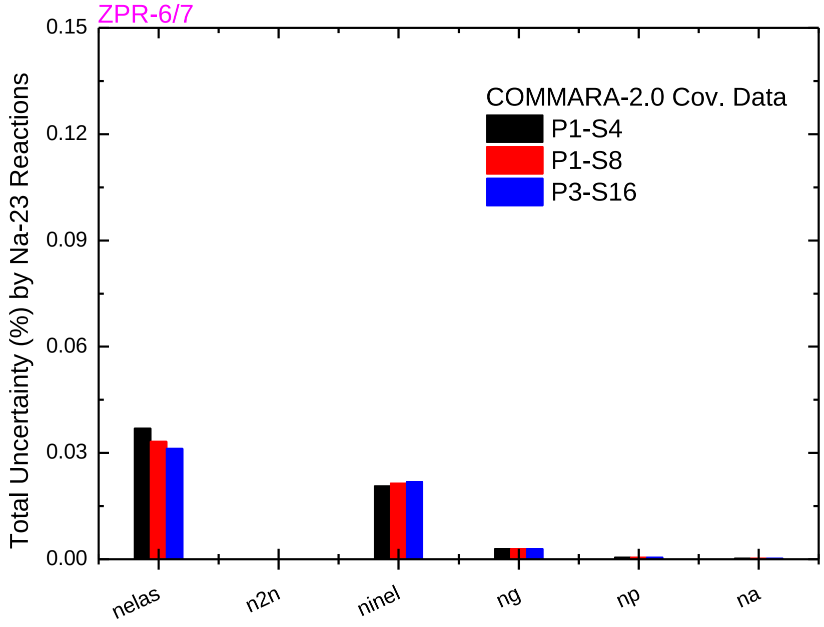
JENDL-4.0 vs. COMMARA-2.0

✓larger differences in Fe-56 elastic & inelastic scattering and capture contributions

< by Reactions of Na-23 >

JENDL-4.0	COMMARA-2.0



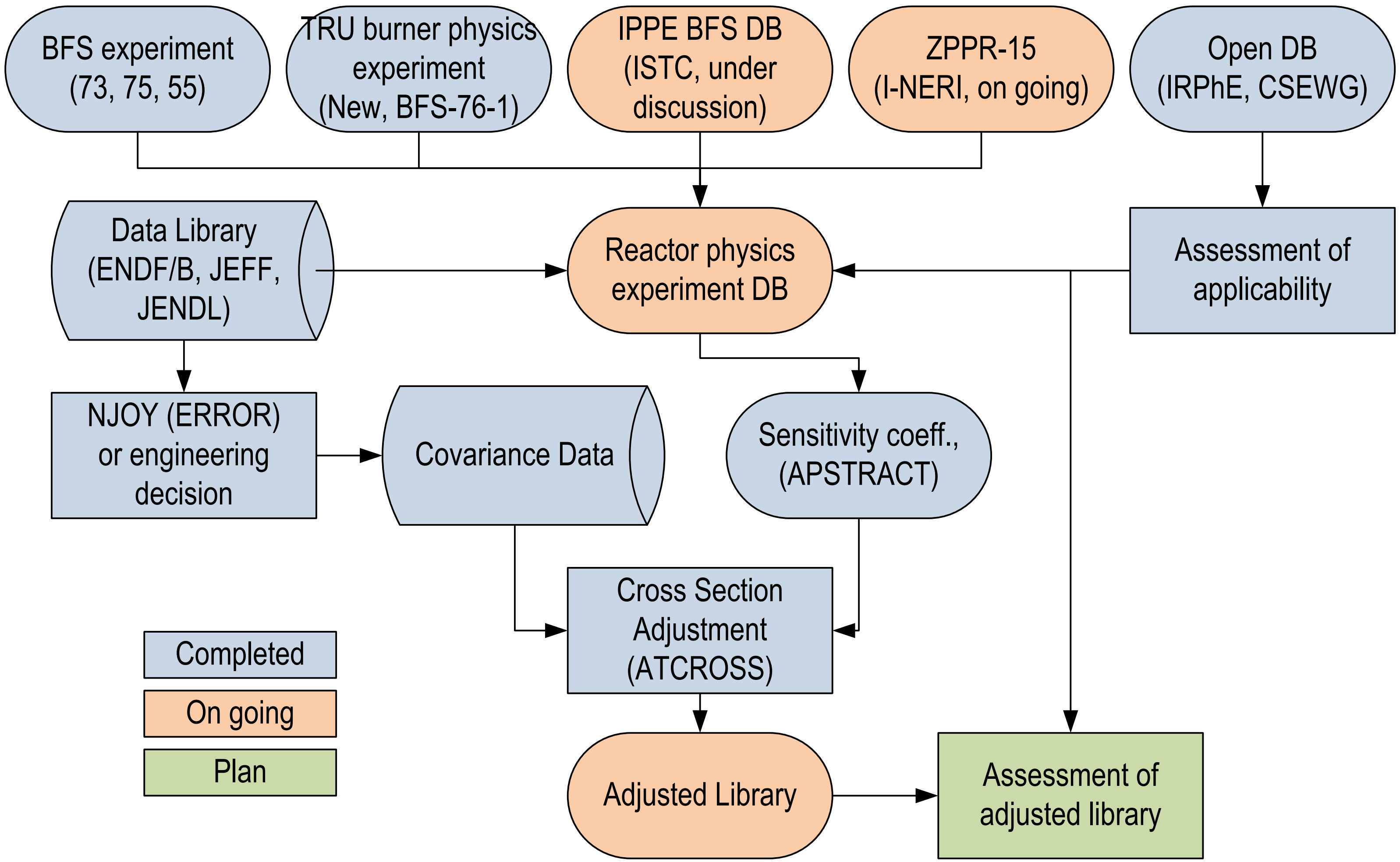


JENDL-4.0 vs. COMMARA-2.0

✓larger differences in Na-23 elastic & inelastic scattering and capture contributions

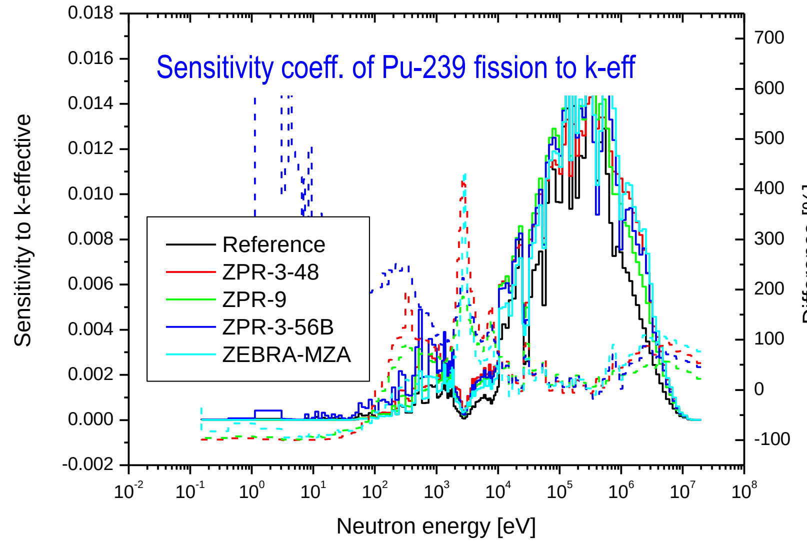
III. Status of V&V Activity at KAERI

Work flow of V&V activity



Development of sensitivity analysis code (APSTRACT)

- Using perturbation theory based S_N transport theory
  - Forward and adjoint flux from TWODANT calculation
  - Using self-shielded cross section in ISOTXS



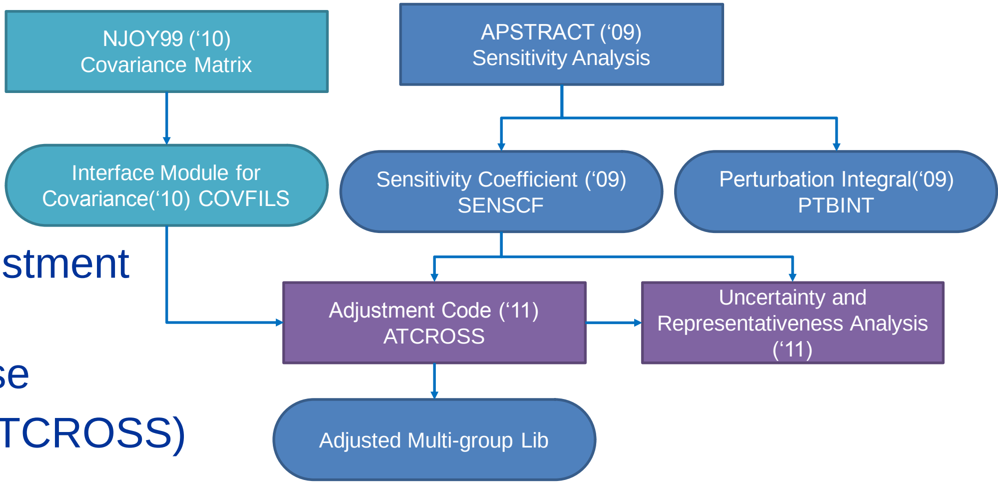
< Comparison of integral sensitivity coefficients of reactor physics exp. with reference core[1]>

		Ref. [1]	ZPR-3-48	ZPR-6-6A	ZPR-9	ZPR-3-56B	ZEBRA-MZA
Pu239	Fission	0.4382	0.5739	-	0.5659	0.5913	0.5569
	Nu	0.6192	0.8219	-	0.7859	0.8581	0.7830
	Capture	-0.0355	-0.0641	-	-0.0517	-0.0714	-0.0478
U238	Fission	0.0574	0.0849	0.0726	0.0953	0.0652	0.0624
	Nu	0.0981	0.1454	0.1198	0.1599	0.1065	0.1033
	Capture	-0.1509	-0.2051	-0.2667	-0.2302	-0.1638	-0.1292
PU241	Fission	0.0419	0.0094	-	0.0173	0.0187	0.0370
	Nu	0.0627	0.0138	-	0.0251	0.0276	0.0531
	Capture	-0.0167	-0.0043	-	-0.0072	-0.0102	-0.0123
Na	Capture	-0.0017	-0.0008	-0.0021	-0.0012	-0.0019	-0.0008
Fe	Capture	-0.0196	-0.0070	-0.0175	-0.0081	-0.0141	-0.0078

[1] Reference core represents the TRU burner core for which BFS-76-1 experiment was performed

Development of cross section adjustment technology

- Major Topics of Research
  - Requirement of cross section adjustment
  - Determination of target accuracy and selection of reactor physics experiment from open documents
- Methodology of adjustment
  - Generalized least square method
- Development of XS adjustment code (ATCROSS)
  - Interface with sensitivity analysis code
  - Interface with NJOY code for covariance (COVFILS format)
  - Uncertainty analysis and representativeness analysis
- Major Achievements and Further Utilization
  - Requirement of cross section adjustment
  - Selection of applicable physics experiment DB from open database
  - Cross section adjustment code (ATCROSS)
  - Utilization for producing adjusted multi-group library



IV. Summary

- Summary
  - Generation of MATXS-format cross section libraries based on ENDF/B-VII.0 and JENDL-4.0
  - Generation of COVFIL-format covariance libraries based on JENDL-4.0 and COMMARA-2.0
  - Calculation of integral parameters for 7 benchmark exercises of WPEC SG33
  - Estimation of nuclear data uncertainties to k-eff
- Future Works
  - GPT Routine Development
  - Adjustment Procedure Development