Processing of JEFF nuclear data libraries for the SCALE Code System

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1. Introduction

In the last years, a new version of the Joint Evaluated Fission and Fusion File (JEFF) data library, namely **JEFF-3.3**, has been released with relevant updated in the neutron reaction and the thermal neutron scattering sub-libraries.

Its application within SCALE system is a valued asset, enabling the use of JEFF state-of-the-art nuclear data libraries with the extensively tested and verified SCALE codes for nuclear analysis. Previous efforts set the first milestones and established the collaboration for the usage of JEFF libraries within SCALE.

Within the EU H2020 SANDA project and as a continuation of that work, **AMPX** is being used in order to process the continuous-energy (CE) JEFF-3.3 neutron library.

The processed library is verified and tested using a comprehensive set of benchmarks from ICSBEP.

C.J. Díez, F. Michel-Sendis, O. Cabellos, D. Wiarda, M.E. Dunn. "**On the processing of JEFF-3.2 neutron data library with AMPX 6.2 for its use with the SCALE tool suite**", EPJ Web of Conferences 111, 06003, 2016. https://doi.org/10.1051/epjconf/201611106003

2. JEFF-3.3 library

JEFF is an evaluated library produced via an international collaboration of NEA Data Bank participating countries. JEFF-3.3, which was officially released on November 20, 2017, is the latest outcome of that collaboration.

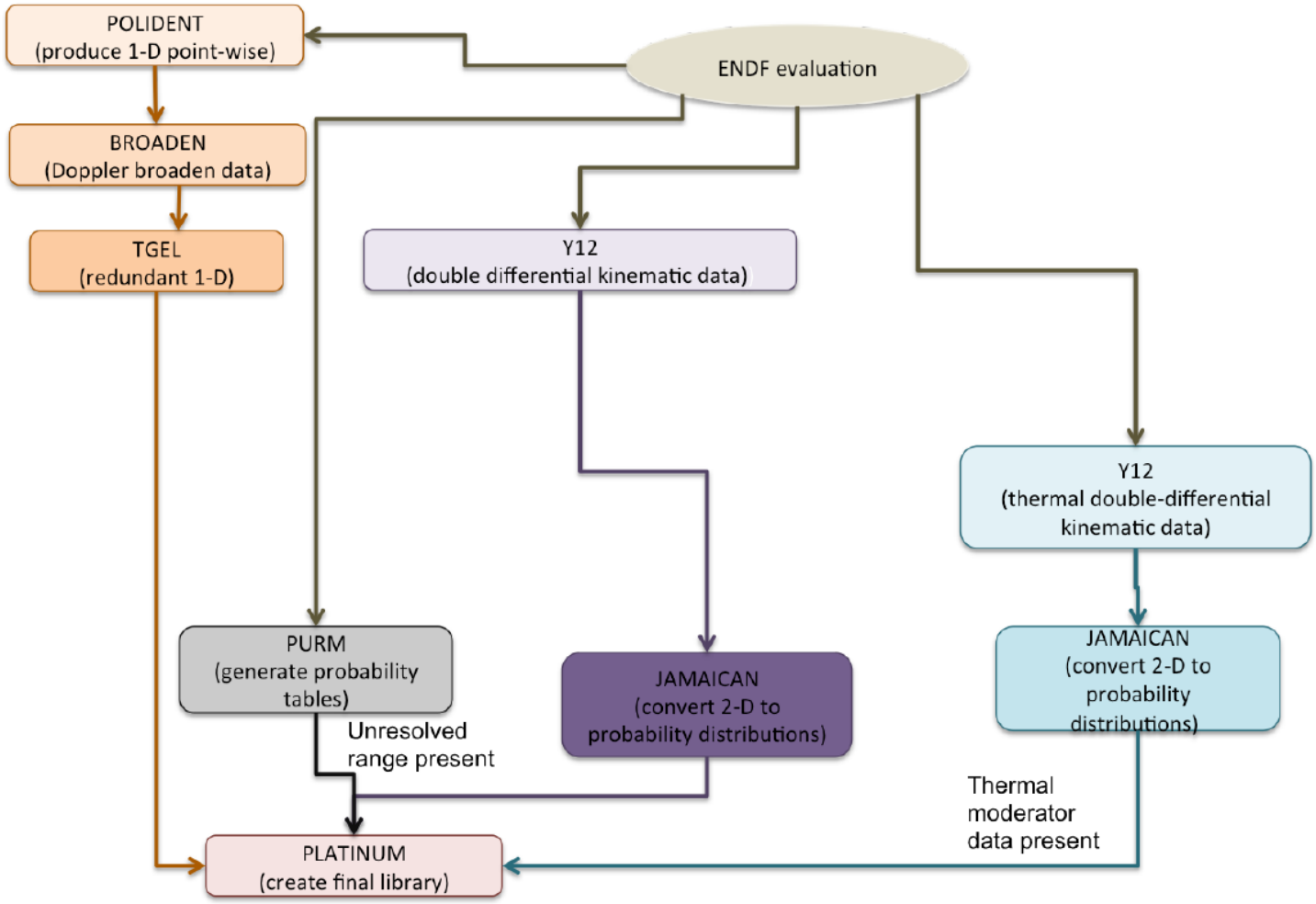
JEFF-3.3 includes new evaluations for neutron-induced interactions with the major actinides U-235, U-238 and Pu-239, on Am-241 and Na-23, Ni-59, Cr, Cu, Zr, Cd, Hf, W, Au, Pb and Bi.

- 562 incident neutron isotopic evaluations
- 20 evaluations for 20 compounds (TSL)

JEFF-3.3 library targeted the needs for the advanced reactors development programs since it contains updated evaluations for both sodium and lead.

A.J.M. Plompen, O. Cabellos, C. De Saint Jean, M. Fleming, et al. "**The joint evaluated fission and fusion nuclear data library, JEFF-3.3**", Eur. Phys. J. A., 56:181, 2020. https://doi.org/10.1140/epja/s10050-020-00141-9

3. Processing of CE libraries with AMPX



4. Testing with critical benchmark experiments

The processed library is tested, comparing k_{eff} from SCALE and MCNP, in a selection of 120 ICSBEP benchmarks.

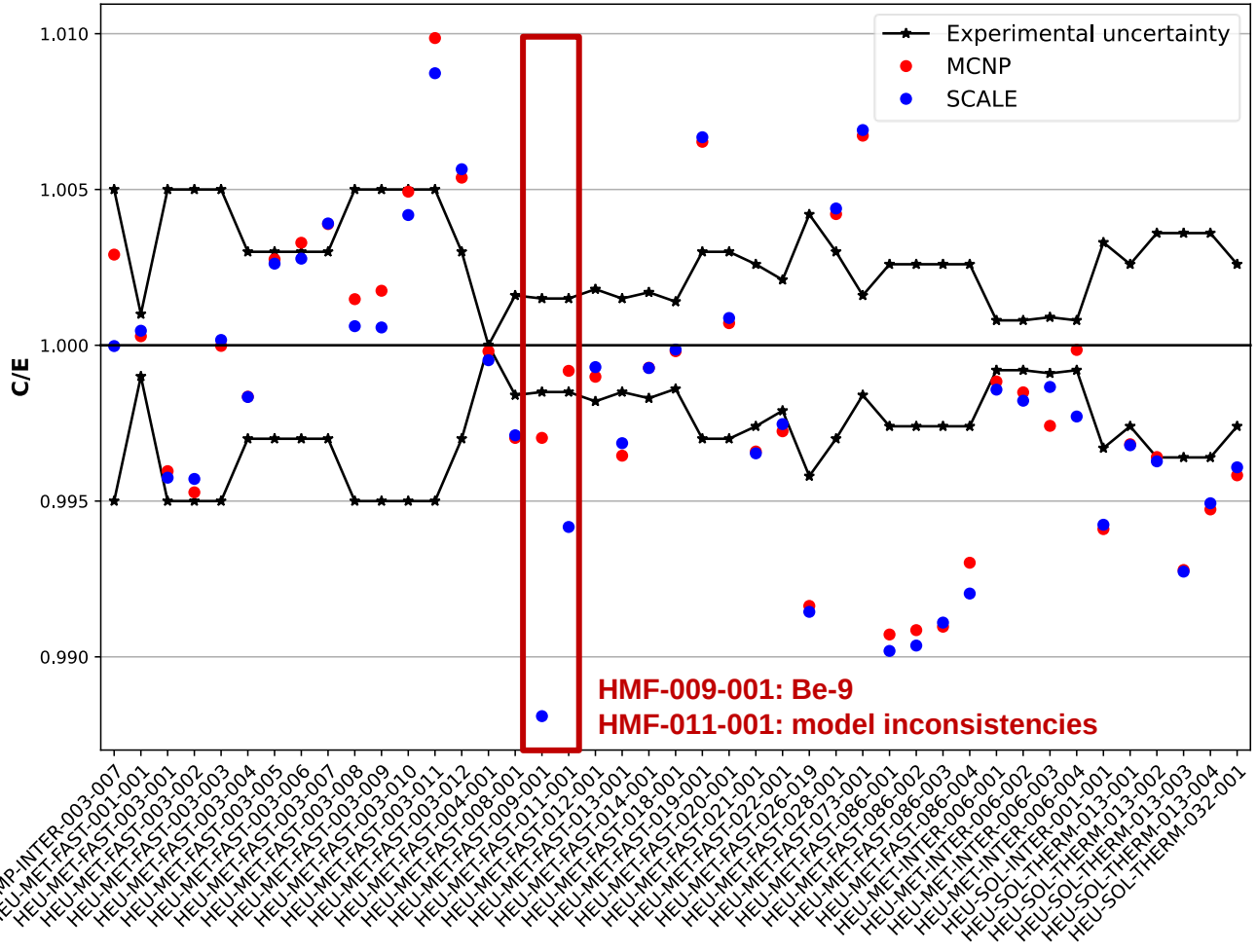
- 43 out of 102 HEU benchmarks*
- 10 out of 12 IEU benchmarks*
- 14 out of 159 LEU benchmarks*
- 8 out of 61 MIX benchmarks*
- 28 out of 93 PU benchmarks*
- 17 out of 190 U233 benchmarks*

Fuel	Number of benchmarks		
	Fast	Intermediate	Thermal
HEU	32	6	5
IEU	10	-	-
LEU	-	-	14
MIX	2	-	6
PU	17	-	11
U233	10	-	7
Total	**71**	**6**	**43**

*Benchmarks for which KENO inputs are available in VALID Suite

4. Testing with critical benchmark experiments

High-enriched uranium (HEU) benchmarks



4. Testing with critical benchmark experiments

Verification regarding the processing of Be-9

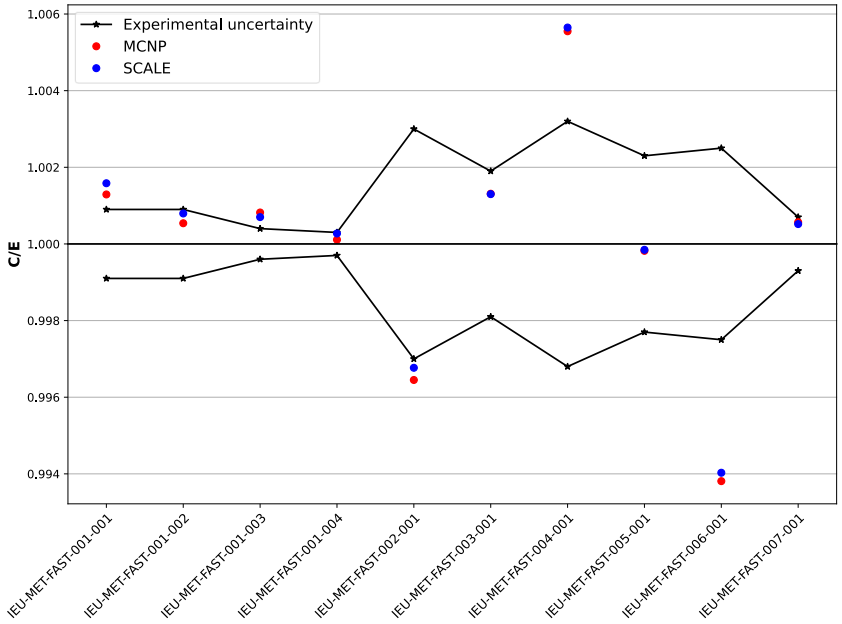
	Library	Code	keff	Dkeff	Δkeff (pcm)
U233-MET-FAST-005-001	JEFF-3.3-UPM	MCNP6.1	0.99721	0.00009	ref
	JEFF-3.3-UPM	SCALE	0.98472	0.00010	1249
	JEFF-3.3-UPM (Be-9 patch)	SCALE	0.99622	0.00010	99
	Library	**Code**	**keff**	**Dkeff**	**Δkeff (pcm)**
U233-MET-FAST-005-002	JEFF-3.3-UPM	MCNP6.1	0.99634	0.00009	ref
	JEFF-3.3-UPM	SCALE	0.97438	0.00010	2196
	JEFF-3.3-UPM (Be-9 patch)	SCALE	0.994692	0.00010	165
	Library	**Code**	**keff**	**Dkeff**	**Δkeff (pcm)**
U233-SOL-INTER-001-001	JEFF-3.3-UPM	MCNP6.1	0.98513	0.00015	ref
	JEFF-3.3-UPM	SCALE	0.93762	0.00013	4751
	JEFF-3.3-UPM (Be-9 patch)	SCALE	0.98198	0.00012	315

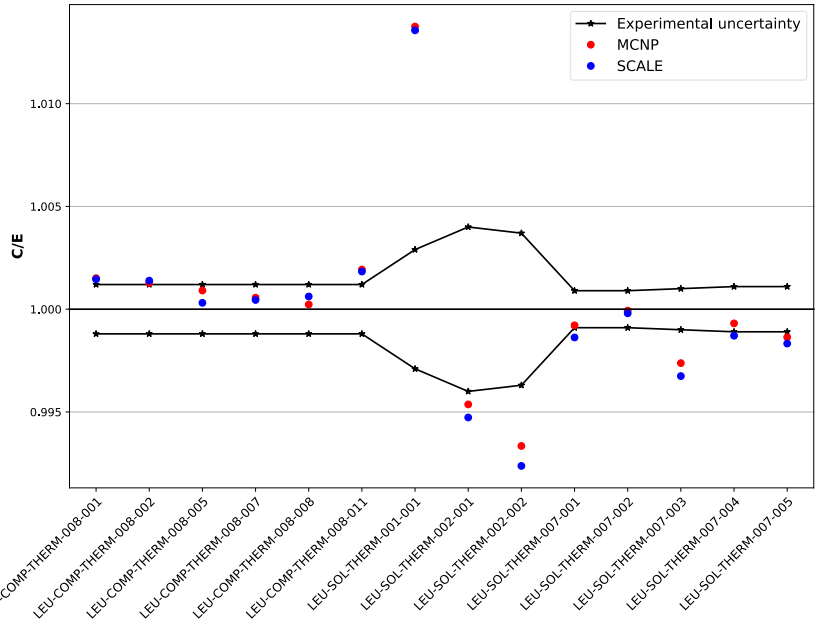
Large differences observed when Be-9 (or Be-9 in BeO) is involved. AMPX does not properly deal with MT875+ reaction channels.

4. Testing with critical benchmark experiments

Intermediate-enrichment uranium (IEU) benchmarks

Low-enriched, natural or depleted uranium (LEU) benchmarks

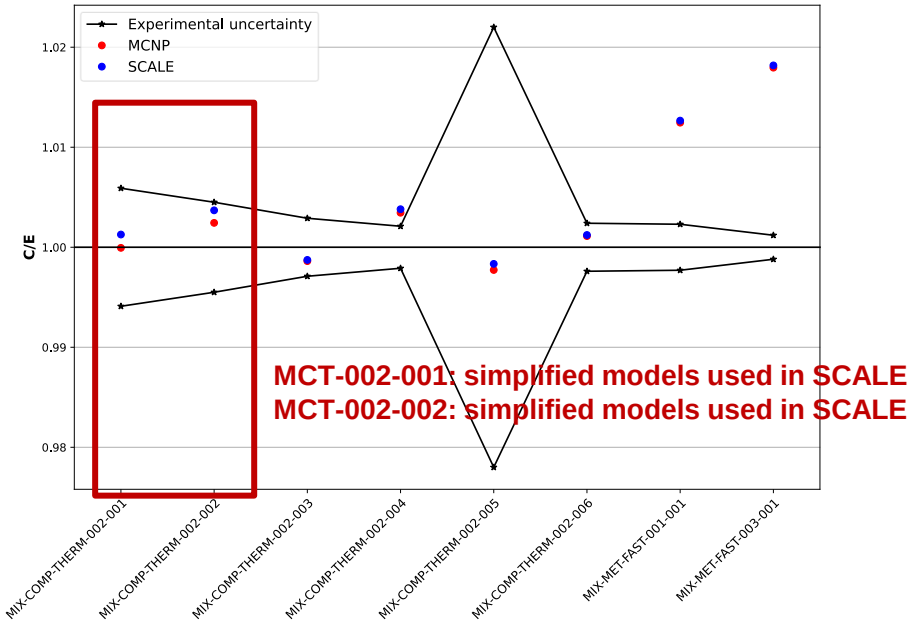


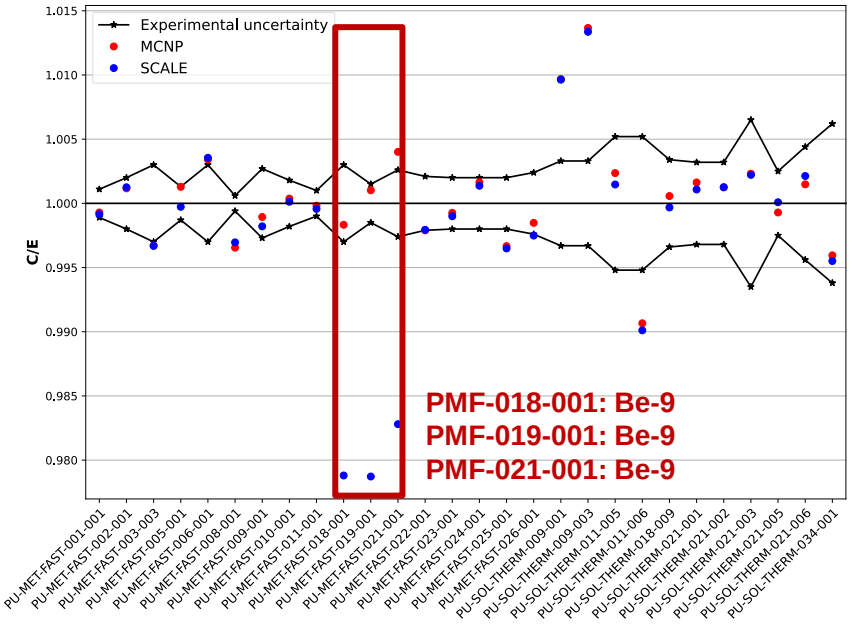


4. Testing with critical benchmark experiments

Mixed uranium and plutonium (MIX) benchmarks

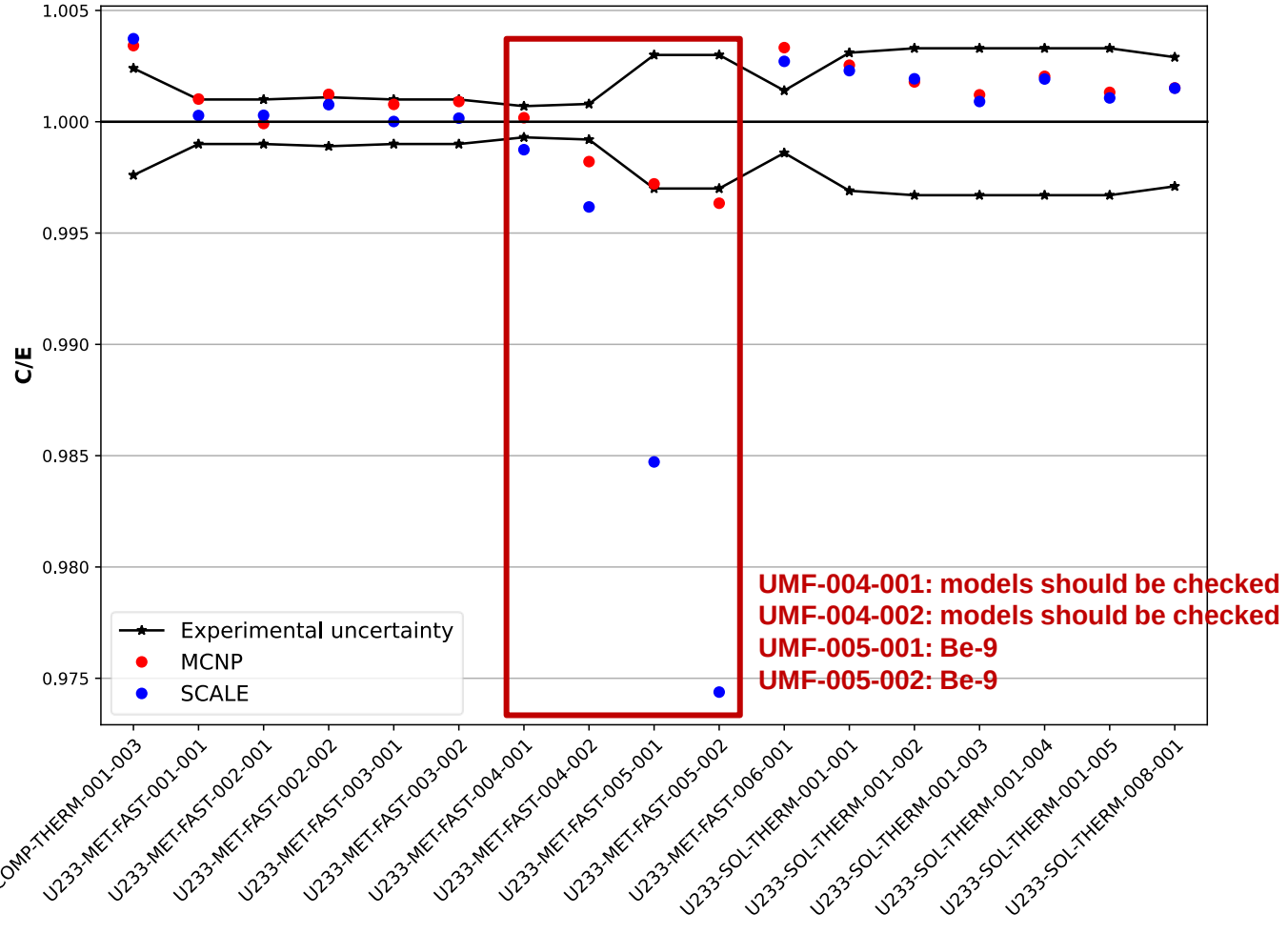
Plutonium (PU) benchmarks





4. Testing with critical benchmark experiments

U-233 (U233) benchmarks



5. Generating JEFF covariance libraries with AMPX

Recently, AMPX was also used to process associated covariance libraries of JEFF-3.3 library. PUFF is the main AMPX module to generate covariance matrices from ENDF files on the user-defined grid.

- Processing of JEFF-3.3 covariance library on 33 groups using a weighting spectrum appropriate for fast systems (IWT=8).
- Verification activities were performed for the ESFR (SANDA Project).

Quantity		$\Delta k_{eff}/k_{eff}$ (%)		
		TSUNAMI-3D + SAMS	MCNP + SUMMON	
			Result	*Ratio*
^{240}Pu (n,f)	^{240}Pu (n,f)	0.582 ± 8.40E-05	0.577 ± 5.93E-04	0.992 ± 1.03E-03
^{238}U (n,n')	^{238}U (n,n')	0.476 ± 1.79E-04	0.464 ± 4.23E-03	0.975 ± 8.90E-03
^{240}Pu (n,f)	^{240}Pu (n,γ)	-0.437 ± 2.02E-05	-0.438 ± 1.09E-04	1.002 ± 2.53E-04
^{239}Pu χ	^{239}Pu χ	0.427 ± 4.17E-04	0.426 ± 1.96E-03	0.997 ± 4.70E-03
^{238}U (n,n')	^{238}U (n,f)	-0.341 ± 5.51E-05	-0.345 ± 9.23E-04	1.014 ± 2.71E-03
^{239}Pu (n,f)	^{239}Pu (n,f)	0.313 ± 1.21E-05	0.313 ± 2.42E-04	0.999 ± 7.73E-04
^{239}Pu nubar	^{239}Pu nubar	0.296 ± 3.93E-06	0.296 ± 3.11E-05	0.998 ± 1.06E-03
^{238}U (n,γ)	^{238}U (n,γ)	0.293 ± 2.73E-06	0.291 ± 8.97E-05	0.995 ± 3.07E-04
^{238}U (n,n')	^{238}U (n,γ)	0.296 ± 7.42E-05	0.289 ± 1.31E-03	0.977 ± 4.42E-03
^{240}Pu (n,γ)	^{240}Pu (n,γ)	0.201 ± 7.20E-07	0.202 ± 2.24E-05	1.010 ± 1.12E-04

S. Panizo, V. Bécares, N. Leclaire, A. Jiménez-Carrascosa, N. García-Herranz, P. Romojaro, F. Álvarez-Velarde, O. Cabellos. "**Comparison of Sensitivity/Uncertainty analysis methodologies in the ESFR**", submitted to Spanish Nuclear Society Annual Meeting, Granada (Spain), 2021.

5. Conclusions and future work

- The JEFF-3.3 neutron cross section library has been processed with the AMPX version released in SCALE6.3b11. A CE library for neutrons is generated for its use with SCALE transport tools such as KENO-VI and MAVRIC-MONACO (of interest for criticality safety applications, reactor physics, etc).
- The generated CE library is tested in a selection of benchmarks from ICSBEP. A comparison of SCALE and MCNP results has been presented with a good agreement. However, inconsistencies were identified for certain isotopes.
- Associated covariance library was also generated and verified against NJOY-processed covariances matrices for fast systems. Further verification exercises are still required.
- The final goal is to release AMPX-formatted CE JEFF-3.3 and JEFF-3.1.1 libraries through the NEA/CPS.
- As next step, the generation of SCALE multi-group libraries with AMPX is highly interesting since they are widely used for a large variety of applications.

Thank you! Questions?

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3. Processing of CE libraries with AMPX (backup)

- 562 nuclides are processed with AMPX along with probability tables for 447 of these nuclides.
  - Negative cross section values found when reconstructing XS from resonance parameters (19 isotopes): Ag-108, Ar-40, As-74, As-77, Ce-137, Fe-54, Gd-151,152,157, Hg-203, La-137,140, Lu-173, Sc-46, Sr-90, Tb-158, Tl-202, V-49 and Yb-175.
  - Total resonance width given in the file differs from calculated for the same 19 isotopes.
  - The lower limit of the URR does not include in its range some unresolved resonance parameters (1 isotope): U-239
- Regarding TSL, data for H-1 in CaH_2, Ca in CaH_2 and Mg in Mg metal are not included since they do not have identification in SCALE.