

On the processing of JEFF-3.2 neutron data library with AMPX 6.2 for its use with the SCALE tool suite

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Abstract. New processing capabilities are under development at the NEA Data Bank (DB) that aim to provide enlarged and enhanced nuclear data services to member countries in the framework of processing, verification and benchmarking of evaluated nuclear data. Within the context of the Joint Evaluated Fission and Fusion Nuclear Data Library Project (JEFF), we undertake to generate, with the latest version of AMPX processing code, a JEFF-3.2 incident-neutron nuclear data application library for the SCALE tool suite. In this paper we describe the requirements, in terms of nuclear data content, for new data to be considered and used in the SCALE tool suite. An overview of how to process and prepare JEFF-3.2 incident-neutron data with AMPX for its application in SCALE neutron transport codes is given. The resulting library is verified and tested at differential and integral level by comparing the performance of JEFF-3.2 in AMPX format with other processing and transport codes.

1 Introduction

The OECD Nuclear Energy Agency (NEA) Data Bank (DB) is host to the Joint Evaluated Fission and Fusion (JEFF) Nuclear Data Library project since its creation in 1981. JEFF official releases of nuclear data are distributed in ENDF-6 format [1]. Historically, the DB has also made available processed versions of neutron cross section libraries in ACE (A Compact ENDF) format for use with Continuous Energy (CE) Monte Carlo codes such as MCNP5 [2]. These processed libraries are available upon request from NEA or freely accessible from the web, e.g. for the latest release of JEFF: JEFF-3.2 library [3].

In order to expand JEFF's user-base to include other widely used neutron transport codes, the DB has undertaken to process neutron data of JEFF-3.2, into application libraries for the SCALE tool suite [4], for criticality and shielding calculations. This task is possible thanks to the AMPX processing code release since SCALE6.2 β 3.

In this paper, we describe how JEFF-3.2 neutron data files are processed with AMPX into CE libraries. Problems encountered during processing are reported and, whenever possible, their implemented solutions. Verification tests and numerical benchmarks are performed to check correct usage of the resulting processed data. Finally, the performance of these CE libraries is assessed with a selection of criticality benchmarks used in MCNP6 validation [5].

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2 Processing evaluated cross section data

2.1 The JEFF-3.2 neutron library

The JEFF nuclear data library is a compilation of evaluated nuclear data files produced by a collaboration of Data Bank member countries which form the JEFF Project. The JEFF library consists in its diverse releases over the year of neutron and proton interaction data libraries, radioactive decay data libraries, fission yields, and thermal scattering law data libraries.

This work only addresses the treatment of JEFF-3.2 neutron data, which is the latest JEFF release of March 2014. The JEFF-3.2 neutron data library provides cross section data for 472 nuclides and thermal scattering libraries (TSL) for 9 different compounds in ENDF-6 formatted files.

2.2 Processing with AMPX

AMPX is a modular code system, developed by the Reactor and Nuclear Systems Division (RNSD) at Oak Ridge National Laboratory (ORNL), for processing ENDF-6 format evaluations into multi-group (MG) and CE cross sections using different formats that suit different particle transport codes.

In this paper, only how to generate CE cross section data is addressed. Such a task consists of generating the different parts of CE cross section data with the corresponding AMPX *module*:

- Point cross section data is the representation of cross section data as pairs of points (σ, E), cross section values at incident particle energy respectively, and linearly interpolating between two points for incident energies not represented. Contributions from the resonance region are added if present. The *Polident* module creates these point-wise data, reconstructing cross section values from resonance parameters, while *Broaden* performs Doppler-broadening. *Tgel* keeps the consistency between partial and total reactions.
- Unresolved resonance data (if present) represents the energy region for incident particles where resonances are so closely spaced in energy that it is either impossible or impractical to "resolve" each resonance. As a result, unresolved resonance parameters are averaged as resolved resonance parameters over energy. They can be treated in a statistical way with Monte Carlo techniques, using the so-called "probability tables". *Purm* generates such probability tables from the Unresolved resonance parameters at different temperatures.
- Scattering kinematics store differential cross section data: outgoing energy particles and angles as a function of incident particle energy. *Y12* is used to generate kinematics data for neutron scattering and gamma-production scattering, producing double-differential data, while *Jamaican* converts the double differential point-wise distributions into marginal probability distributions in angle and conditional probability distributions in exit energy. The same codes are used for processing thermal scattering libraries.

An additional module, *Platinum*, is required for merging all the parts into final CE libraries.

2.3 Processing JEFF-3.2 cross section data with AMPX

The JEFF-3.2 cross section data is processed with AMPX into CE libraries and TSL for their use in SCALE transport codes. Files for ^{49}V and ^{13}C are not considered as long as cross section files for natural isotopic compositions are given, ^{nat}V and ^{nat}C correspondingly. Regarding TSL, data for ^1H in CaH_2 , Ca in CaH_2 and Mg in Mg metal are not processed as long as the presented bound states have not been considered nor included yet in SCALE.

Different issues arise during processing which should be reviewed, and then, communicated to evaluators if necessary:

- Negative cross section values found when reconstructing cross sections from resonance parameters (12 isotopes): ^{40}Ar , ^{141}Ce , ^{54}Fe , $^{152,157}\text{Gd}$, ^{22}Na , ^{128}Te , $^{46,49,50}\text{Ti}$, ^{89}Y and ^{90}Zr . Any negative cross section value obtained during reconstruction is set to zero.
- Total resonance width given in the file differs from calculated (3 isotopes): ^{141}Ce , ^{22}Na and ^{90}Zr .
- The lower limit of the Unresolved Resonance Range (URR) does not include in its range some unresolved resonance parameters given (1 isotope): ^{239}U . Parameters are interpolated in order to have values within the boundaries of URR when processed with AMPX.
- Sampling negative cross sections when generating probability tables (1 isotope): ^{22}Na . It is not considered further in this work.

3 Verifying the processed CE libraries from JEFF-3.2

By verification, we mean that CE libraries generated can be used in the SCALE tool suite, and their performance in test cases are comparable with results from other codes/applications. Two different test cases are used for this purpose.

3.1 Infinite dilution calculations

They consist of criticality (k_{eff}) calculations of an infinite dilution of fissionable material (^{235}U as default) in a solution of the nuclide whose CE data is tested. Their results show that all CE libraries generated can be used except for two isotopes: ^{152m}Eu and ^{131m}Te . They have not yet been implemented in SCALE, in the modules where compositions and density mixtures are calculated. For the rest, the generated CE libraries successfully pass this test.

3.2 Transmission calculations

They consist in a mono-energetic and mono-directional neutron beam which impinges perpendicularly onto a slab of 25x25x5 cm of the nuclide to test, tallying the neutron spectrum behind the slab in a 2x2x2 cm cube situated 1.5 cm away from the slab (between the slab rear face and the cube's nearest face to the slab). The neutron energies used range from 14.0155 MeV to 0.1125 eV. Fission events are not considered in these calculations.

The total neutron flux observed in the volume tally is compared between MCNP5 [2], using cross section data processed with NJOY2012 [6], and SCALE. Due to issues arising during calculations, the isotopes (76 in total) in Table 1 were not assessed.

For the rest, differences larger than 10% are registered for 152 isotopes (see Table 1) when the statistical uncertainty associated with results is smaller than 10%. No discrepancies are found for incident neutrons at 0.1125 eV. Without probability tables, the number of isotopes with discrepancies decreases to 17 isotopes: 5 falling within statistical uncertainty, while the rest have different issues presented in Table 2.

Differences due to usage of probability tables come from the different handling of cross sections in URR during processing, where AMPX calculates values at the energy of reference and then interpolates on cross section to add additional points if needed, while NJOY calculates at the energy of reference and then interpolates on URR resonance parameters. The ENDF-6 manual says interpolation should be done on cross section. For isotopes whose cross sections are reconstructed from URR parameters, this could lead to differences between NJOY and AMPX. Also, MCNP and SCALE use probability tables in slightly different ways, especially while re-sampling cross sections in that range. In addition, differences can come from scattering data, when incident neutron energies are close to reaction thresholds which use Kalbach-Mann representation [1].

Table 1. Isotopes with differences between SCALE and MCNP larger than 10% in total neutron flux tallied in the cubic volume behind the slab for different mono-energetic neutron beams transmission calculations, not considering fission reactions. Below, those isotopes which could not be compared.

¹⁰⁷ Ag	^{110m1} Ag	^{242m1} Am	³⁶ Ar	³⁸ Ar	¹⁹⁷ Au	¹⁰ B	¹³⁰ Ba	¹³² Ba	¹³³ Ba	¹³⁵ Ba
⁹ Be	²⁴⁷ Bk	²⁴⁹ Bk	¹⁰⁶ Cd	¹⁰⁸ Cd	¹¹⁰ Cd	¹¹¹ Cd	¹¹² Cd	¹¹⁴ Cd	¹³⁶ Ce	¹³⁸ Ce
¹³⁹ Ce	¹⁴³ Ce	¹⁴⁴ Ce	²⁴⁹ Cf	²⁵⁰ Cf	²⁵¹ Cf	²⁵² Cf	²⁴² Cm	²⁴⁶ Cm	²⁴⁷ Cm	²⁴⁸ Cm
²⁵⁰ Cm	¹³³ Cs	¹³⁵ Cs	¹³⁷ Cs	¹⁵⁶ Dy	¹⁵⁸ Dy	¹⁶⁰ Dy	¹⁶¹ Dy	¹⁶² Dy	¹⁶³ Dy	¹⁶⁴ Dy
²⁵³ Es	¹⁵¹ Eu	¹⁵² Eu	¹⁵³ Eu	¹⁵⁴ Eu	¹⁵⁵ Eu	¹⁵⁶ Eu	¹⁵⁷ Eu	⁵⁸ Fe	⁶⁹ Ga	⁷¹ Ga
¹⁵² Gd	¹⁵³ Gd	¹⁵⁴ Gd	¹⁵⁵ Gd	¹⁵⁶ Gd	⁷⁰ Ge	⁷² Ge	⁷⁴ Ge	¹⁷⁴ Hf	¹⁷⁶ Hf	¹⁷⁷ Hf
¹⁷⁸ Hf	¹⁷⁹ Hf	¹⁸⁰ Hf	^{166m1} Ho	¹²⁷ I	¹³¹ I	¹¹³ In	¹⁹³ Ir	³⁹ K	⁷⁸ Kr	⁸⁰ Kr
⁸² Kr	⁸⁴ Kr	¹³⁸ La	¹⁴⁰ La	¹⁷⁶ Lu	⁵⁵ Mn	¹⁴³ Nd	¹⁴⁴ Nd	¹⁴⁵ Nd	¹⁴⁶ Nd	¹⁴⁷ Nd
¹⁴⁸ Nd	²³² Pa	¹⁰⁷ Pd	¹¹⁰ Pd	¹⁴⁷ Pm	¹⁴⁸ Pm	¹⁴⁹ Pm	¹⁵¹ Pm	¹⁴¹ Pr	¹⁴³ Pr	²³⁶ Pu
²³⁸ Pu	²²⁵ Ra	¹⁰⁵ Rh	¹⁰¹ Ru	³⁴ S	⁴⁵ Sc	⁷⁴ Se	⁷⁶ Se	⁷⁷ Se	⁷⁸ Se	⁸⁰ Se
⁸² Se	¹⁴⁴ Sm	¹⁴⁷ Sm	¹⁴⁸ Sm	¹⁴⁹ Sm	¹⁵⁰ Sm	¹⁵¹ Sm	¹⁵² Sm	¹⁵³ Sm	¹⁵⁴ Sm	¹¹² Sn
¹¹⁶ Sn	¹¹⁸ Sn	¹¹⁹ Sn	¹²² Sn	¹²⁴ Sn	⁸⁴ Sr	⁸⁶ Sr	⁸⁹ Sr	⁹⁰ Sr	¹⁸² Ta	¹⁶⁰ Tb
¹²² Te	¹²⁴ Te	¹⁷⁰ Tm	²⁴⁰ U	¹⁸² W	¹⁸³ W	¹⁸⁴ W	¹⁸⁶ W	¹²⁸ Xe	¹²⁹ Xe	¹³² Xe
¹³³ Xe	⁹¹ Y	⁶⁴ Zn	⁶⁶ Zn	⁶⁸ Zn	⁷⁰ Zn	⁹⁰ Zr	⁹² Zr	⁹⁴ Zr		

Failed to run in MCNP (x10):									
³¹ P	⁶² Ni	⁷⁶ Ge	¹⁰⁹ Ag	¹¹⁵ In	¹³⁴ Cs	¹⁶² Er	¹⁸⁷ Re	²³³ Th	²⁴² Am

Failed to run in SCALE (x66):										
³⁹ Ar	⁴¹ Ar	¹³⁹ Ba	⁴¹ Ca	⁴⁵ Ca	¹⁰⁹ Cd	³⁶ Cl	⁵⁷ Co	⁶⁰ Co	⁵¹ Cr	⁶⁴ Cu
⁶⁶ Cu	¹⁶⁵ Dy	¹⁶⁹ Er	¹⁷¹ Er	¹⁷² Er	¹⁴⁸ Gd	¹⁶¹ Gd	¹⁸¹ Hf	¹²⁶ I	¹²⁸ I	¹⁹² Ir
¹⁷⁷ Lu	²⁷ Mg	⁵³ Mn	⁵⁴ Mn	²⁰ Ne	²¹ Ne	²² Ne	⁶³ Ni	¹⁸ O	¹⁸⁴ Os	¹⁸⁶ Os
²⁰⁵ Pb	²⁰⁹ Po	¹⁹⁰ Pt	¹⁹² Pt	¹⁸⁷ Os	¹⁸⁸ Os	¹⁸⁹ Os	¹⁹⁰ Os	¹⁹¹ Os	¹⁹² Os	¹⁹³ Os
¹⁹⁴ Pt	¹⁹⁵ Pt	¹⁹⁶ Pt	¹⁹⁸ Pt	⁸⁸ Rb	¹⁸⁸ Re	¹⁰⁴ Rh	⁴⁶ Sc	³¹ Si	³² Si	^{180m1} Ta
⁹⁸ Tc	²⁰⁴ Tl	¹⁷¹ Tm	¹⁶⁸ Yb	¹⁶⁹ Yb	¹⁷⁰ Yb	¹⁷¹ Yb	¹⁷² Yb	¹⁷³ Yb	¹⁷⁴ Yb	¹⁷⁶ Yb

Table 2. Summary of sources for issues on isotopes in Table 1 when probably tables are not used.

Isotope	Energy	Region	Issue
¹⁰⁷ Ag	1.10 keV	RRR → Fast	Different amount of interpolation points in AMPX and NJOY
¹⁹⁷ Au	9.86 keV	URR	AMPX issue using scattering radius as function of energy (corrected)
⁹ Be	> 3.87 MeV	-	AMPX cannot handle (n,2n + excited residual) reactions (MT875+)
²⁴⁷ Bk	1.10 keV	RRR → Fast	Different amount of interpolation points in AMPX and NJOY
²⁵³ Es	90.1 eV	RRR	Discrepancies in RRR reconstruction, difference within statistical uncertainty
¹⁵⁴ Gd	9.86 keV	URR	AMPX and NJOY generate different average cross section values in URR
¹⁴⁷ Nd	1.10 keV	URR	AMPX and NJOY generate different average cross section values in URR
²³⁶ Pu	90.1 eV	URR	AMPX and NJOY generate different average cross section values in URR
²²⁵ Ra	90.1 eV	10 - 100 eV	Integral cross section value differs 0.6% and close to statistical uncertainty
⁴⁵ Sc	104 keV	-	ENDF-6 evaluation provides two cross section values at 100 keV
¹⁵⁰ Sm	2.94 MeV	Fast	Origin not found (probable issue with differential cross section)
⁹⁰ Zr	104 keV	RRR	Different treatment of total width in RRR between AMPX and NJOY

4 Benchmarking the processed CE libraries from JEFF-3.2 for criticality

The processed libraries are benchmarked, comparing k_{eff} from SCALE6.2b3 and MCNP6.1 results [7]. The benchmarks to calculate are selected, due to input availability in both codes, from those in the criticality validation suite for MCNP6 [5], shown in Table 3 using the ICSBEP identifiers [8].

Results are presented in Table 3, marked in grey those cases where SCALE and MCNP k_{eff} values differ more than 60 pcm. The source of differences for the highlighted cases are discussed:

- HEU-COMP-INTER-003-006 (82 pcm) whose difference comes partially from ^{197}Au , due to differences in reconstruction of ^{197}Au cross sections in URR. However, not including ^{197}Au in calculations yields a difference between MCNP and SCALE of 154 pcm, so the equivalence of MCNP and SCALE models shall be checked.
- HEU-MET-FAST-026-021 (93 pcm) has differences between in MCNP and SCALE models, such as the amount of paraffin. Once equaled, the difference increases up to 343 pcm. Model representations in both cases shall be reviewed.
- U233-COMP-THERM-001-003 (204 pcm) has ^{90}Zr in its composition, for which large discrepancies have been observed in transmission tests. It has a large impact in k_{eff} as seen from sensitivity analysis, so when it is not included in calculations, differences are reduced to 23 pcm.
- U233-MET-FAST-005-002 (2210 pcm) is a ^{233}U sphere reflected by ^9Be which involves fast neutron spectrum. As seen in transmission cases, large differences will be encountered using ^9Be due to issues in handling MT875+ reaction channels with AMPX.

Therefore, despite HEU-COMP-INTER-003-006 and HEU-MET-FAST-026-021 cases where equivalence between MCNP and SCALE models shall be reviewed, a good agreement is achieved between MCNP and SCALE processing the JEFF-3.2 neutron cross section libraries with AMPX and NJOY.

Table 3. Results for k_{eff} in criticality benchmarks using SCALE6.2b3 and MCNP6.1, marked in grey are those with differences between MCNP and SCALE larger than 60 pcm.

Identifier	Experiments		MCNP6.1		SCALE6.2b3		Diff. (pcm)
	k_{eff}	unc.	k_{eff}	unc.	k_{eff}	unc.	
HEU-COMP-INTER-003-006	1.00000	0.00470	0.99793	0.00003	0.99875	0.000027	-82
HEU-MET-FAST-026-021	1.00000	0.00380	0.99885	0.00002	0.99792	0.000099	93
HEU-MET-FAST-028-001	1.00000	0.00300	1.00502	0.00002	1.00539	0.000035	-37
HEU-SOL-THERM-032-001	1.00150	0.00260	0.99903	0.00002	0.99908	0.000041	-5
IEU-MET-FAST-003-001 (Detailed)	1.00000	0.00170	1.00245	0.00002	1.00289	0.000099	-44
IEU-MET-FAST-004-001 (Detailed)	1.00000	0.00300	1.00705	0.00002	1.00748	0.000091	-43
LEU-COMP-THERM-008-002	1.00070	0.00120	1.00069	0.00005	1.00019	0.00005	50
LEU-SOL-THERM-002-002	1.00240	0.00370	0.99618	0.00002	0.99582	0.000099	36
LEU-SOL-THERM-007-004	0.99880	0.00110	0.99898	0.00002	0.99838	0.000043	60
MIX-COMP-THERM-002-004	1.00240	0.00240	1.00679	0.00002	1.00693	0.000097	-14
PU-COMP-INTER-001-001	1.00000	0.01100	1.00603	0.00002	1.00612	0.000073	-9
PU-MET-FAST-001-001 (Detailed)	0.99999	0.00129	1.00021	0.00002	1.00056	0.000029	-35
PU-MET-FAST-002-001	1.00000	0.00200	1.00258	0.00002	1.00296	0.000099	-38
PU-MET-FAST-003-003	1.00000	0.00300	0.99679	0.00002	0.99666	0.000063	13
PU-MET-FAST-006-001	1.00000	0.00300	1.00218	0.00002	1.00262	0.000099	-44
PU-MET-FAST-011-001	1.00000	0.00100	0.99786	0.00002	0.99795	0.00011	-9
U233-COMP-THERM-001-003	1.00000	0.00240	1.00288	0.00002	1.00493	0.0001	-204
U233-MET-FAST-001-001	1.00000	0.00100	0.99985	0.00002	1.00008	0.000099	-23
U233-MET-FAST-005-002	1.00000	0.00300	0.99515	0.00002	0.97363	0.000026	2210
U233-MET-FAST-006-001	1.00000	0.00140	1.0008	0.00002	1.00123	0.000049	-43

5 Conclusions

The JEFF-3.2 neutron cross section library has been processed with the AMPX version released in SCALE6.2b4. A continuous energy library for neutrons is generated for its use with SCALE transport calculations tools: KENO for criticality and MAVRIC-MONACO for shielding.

This work has identified different issues to address during the processing of JEFF-3.2 data with AMPX, which concern 17 isotopes (see Sec. 2.3). Those issues which are more relevant due to their impact in benchmarking are due to ^{22}Na and ^{90}Zr . Therefore, for these 17 isotopes, processing and evaluations shall be reviewed.

The verification of processed files is carried out by performing criticality calculations in infinite dilution cases and transmission tests. These tests show the need to implement the definition of some isotopes in SCALE: ^{152m}Eu , ^{180m}Ta and ^{131m}Te , as well as those marked in Table 1 for transmission tests. When comparing SCALE and MCNP results in transmissions tests, large differences were found for 150 isotopes (Table 1), due to a different treatment of the URR in processing and its usage in transport codes. The number of discrepant isotopes sharply decreases when probability tables are not used, where important differences are only found for 12 isotopes, with their likely issues being described in Table 2.

Finally, the generated CE library from JEFF-3.2 is used in a selection of benchmarks from the criticality validation suite for MCNP6. A comparison of SCALE and MCNP results is given. In general, a good agreement is obtained, within 60 pcm differences except for 4 cases. For 3 of these 4 cases, isotopes with large differences found in transmission tests are involved, such as ^{197}Au , ^9Be and ^{90}Zr . The differences found are however not completely explained, and would require the further review of both the MCNP and SCALE input models used.

Once the missing isotopes have been implemented in SCALE libraries, further study on transmission tests should be carried out with a wider selection of benchmarks in order to expand the application cases. Although, this latter work depends also in availability of inputs, for which checks on equivalence shall be carried out.

This work has focused on processing the entire JEFF-3.2 neutron data library with the AMPX version released in SCALE6.2b4. Although most of the evaluations are processed successfully, the goal of releasing the thoroughly processed CE library from JEFF-3.2 library for SCALE would still need some necessary actions and decisions to be taken and which concern the issues mentioned. Nevertheless, this work has set the first milestones and established a successful collaboration for the future usage of JEFF libraries within SCALE.

References

- [1] CSEWG, Tech. Rep. BNL-90365-2009 Rev.2, BNL (2012)
- [2] X-5 Monte Carlo Team, Tech. Rep. LA-CP-03-0245, LANL (2003), Version 5
- [3] OECD/NEA Data Bank, *JEFF-3.2 Evaluated Data Library - Neutron data* (2014), http://www.oecd-nea.org/dbforms/data/eva/evatapes/jeff_32/
- [4] ORNL, *SCALE: A comprehensive modeling and simulation suite for nuclear safety analysis and design* (2011), ORNL/TM-2005/39, Version 6.1
- [5] R.D. Mosteller, Tech. Rep. LA-UR-02-0878, LANL (2002)
- [6] R.E. MacFarlane, D.W. Muir, R.M. Boicourt, A.C. Kahler, Tech. Rep. LA-UR-12-27079, LANL (2015)
- [7] T. Goorley, M. James, T. Booth, F. Brown, J. Bull, L. Cox, J. Durkee, J. Elson, M. Fensin, R. Forster et al., *Nuclear Technology* **180**, 298 (2012)
- [8] J.B.B. editor, Tech. Rep. NEA/NSC/DOC(95)03, OECD Nuclear Energy Agency (2010)