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1 Introduction

The goal of this study is to compare the various libraries JEFF-3.3[1], TENDL-17[2] and ENDF/B-VIII[3] on a series of criticality benchmarks using identical processing method and various Monte Carlo simulations, TRIPOLI-4®[4] and MCNP[5] . In this document, the criticality calculations are performed with the Monte Carlo code TRIPOLI-4®.
TRIPOLI-4 is the fourth generation of the continuous-energy three-dimensional transport Monte Carlo code developed by the Service d'Études des Réacteurs et de Mathématiques Appliquées (SERMA) at CEA Saclay (FRANCE). TRIPOLI-4 is devoted to shielding, reactor physics with depletion, criticality safety and nuclear instrumentation for both fission and fusion systems. The code has been has been developed starting from the mid 90s in C++, with a few parts in C and Fortran. The latest release of TRIPOLI-4 is version 11, as of November 2018.

2 Nuclear Data Treatment

The three nuclear data libraries for neutron transport have been produced in a similar way with the nuclear data processing code NJOY2016.49[6] . The cross section files used by TRIPOLI-4 require the use of NJOY's RECONR and BROADR modules to produce "free gas" cross sections in PENDF files.

- RECONR : Reconstruction using linearization precision of 0.1%
- BROADR : Doppler broadening using 0.1% precision

TRIPOLI-4 code uses additional data produced from evaluation files. These data are generated and stored in ENDF-like files[10] the first time the TRIPOLI-4 code is used with the evaluation files. These files contain kinematic data of the particles coming out of the reactions induced by the incident particle (energetic and angular distributions for example). These files will be available for later use of the materials in various simulations, regardless of the temperature of the materials. Finally, the thermal scattering data (H1/H2O, H1/CH2, C/Graphite) are produced using the THERMR module of NJOY2016.49.

Probability tables The probability tables in the unresolved domain are produced by the CALENDF code [7]. This type of file is the one used since the 1980s. The probability tables are given in multigroup forms and not in point form as those produced by NJOY's PURR module. These probability tables cover the total, elastic and radiative capture, fission cross sections but also other reactions existing in the unresolved range (e. g. inelastic scattering in the case of U238).

2.1 Nuclear data corrections on evaluation files

The processing of these three libraries, JEFF-3.3, TENDL-17 and ENDF/B-VIII for the TRIPOLI-4 code implies the verification of nuclear data contained in evaluation files. Sometimes, corrections are required so that these files can be used with the TRIPOLI-4 code. To carry out the calculations presented later, many corrections have been made to a number of evaluation files of the nuclei present in the compositions of the benchmarks studied in this document.

JEFF-3.3 The JEFF-3.3 library released in November 2017 had been extensively tested in its beta versions. There are no major corrections required for use with TRIPOLI-4.

ENDF/B-VIII.0 The prompt fission neutron and gamma-ray multiplicity probabilities have been included for the first time in evaluation files in ENDF/B-VII library. The latest version of TRIPOLI-4 is able to read this evolution of the ENDF format. However, these data are not currently used in Monte Carlo TRIPOLI-4 simulations.
The CALENDF code is not capable to process energy-dependent scattering radius in the unresolved domain as it is the case for the U238 evaluation. We have imposed a constant scattering radius as it was the case in previous evaluations. The value used is 0.9295.
The first calculations made with TRIPOLI-4 using this library showed very significant differences with TRIPOLI-4 calculations with the ENDF/B-VII.1 library[8] and MCNP calculations with ENDF/B-VIII.0 for benchmarks that

contain Pu239. Figure 1 shows different results on a series of benchmarks containing Pu239:

- MCNP + ENDF/B-VII.1 in blue
- MCNP + ENDF/B-VIII in green
- TRIPOLI-4, version 10.2 + ENDF/B-VII.1 in black
- TRIPOLI-4, version 10.2 + ENDF/B-VIII in red

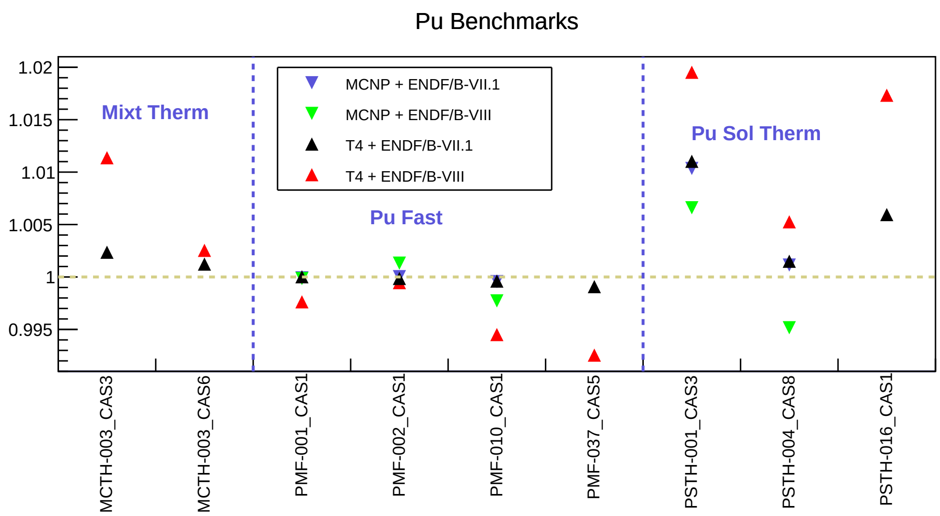

Figure 1: MCNP and TRIPOLI-4 k_{eff} calculations on a series of Pu benchmarks using ENDF/B-VII.1 and ENDF/B-VIII libraries

A very good agreement is obtained between the MCNP and TRIPOLI-4 results for the ENDF/B-VII.1 library (blue and black results). However, the change of library from ENDF/B-VII.1 to ENDF/B-VIII does not produce the same modifications for the MCNP and TRIPOLI-4 codes. The analysis of the modifications on the Pu239 nuclear data between the ENDF/B-VII.1 and ENDF/B-VIII evaluations shows that the total cross section (MF=3, MT=1) is not equal to the sum of the partial cross sections in the unresolved resonance range. The use of the LSSF=1 flag in this range implies that the probability tables must be normalized to the cross sections given in MF=3. CALENDF does not calculate correctly the probability tables if this legitimate equality is not verified. We have corrected the total cross section in the unresolved range and obtained the new results presented in Figure 2. The TRIPOLI-4 results obtained using this corrected evaluation file (black star) are in a very good agreement with the expected values and with the MCNP results.

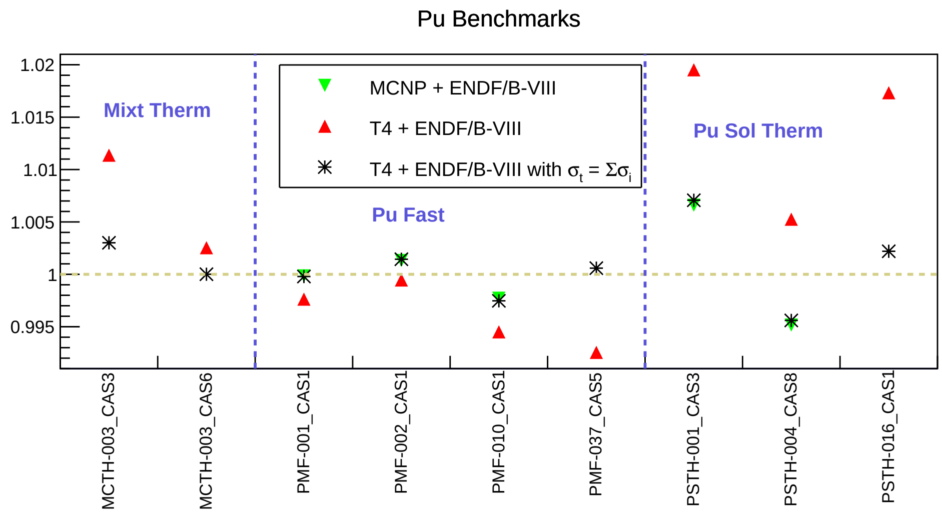

Figure 2: MCNP and TRIPOLI-4 calculations on a serie of Pu benchmarks using ENDF/B-VIII libraries

TENDL17 Corrections applied to the evaluation files U238 and Pu239 for the ENDF/B-VIII library were reported in TENDL17 evaluation files. In order to calculate all the ICSBEP configurations selected for this comparison, we had applied corrections to part of the library's evaluation files. These corrections concern the normalization of PFNS distributions for the following nuclei: Am241, Pu238, Pu240, Pu241, Pu242, U234 and U236.
Other nuclei could be concerned by this correction but they do not appear in the configurations studied in this report.

3 Criticality Benchmarks calculations

Several configurations from ICSBEP database[9] were studied with the three libraries ENDF/B-VIII, JEFF-3.3 and TENDL-17. Table 1 summarizes results for the list of benchmarks selected for this study. Table 2 presents additional results on a list of benchmarks generally used for library reviews performed with TRIPOLI-4. The blue results identify differences greater than or equal to 100 pcm between at least two libraries. The general trends of these three libraries are quite consistent.

4 Conclusion

The processing of the three libraries JEFF-3.3, ENDF/B-VIII and TENDL-17 for use with the Monte Carlo code TRIPOLI-4 gives the opportunity to test these libraries in similar conditions of use. We were able to identify deficiencies, for example for Pu239 of ENDF/B-VIII and TENDL-17, which were not systematically observed by other Monte Carlo codes coupled to their processing systems. The comparison of some benchmarks containing Plutonium shows the very good agreement between MCNP and TRIPOLI-4 with the same nuclear data libraries. Not surprisingly, the results obtained with the TENDL-17 and ENDF/B-VIII libraries are in very good agree-ment, since major actinide evaluations are quite similar between the two libraries. Overall, the trends are consistent across the three libraries. In particular, a detailed analysis of reaction rates will provide a better understanding of the differences.

5 TRIPOLI-4 k_{eff} calculations

Ident	ENDF/B-VIII (σ)	JEFF-3.3 (σ)	TENDL-17 (σ)
hmf001c1	1.00018 (12)	1.00029 (12)	1.00008 (12)
hmf001c2	0.99994 (12)	1.00032 (12)	0.99980 (12)
hmf028	1.00075 (11)	1.00429 (11)	1.00072 (11)
hst001c1	0.99907 (17)	1.00042 (17)	0.99922 (17)
hst001c2	0.99542 (17)	0.99883 (17)	0.99550 (17)
hst001c3	1.00267 (17)	1.00394 (17)	1.00211 (17)
hst001c4	0.99808 (17)	1.00105 (17)	0.99770 (17)
hst001c5	0.99935 (16)	1.00054 (16)	0.99949 (16)
hst001c6	1.00312 (16)	1.00351 (16)	1.00264 (16)
hst001c7	0.99865 (17)	1.00036 (17)	0.99839 (17)
hst001c8	0.99918 (16)	1.00030 (17)	0.99888 (17)
hst001c9	0.99334 (17)	0.99735 (17)	0.99371 (17)
hst009c1	1.00144 (17)	1.00301 (17)	1.00119 (16)
hst009c2	1.00240 (16)	1.00333 (16)	1.00243 (16)
hst009c3	1.00262 (16)	1.00248 (16)	1.00245 (16)
hst009c4	0.99788 (16)	0.99665 (16)	0.99713 (16)
hst010c1	1.00284 (16)	1.00188 (16)	1.00269 (16)
hst010c2	1.00312 (16)	1.00206 (16)	1.00314 (16)
hst010c3	1.00033 (16)	0.99985 (16)	1.00088 (16)
hst010c4	0.99838 (16)	0.99775 (16)	0.99858 (16)
hst011c1	1.00596 (16)	1.00512 (16)	1.00554 (16)
hst011c2	1.00200 (16)	1.00115 (16)	1.00169 (16)
hst012c1	1.00088 (16)	1.00053 (16)	1.00090 (16)
hst013c1	0.99860 (16)	0.99828 (16)	0.99831 (16)
hst013c2	0.99772 (16)	0.99734 (16)	0.99797 (16)
hst013c3	0.99460 (16)	0.99378 (16)	0.99456 (16)
hst013c4	0.99627 (16)	0.99540 (16)	0.99597 (16)
hst014c1	0.99517 (16)	0.99484 (16)	0.99494 (16)
hst014c2	1.01117 (16)	1.01118 (16)	1.01086 (16)
hst014c3	1.01983 (16)	1.01932 (16)	1.01920 (16)
hst018c1	0.99088 (16)	0.99100 (16)	0.99055 (16)
hst018c2	0.98517 (17)	0.98659 (16)	0.98493 (17)
hst018c3	0.98911 (16)	0.98953 (16)	0.98903 (16)
hst019c1	0.99742 (16)	0.99874 (17)	0.99724 (16)
hst032	0.99863 (16)	0.99746 (16)	0.99822 (16)
imf001c2	0.99708 (13)	0.99837 (13)	0.99705 (13)
imf001c3	0.99826 (12)	0.99959 (12)	0.99820 (13)
imf001c4	0.99895 (12)	1.00064 (13)	0.99907 (12)

imf002c1	0.99633 (11)	0.99663 (11)	0.99623 (11)
imf007d	1.00466 (13)	1.00525 (13)	1.00511 (13)
imf007s	1.00415 (13)	1.00447 (13)	1.00410 (13)
imf010c1	0.99660 (12)	0.99906 (12)	0.99705 (12)
imf012c1	1.00184 (13)	1.00463 (13)	1.00045 (13)
imf7tzh	0.99511 (13)	0.99548 (13)	0.99531 (12)
lct005c1	1.00266 (13)	1.00360 (13)	1.00278 (13)
lct005c10	0.99986 (13)	1.00804 (13)	0.99997 (13)
lct005c11	1.00047 (13)	1.00856 (13)	1.00009 (13)
lct005c12	1.00420 (13)	1.00912 (13)	1.00417 (13)
lct005c13	1.01021 (13)	1.01609 (13)	1.00958 (13)
lct005c14	0.99824 (13)	0.99961 (13)	0.99851 (13)
lct005c15	1.01719 (13)	1.01908 (13)	1.01707 (13)
lct005c16	1.01248 (13)	1.01469 (13)	1.01232 (13)
lct005c2	0.99987 (13)	1.00117 (13)	0.99999 (13)
lct005c3	0.99901 (13)	1.00228 (13)	0.99880 (13)
lct005c4	0.99763 (13)	1.00135 (13)	0.99759 (13)
lct005c5	1.00374 (13)	1.00733 (13)	1.00347 (13)
lct005c6	1.00468 (13)	1.00945 (13)	1.00476 (13)
lct005c7	0.99989 (13)	1.00591 (13)	0.99971 (13)
lct005c8	0.99985 (13)	1.00720 (13)	0.99979 (13)
lct005c9	1.00077 (13)	1.00854 (13)	1.00027 (13)
lct006c01	0.99995 (12)	1.00131 (12)	0.99984 (12)
lct006c03	1.00022 (9)	1.00196 (9)	1.00007 (9)
lct006c04	1.00006 (12)	1.00113 (12)	0.99996 (12)
lct006c08	1.00018 (12)	1.00133 (12)	1.00011 (12)
lct006c09	1.00033 (12)	1.00082 (12)	1.00019 (12)
lct006c13	1.00004 (12)	1.00089 (12)	0.99982 (12)
lct006c14	1.00012 (12)	1.00041 (12)	1.00004 (12)
lct006c18	0.99986 (12)	1.00051 (12)	0.99981 (12)
lct007c01	0.99761 (12)	0.99957 (34)	0.99735 (12)
lct007c02	0.99960 (15)	1.00046 (15)	0.99948 (15)
lct007c03	0.99896 (15)	0.99816 (15)	0.99843 (15)
lct007c05	0.99688 (15)	0.99910 (15)	0.99662 (15)
lct007c06	0.99976 (15)	1.00018 (15)	0.99971 (15)
lct007c07	0.99958 (15)	0.99927 (15)	0.99971 (15)
lct010c01	1.00577 (12)	1.00932 (12)	1.00496 (12)
lct010c20	1.00392 (12)	1.00751 (12)	1.00315 (12)
lct027c01	1.00302 (12)	1.01022 (12)	0.99919 (12)
lct035c1	0.99994 (9)	1.00166 (9)	0.99991 (9)
lct035c2	0.99895 (9)	1.00066 (9)	0.99895 (9)
lct035c3	0.99530 (9)	0.99725 (9)	0.99539 (9)

lct039c01	0.99716 (15)	0.99849 (15)	0.99702 (15)
lct039c04	0.99663 (15)	0.99765 (15)	0.99679 (15)
lct039c06	0.99796 (15)	0.99885 (15)	0.99753 (15)
mct004c1	0.99536 (13)	0.99628 (13)	0.99499 (13)
mct004c10	0.99662 (13)	0.99587 (13)	0.99571 (13)
mct004c4	0.99570 (13)	0.99616 (13)	0.99485 (13)
mct004c7	0.99597 (13)	0.99624 (13)	0.99547 (13)
pmf001	0.99986 (15)	0.99931 (15)	1.00014 (15)
pmf002	1.00136 (15)	1.00142 (15)	1.00496 (15)
pst001c01	1.00152 (12)	1.00096 (12)	1.00145 (13)
pst001c02	1.00396 (13)	1.00276 (12)	1.00375 (13)
pst001c03	1.00711 (12)	1.00574 (12)	1.00718 (13)
pst001c04	1.00182 (13)	1.00014 (12)	1.00161 (13)
pst001c05	1.00590 (13)	1.00408 (12)	1.00555 (12)
pst001c06	1.00869 (13)	1.00757 (13)	1.00831 (13)
pst009c1a	1.03943 (11)	1.04017 (11)	1.03965 (11)
pst009c2a	1.01294 (11)	1.01380 (11)	1.01328 (11)
pst009c3a	1.01294 (11)	1.01382 (11)	1.01294 (11)
pst011c16-1	1.00398 (13)	1.00641 (13)	1.00417 (13)
pst011c16-5	1.00041 (13)	1.00251 (13)	1.00053 (13)
pst011c18-1	0.98799 (13)	0.99102 (13)	0.98808 (13)
pst011c18-6	0.99385 (13)	0.99689 (13)	0.99397 (13)
pst013c01	1.00029 (13)	1.00061 (12)	1.00015 (13)
pst013c02	1.00002 (13)	1.00051 (12)	0.99984 (13)
pst013c04	0.99281 (13)	0.99332 (12)	0.99258 (13)
topsyni	1.00354 (17)	1.01010 (18)	1.02598 (18)
topsyu	1.00854 (16)	1.01421 (16)	1.00872 (16)

Table 1: ICSBEP Benchmarks : TRIPOLI-4 calculations using ENDF/B-VIII, JEFF-3.3 and TENDL-17 libraries

6 TRIPOLI-4 k_{eff} calculations

Ident	ENDF/B-VIII (σ)	JEFF-3.3 (σ)	TENDL-17 (σ)
HMF-0013_CAS1	0.99897 (11)	0.99625 (11)	0.99930 (11)
HMF-001_CAS1	1.00005 (11)	1.00046 (11)	0.99999 (11)
HMF-004_CAS1_1D	0.99924 (12)	0.99820 (12)	0.99936 (12)
HMF-004_CAS1_3D	1.00204 (12)	1.00120 (12)	1.00203 (12)
HMF-014_CAS1	0.99997 (10)	0.99670 (10)	1.00079 (10)
HMF-015_CAS1	0.99493 (9)	0.99483 (9)	0.99488 (9)
HMF-028_CAS1	1.00075 (11)	1.00429 (11)	1.00072 (11)
HMF-032_CAS1	1.00176 (9)	1.00479 (9)	1.00159 (9)
HMF-032_CAS2	1.00211 (9)	1.00575 (9)	1.00233 (9)
HMF-032_CAS3	0.99820 (9)	1.00092 (9)	0.99819 (9)
HMF-032_CAS4	0.99979 (9)	1.00190 (9)	0.99998 (9)
LCTH-007_CAS4	1.00133 (6)	1.00345 (5)	1.00124 (5)
LCTH-045_CAS1	1.01151 (6)	1.01509 (4)	1.01162 (4)
MCTH-003_CAS3	1.00291 (6)	1.00445 (4)	1.00395 (4)
MCTH-003_CAS6	1.00008 (6)	0.99747 (5)	1.00052 (5)
MCTH-004_CAS11	0.99695 (6)	0.99611 (4)	0.99636 (4)
MMF-001_CAS1	0.99920 (10)	0.99880 (10)	0.99961 (10)
MMF-009_CAS1	0.99957 (10)	0.99956 (10)	1.00009 (10)
MSTH-002_CAS58	0.99545 (12)	0.99654 (7)	0.99576 (4)
PMF-010_CAS1	0.99737 (12)	0.99983 (12)	0.99767 (12)
PMF-016_CAS1	1.02428 (10)	1.02127 (10)	1.02382 (10)
PMF-016_CAS2	1.01363 (10)	1.01029 (10)	1.01340 (10)
PMF-016_CAS3	1.01166 (10)	1.00832 (10)	1.01157 (10)
PMF-016_CAS4	1.01135 (10)	1.00785 (10)	1.01104 (10)
PMF-016_CAS5	1.01104 (10)	1.00761 (10)	1.01050 (10)
PMF-016_CAS6	1.01364 (10)	1.01005 (10)	1.01338 (10)
PMF-022_CAS1	0.99807 (9)	0.99812 (9)	0.99868 (9)
PMF-024_CAS1_detail	1.00088 (12)	1.00164 (12)	1.00141 (12)
PMF-024_CAS1_simple	1.00063 (12)	1.00158 (12)	1.00145 (12)
PMF-028_CAS1	1.00297 (30)	0.99926 (30)	1.00355 (30)
PMF-029_CAS1	0.99603 (9)	0.99553 (9)	0.99670 (9)
PMF-037_CAS1	1.00278 (10)	1.00250 (10)	1.00258 (10)
PMF-037_CAS10	1.00028 (10)	0.99892 (10)	1.00010 (10)
PMF-037_CAS11	0.99720 (10)	0.99633 (10)	0.99696 (10)
PMF-037_CAS12	1.00306 (10)	1.00141 (10)	1.00239 (10)
PMF-037_CAS13	0.99771 (10)	0.99553 (10)	0.99726 (10)
PMF-037_CAS14	1.00595 (10)	1.00405 (10)	1.00551 (10)
PMF-037_CAS15	0.99837 (10)	0.99673 (10)	0.99820 (10)

PMF-037_CAS16	0.99900 (10)	0.99743 (10)	0.99850 (10)
PMF-037_CAS2	1.00207 (10)	1.00137 (10)	1.00210 (10)
PMF-037_CAS3	1.00031 (10)	0.99969 (10)	1.00002 (10)
PMF-037_CAS4	1.00390 (10)	1.00296 (10)	1.00362 (10)
PMF-037_CAS5	1.00063 (10)	1.00003 (10)	1.00051 (10)
PMF-037_CAS6	1.00282 (10)	1.00185 (10)	1.00241 (10)
PMF-037_CAS7	1.00134 (10)	1.00039 (10)	1.00087 (10)
PMF-037_CAS8	1.00222 (10)	1.00084 (10)	1.00190 (10)
PMF-037_CAS9	1.00095 (10)	0.99959 (10)	1.00074 (10)
PSTH-004_CAS11	0.99532 (11)	0.99600 (11)	0.99525 (11)
PSTH-004_CAS2	0.99311 (11)	0.99439 (11)	0.99266 (11)
PSTH-004_CAS3	0.99511 (11)	0.99644 (11)	0.99485 (11)
PSTH-004_CAS5	0.99378 (11)	0.99538 (11)	0.99382 (11)
PSTH-004_CAS6	0.99601 (11)	0.99715 (11)	0.99576 (11)
PSTH-004_CAS8	0.99568 (11)	0.99679 (11)	0.99567 (11)
PSTH-016_CAS1	1.00223 (9)	1.00305 (9)	1.00211 (9)
PSTH-016_CAS2	1.00209 (9)	1.00309 (9)	1.00202 (9)
PSTH-016_CAS3	1.00290 (9)	1.00355 (9)	1.00282 (9)
PSTH-016_CAS4	1.00297 (9)	1.00372 (9)	1.00276 (9)
PSTH-016_CAS5	1.00076 (9)	1.00131 (9)	1.00046 (9)
PSTH-016_CAS6	1.00101 (9)	1.00167 (9)	1.00090 (9)
PSTH-016_CAS7	1.00155 (9)	1.00242 (9)	1.00153 (9)

Table 2: ICSBEP Benchmarks : TRIPOLI-4 calculations using ENDF/B-VIII, JEFF-3.3 and TENDL-17 libraries

References

[1] Cabellos, O., et al. ”Benchmarking and validation activities within JEFF project.” EPJ Web of Conferences. **146**. EDP Sciences, 2017. https://www.oecd-nea.org/dbdata/jeff/jeff33/

[2] KONING, A. J., ROCHMAN, D., SUBLET, J.-Ch, et al. “TENDL: complete nuclear data library for innovative nuclear science and technology”. Nuclear Data Sheets, 2019, **155**, p. 1-55.

[3] BROWN, David A., CHADWICK, M. B., CAPOTE, R., et al. “ENDF/B-VIII. 0: the 8th major release of the nuclear reaction data library with CIELO-project cross sections, new standards and thermal scattering data”. Nuclear Data Sheets, 2018, **148**, p. 1-142.

[4] BRUN, E. et al., “Tripoli-4®, CEA, EDF and AREVA reference Monte Carlo code”, Annals of Nuclear Energy **82**, 151-160 (2015).

[5] MCNP 5.1.40 RSICC Release Notes, Los Alamos Report, LA-UR-05-8617, (2005).

[6] KAHLER III, A. C. and MACFARLANE, R. NJOY2016. Los Alamos National Lab. (LANL), Los Alamos, NM (United States), 2016. LA-UR-17_20093 (2017).

[7] SUBLET, J.-Ch, RIBON, P., and COSTE-DELCLAUX, M. “CALENDF-2010: user manual”. 2011. CEA-R-6277 (2011).

[8] CHADWICK, M. B., HERMAN, M., OBLOŽINSKÝ, P., et al. “ENDF/B-VII. 1 nuclear data for science and technology: cross sections, covariances, fission product yields and decay data”. Nuclear data sheets, 2011, **112**, no 12, p. 2887-2996.

[9] BRIGGS, J., et al. “International handbook of evaluated criticality safety benchmark experiments”. Nuclear Energy Agency, NEA/NSC/DOC (95), 2004, **3**, p. l.

[10] MCLANE, V. “ENDF-102 data formats and procedures for the evaluated nuclear data file ENDF-6”. Brookhaven National Lab., 2001.