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Title: Release of Lib81: ENDF/B-VIII.1-Based ACE Data Files for Neutron Transport

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Intended for: Accompanying dataset will be posted on nucleardata.lanl.gov for unlimited release.
Report

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Memorandum
XCP-5 Materials and Physical Data

Subject: Release of Lib81: ENDF/B-VIII.1-Based ACE Data Files for Neutron Transport

1 Introduction

On August 30, 2024, the National Nuclear Data Center (NNDC) released the ENDF/B-VIII.1 nuclear data library [1]. The library was released in the standard Evaluated Nuclear Data File (ENDF) format [2]. The files can be accessed on the NNDC's website `www.nndc.bnl.gov`. The files provided in the neutron sublibrary were processed into A Compact ENDF (ACE)-formatted files [3], verified, and validated by the XCP-5 Nuclear Data Team, resulting in the **Lib81** application library. This report details the processing of these files and the quality assurance approach taken. This is not intended to be a full validation effort; rather, this library is intended to simply reproduce the released files for further validation testing by the community. The validation basis and details of the evaluations are documented in the forthcoming "Big Paper" [1]. Lib81 is available on LANL computing resources and will be made available without restriction via `nucleardata.lanl.gov`.

2 Library Details

2.1 Temperatures

Lib81 uses 8 temperatures, including 6 that match the first 6 temperatures of the previous library Lib80x [4] plus two additional. These temperatures in Kelvin are 293.6, 600, 900, 1200, 2500, 0.1, 233.15, 273.15.

2.2 ZAID

ZA identifiers (ZAID) are used by MCNP inputs to associate data files with nuclide specifications. As is typical, the first several digits of the ZAID follow a convention related to the atomic number Z, mass number A, and isomeric state S. For the ground state:

$$\mathrm{ZA} = Z * 1000 + A, \quad (1)$$

and for any excited states:

$$\mathrm{ZA} = Z * 1000 + A + 300 + S * 100. \quad (2)$$

Table 1: Temperatures and ZAID extensions in Lib81.

Temperature (K)	ZAID Extension
293.6	.10c
600	.11c
900	.12c
1200	.13c
2500	.14c
0.1	.15c
233.15	.16c
273.15	.17c

The extensions ".10c" through ".17c" are used for this library. The "c" indicates the library type, continuous energy fast neutron data. In a few cases, this set of extensions includes the same ZAID as some previously released MCNP data. It is not expected that these overlapping ZAIDs will affect any use case, but users of legacy data should ensure that this does not cause unexpected data to be used. The mapping of extension to temperature is given in Table 1.

2.3 Deviations from ENDF/B-VIII.1

After verification testing, as described in Section 4, changes were made to the evaluated files before processing:

- For 17 files, ENDF/B-VIII.1 added photon production data from two different sources, and they were not consistent. For these files, both MF12/MT3 data and MF12/MT102 data was included. Because they were not consistent and MT3 contains production from additional reactions, the MF12/MT102 data was removed from the files before processing. The affected target nuclides included Se-78, Kr-84, In-113, Yb-168,170,171,172,173,174,176, and Hf-174,176,178,179,180,181,182. After this correction, these nuclides still show negative KERMA values due to deficiencies in the MT3 data, but the magnitudes are very small.
- Probability tables using ENDF/B-VIII.1 unresolved resonance parameters led to negative cross sections for 4 target nuclides. For each of these, probability tables were omitted in the processing. The affected target nuclides were Na-22, Ar-36, Cd-106, and Cd-111.
- Negative CDF values were detected for Ne-20 MT22 neutron distributions. The issue was traced back to the 2nd through 6th incident energy point for the outgoing neutron in MT22 in this evaluation. For these incident energies, the outgoing energy grid generated by ACER in NJOY2016 was not in order which causes the negative values while integrating the PDF to a CDF. To fix the issue, an extra outgoing energy point at 0 eV with an emission probability of 1e-19 have been added for all affected distributions (originally, the first outgoing energy value for these distributions was not 0 eV but 1.45 MeV with an emission probability of 1e-19). These modifications resolved the issue of negative CDF values.

- O-16 was found to have significant negative KERMA. ENDF/B-VIII.1 added more detailed, transition-based photon production for inelastic channels, but the lumped, experimentally-driven photon production was retained, leading to double counting. After discussion with the evaluators, the legacy lumped photon production was used for these ACE files and the new evaluation will be updated before inclusion in a LANL application library.
- Ca-41 and S-35 were found to have a small number of very unphysical transition probabilities, leading to excessive photon production and negative KERMAs. The offending values were updated, and patched files have already been committed to the ENDF working repository.

In addition to these physics changes, Am-239 was added to the library (taken from TENDL-2019 [5]) and the neutron-neutron scattering file was omitted (as it cannot be used in MCNP).

2.4 Target Nuclides

Table 2 gives a complete listing the ZAID (without extension) avaiable in this library. There are 558 files corresponding to 557 of the 558 nuclides available in ENDF/B-VIII.1 (excluding the neutron target, Ta-180m new since ENDF/B-VIII.0) and Am-239 (taken from TENDL-2019). For historical reasons, ZAID 95242 refers to the excited state of Am-242 and 95642 refers to the ground state, which goes against the convention used in the rest of the library.

Table 2: ZAID for nuclei included in Lib81.

1001	1002	1003	2003	2004	3006	3007	4007	4009	5010
5011	6012	6013	7014	7015	8016	8017	8018	9019	10020
10021	10022	11022	11023	12024	12025	12026	13426**	13027	14028
14029	14030	14031	14032	15031	16032	16033	16034	16035	16036
17035	17036	17037	18036	18037	18038	18039	18040	18041	19039
19040	19041	20040	20041	20042	20043	20044	20045	20046	20047
20048	21045	22046	22047	22048	22049	22050	23049	23050	23051
24050	24051	24052	24053	24054	25054	25055	26054	26055	26056
26057	26058	27058	27458**	27059	28058	28059	28060	28061	28062
28063	28064	29063	29064	29065	30064	30065	30066	30067	30068
30069	30070	31069	31070	31071	32070	32071	32072	32073	32074
32075	32076	33073	33074	33075	34074	34075	34076	34077	34078
34079	34080	34081	34082	35079	35080	35081	36078	36079	36080
36081	36082	36083	36084	36085	36086	37085	37086	37087	38084
38085	38086	38087	38088	38089	38090	39089	39090	39091	40090
40091	40092	40093	40094	40095	40096	41093	41094	41095	42092
42093	42094	42095	42096	42097	42098	42099	42100	43098	43099
44096	44097	44098	44099	44100	44101	44102	44103	44104	44105
44106	45103	45104	45105	46102	46103	46104	46105	46106	46107
46108	46109	46110	47107	47108	47109	47510**	47111	47112	47113

Continued on next page

Table 2: ZAID for nuclei included in Lib81. *(continued).*

47114	47115	47116	47117	47518**	48106	48107	48108	48109	48110
48111	48112	48113	48114	48515**	48116	49113	49114	49115	50112
50113	50114	50115	50116	50117	50118	50119	50120	50521**	50122
50123	50124	50125	50126	51121	51122	51123	51124	51125	51126
52120	52121	52521**	52122	52123	52124	52125	52126	52527**	52128
52529**	52130	52131	52531**	52132	53127	53128	53129	53130	53131
53132	53532**	53133	53134	53135	54123	54124	54125	54126	54127
54128	54129	54130	54131	54132	54133	54134	54135	54136	55133
55134	55135	55136	55137	56130	56131	56132	56133	56134	56135
56136	56137	56138	56139	56140	57138	57139	57140	58136	58137
58537**	58138	58139	58140	58141	58142	58143	58144	59141	59142
59143	60142	60143	60144	60145	60146	60147	60148	60149	60150
61143	61144	61145	61146	61147	61148	61548**	61149	61150	61151
62144	62145	62146	62147	62148	62149	62150	62151	62152	62153
62154	63151	63152	63153	63154	63155	63156	63157	64152	64153
64154	64155	64156	64157	64158	64159	64160	65158	65159	65160
65161	66154	66155	66156	66157	66158	66159	66160	66161	66162
66163	66164	67165	67566**	68162	68163	68164	68165	68166	68167
68168	68169	68170	69168	69169	69170	69171	70168	70169	70170
70171	70172	70173	70174	70175	70176	71175	71176	72174	72175
72176	72177	72178	72179	72180	72181	72182	73180	73580**	73181
73182	74180	74181	74182	74183	74184	74185	74186	75185	75586**
75187	76184	76185	76186	76187	76188	76189	76190	76191	76192
77191	77192	77193	77594**	78190	78191	78192	78193	78194	78195
78196	78197	78198	79197	80196	80197	80597**	80198	80199	80200
80201	80202	80203	80204	81203	81204	81205	82204	82205	82206
82207	82208	83209	83610	84208	84209	84210	88223	88224	88225
88226	89225	89226	89227	90227	90228	90229	90230	90231	90232
90233	90234	91229	91230	91231	91232	91233	92230	92231	92232
92233	92234	92235	92236	92237	92238	92239	92240	92241	93234
93235	93236	93636**	93237	93238	93239	94236	94237	94238	94239
94240	94241	94242	94243	94244	94245	94246	95239	95240	95241
95242**	95642	95243	95244	95644**	96240	96241	96242	96243	96244
96245	96246	96247	96248	96249	96250	97245	97246	97247	97248
97249	97250	98246	98247	98248	98249	98250	98251	98252	98253
98254	99251	99252	99253	99254	99654**	99255	100255		

** Excited state evaluation

† From TENDL-2019

3 File Processing

All ENDF-formatted files were processed at room temperature (293.6 K) with NJOY2016[1] Version 74 into the ACE format. The same processing path as for the previous Lib80x [4] was used, and thus the inputs are not reproduced in this documentation. The modules used include MODER, RECONR, BROADR, HEATR, GASPR, PURR, and ACER.

4 Verification

Multiple verification tests were performed on the processed ACE files. The nuclear data toolkit, ACEtk[2], was used to ensure all nuclear data files are readable. Next, the ACE files were tested with a tool called checkACE [6], which is a collection of Fortran routines designed to test different aspects of ACE files prepared by NJOY for the Monte Carlo N-Particle® (MCNP) code[3] [7].

4.1 ACEtk Test

ACEtk is a toolkit for reading and interacting with ACE nuclear data files. This toolkit is part of the NJOY modernization and provides a full C++ library along with Python bindings. It currently supports the following ACE file types: (1) incident neutron and charged particle ACE files, (2) photoatomic and photonuclear ACE files, (3) thermal scattering ACE files, and (4) dosimetry ACE files. When reading ACE files, ACEtk will break up the underlying data array into smaller blocks and provide an interface on top of those blocks to make interacting with the data easier for a user. These block interfaces effectively abstract away the internal locators in the data array of the ACE file. As a result, ACEtk is useful for doing a basic ACE format check since errors in the internal locators will lead to errors being thrown by the tool upon reading the ACE files. ACEtk was used to read all ACE files that were produced and no errors were detected.

4.2 checkACE Test

The checkACE Fortran routines provide basic consistency checks/common sense testing of ACE files. This report does not contain documentation for each specific test that checkACE performs; the documentation for each checkACE test can be found in Reference 6. The following subsections provide details of specific tests that produced an error or warning message.

These errors are generally associated with the evaluation and not the processing. While these tests motivated some of the deviations from the ENDF/B-VIII.1 library discussed in Section 2.3,

[1] https://github.com/njoy/NJOY2016

[2] https://github.com/njoy/ACEtk

[3] MCNP® and Monte Carlo N-Particle® are registered trademarks owned by Triad National Security, LLC, manager and operator of Los Alamos National Laboratory. Any third party use of such registered marks should be properly attributed to Triad National Security, LLC, including the use of the designation as appropriate. For the purposes of visual clarity, the registered trademark symbol is assumed for all references to MCNP within the remainder of this paper.

concerns about remaining errors should be addressed with nuclear data evaluators.

4.2.1 check5

Some evaluations have been seen to emit very large number of neutrons via the MT=5 (z,anything) reaction. Based on a limit of secondary neutrons produced in a single reaction in older versions of MCNP, this test looks for neutron multiplicities greater than 11. This is observed in Lib81 for Os-191, Ir-192, Pa-231, and Pa-233. In all cases, this behavior is only seen above 30 MeV and is unlikely to be seen by typical users of ENDF data in MCNP. For Pa-231, the neutron multiplicity exceeds 20 above 50 MeV, and this is above the limit for MCNP 6.2 and 6.3.

4.2.2 check_heat

Many nuclides were found to have some degree of negative KERMA values. The most significant issues were corrected, as documented in Section 2.3. The remaining issues are primarily due to the addition of exit distributions from TENDL or elsewhere, a significant effort for ENDF/B-VIII.1. While these new exit distributions have a number of benefits, unfortunately, small negative KERMA values are a side effect, as these were not evaluated consistently with the rest of the file. The affected nuclides are: Ag-118m, Cd-115m, Te-121m, Te-131m, I-132m, Ce-137m, Ho-166m, Ir-194m, Hg-197m, Bi-210m, S-33, S-36, Zr-92, Zr-93, Zr-94, Zr-95, Zr-96, Nb-93, Mo-92, Mo-94, Mo-96, Mo-97, Mo-98, Cd-111, In-113, Cs-133, Ce-143, Nd-145, Nd-147, Pm-144, Sm-147, Sm-149, Sm-151, Gd-153, Gd-155, Ho-165, Er-166, Tm-168, Yb-168, Yb-170, Yb-171, Yb-172, Yb-173, Yb-174, Yb-176, Hf-174, Hf-176, Hf-178, Hf-179, Hf-180, Hf-181, Hf-182, Au-197, Hg-196, Hg-202, Tl-203, Tl-205, Bi-209, and Po-208.

5 Validation

Validation testing of the processed ACE files was performed with the LANL legacy suite of fast critical assemblies. These tests demonstrate that the processed ACE files were able to be read into MCNP and used for enhanced predictive capabilities. This is not a complete validation analysis; instead, this is being used as a further verification test to ensure that files can be read in MCNP and do not cause egregiously incorrect errors due to processing. These results are consistent with the full validation basis presented in the ENDF/B-VIII.1 Big Paper [1].

The LANL legacy benchmark suite has been used extensively to validate new nuclear data libraries. The benchmarks and associated International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook [8] designations included in the legacy suite: (1) Godiva, HEU-MET-FAST-001 Revision 2, (2) Flattop with HEU core (Flattop-25), HEU-MET-FAST-028 Revision 2, (3) The Early Jemima Experiments (Jemima), IEU-MET-FAST-001-001 (4) Bigten, IEU-MET-FAST-007 Revision 1, (5) Jezebel, PU-MET-FAST-001 Revision 5, (6) Dirty Jezebel (Jezebel-Pu), PU-MET-FAST-002 Revision 1, (7) Flattop with Pu core (Flattop-Pu), PU-MET-FAST-006 Revision 1, (8) U-233 Jezebel (Jezebel-23), U233-MET-FAST-001 Revision 3, and (9) Flattop with U-233 core (Flattop-23), U233-MET-FAST-006 Revision 1. Version 6.3 of the MCNP code was used with the

Lib80x and Lib81 nuclear data libraries for validation testing. Validation results for the criticality experiments are shown in Table 3.

Table 3: Criticality validation of LANL legacy suite benchmarks.

		Calculated k_{eff}	
Experiment	**Measured k_{eff}**	**ENDF/B-VIII.0**	**ENDF/B-VIII.1**
Godiva	1.00000 (100)	1.00005 (3)	0.99989 (3)
Flattop	1.00000 (130)	1.00078 (3)	1.00066 (3)
Jemima	0.99880 (109)	0.99900 (9)	0.99892 (9)
Big Ten	1.00450 (107)	1.00425 (7)	1.00466 (7)
Jezebel	1.00000 (111)	1.00056 (1)	1.00010 (1)
Jezebel-Pu	1.00000 (120)	1.00147 (8)	1.00075 (8)
Flattop-Pu	1.00000 (130)	0.99968 (3)	0.99998 (3)
Jezebel-23	1.00000 (110)	1.00056 (8)	0.99991 (8)
Flattop-23	1.00000 (114)	0.99988 (10)	1.00019 (10)

6 Quality Assurance

The ENDF files, processing scripts, and other associated files for this release are stored in HPSS in `/hpss/nucldata/archive/2025/xcp-5-25-022`.

7 Conclusions

The ENDF/B-VIII.1 neutron sub-library has been processed into the Lib81 ACE library. With only minimal changes to the underlying ENDF files compared to the official release, the processing effort is deemed to be of sufficient quality for all use cases. The library is available on LANL HPC resources and will be released publicly via `nucleardata.lanl.gov`.

References

[1] G. Nobre, et al., "ENDF/B-VIII.1: Updated Nuclear Reaction Data Library for Science and Applications," *Nuclear Data Sheets*, (in review).

[2] A. Trkov, M. Herman, and D. A. Brown, "ENDF-6 Formats Manual: Data Formats and Procedures for the Evaluated Nuclear Data Files," Brookhaven National Laboratory Technical Report BNL-203218-2018-INRE (2018). DOI:10.2172/1425114

[3] J. Conlin, and P. Romano, "A Compact ENDF (ACE) Format Specification," Los Alamos National Laboratory (2019). LA-UR-19-29016 DOI:10.2172/1561065

[4] J. Conlin, W. Haeck, D. Neudecker, D. Parsons, and M. White, "Release of ENDF/B-VIII.0-Based ACE Data Files," Los Alamos National Laboratory (2018). LA-UR-18-24034 DOI:10.2172/1438139

[5] A. J. Koning, et. al, "TENDL: Complete Nuclear Data Library for Innovative Nuclear Science and Technology," *Nuclear Data Sheets*, **155** (2019).

[6] D. Kent Parsons, "The Rules of CHECKACE – a Suite of Checking Codes for MCNP ACE Cross Section Files," Memo XCP-5:15-032. Los Alamos National Laboratory, Apr. 2015.

[7] J. A. Kulesza, T. R. Adams, J. C. Armstrong, S. R. Bolding, F. B. Brown, J. S. Bull, T. P. Burke, A. R. Clark, R. A. Forster III, J. F. Giron, T. S. Grieve, C. J. Josey, R. L. Martz, G. W. McKinney, E. J. Pearson, M. E. Rising, C. J. Solomon Jr., S. Swaminarayan, T. J. Trahan, S. C. Wilson, A. J. Zukaitis. MCNP® Code Version 6.3.0 Theory & User Manual. Los Alamos National Laboratory Tech. Rep. LA-UR-22-30006, Rev. 1. Los Alamos, NM, USA. September 2022. DOI:10.2172/1889957

[8] "International Handbook of Evaluated Criticality Safety Benchmark Experiments." Organisation for Economic Cooperation and Development Nuclear Energy Agency, NEA/NSC/DOC(95)03 (2021 Edition).

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