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Title: MT71x: Multi-Temperature Library Based on ENDF/B-VII.1

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MT71x

Multi-Temperature Library Based on ENDF/B-VII.1

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Contents

1. Summary

The Nuclear Data Team has released a multi temperature transport library, MT71x, based upon ENDF/B-VII.1 with a few modifications as well as additional evaluations for a total of 427 isotope tables. The library was processed using NJOY2012.39 into 23 temperatures.

MT71x consists of two sub-libraries; MT71x_{MG} for multigroup energy representation data and MT71x_{CE} for continuous energy representation data. These sub-libraries are suitable for deterministic transport and Monte Carlo transport applications, respectively. The `SZA`s used are the same for the two sub-libraries; that is, the same `SZA` can be used for both libraries. This makes comparisons between the two libraries and between deterministic and Monte Carlo codes straightforward.

Both the multigroup energy and continuous energy libraries were verified and validated with our checking codes `checkmg` [1] and `checkace` [2] (multigroup and continuous energy respectively) Then an expanded suite of tests was used for additional verification and finally, verified using an extensive suite of critical benchmark models. We feel that this library is suitable for all calculations and is particularly useful for calculations sensitive to temperature effects.

2. Introduction

ENDF/B-VII.1 was released by the National Nuclear Data Center (NNDC) in December 2011 [3]. Since that time, LANL has produced two libraries based on that data; ENDF71x [4], a continuous energy library in 7 temperatures suitable for reactor applications, and MENDF71x [5], a multigroup energy library at room temperature without upscatter data.

In the same time frame, two multi-temperature, multigroup libraries (`mtmg01` and `mtmg01ex`) were released by the Nuclear Data Team [6, 7]. These libraries were based on data evaluations prior to the release of ENDF/B-VII.0. Our users had requested an updated multi-temperature library, based on ENDF/B-VII.1, for both multigroup energy and continuous energy data. Based on these requests, we have created the MT71x library.

This paper serves to document the library, its features, the way in which it was processed, and the verification and validation that was performed. The remainder of this Section discusses the origination of the data and the changes that were made from the original evaluation. It also gives the properties of the library that are applicable to both the multigroup energy and continuous energy sub-libraries.

Section 3 discusses the specifics of the multigroup energy sub-library while Section 4 discusses the specifics of the continuous energy sub-library. In each of those sections, the verification and validation for the sub-library is detailed.

2.1. Changes in MT71x from ENDF/B-VII.1

A handful of changes have been made to the official ENDF/B-VII.1 evaluations. We have made these changes based upon our experience and judgement of the quality of these

evaluations. The vast majority of the ENDF/B-VII.1 evaluations were not altered. In this section, we document what changes we have made to the ENDF/B-VII.1 evaluations.

2.1.1. ^{56}Fe and ^{61}Ni

In the ^{56}Fe and ^{61}Ni evaluations, there was one cross section that had values that were zero, which is unphysical. These occurred at 1.1971 MeV in ^{56}Fe; and at 0.742 925 MeV and 0.743 962 MeV to 0.818 412 0 MeV in ^{61}Ni. In both evaluations, the cross section value was chosen to be 1×10^{-6} b, the smallest reasonable value [8]. This is the same evaluation used in the MENDF71x library.

2.1.2. ^{168}Tm

The official ENDF/B-VII.1 version of ^{168}Tm has an error in the energy-angle distribution (MF 6, MT102) for output gammas from low energy incident neutrons. The error affects the kerma values for low energy incident neutrons. David Brown of BNL has supplied us with a corrected evaluation. The correction should appear in a future ENDF release. This is the same evaluation used in the MENDF71x library.

2.1.3. ^{153}Eu

The official ENDF/B-VII.1 version of ^{153}Eu has an error in the gamma yield per incident neutron energy for low incident energy neutrons. The error affects the kerma values for low energy incident neutrons. We have corrected the error and have submitted the correction to David Brown of BNL. We anticipate that the correction will appear in a future ENDF release. This is the same evaluation used in the MENDF71x library.

Another problem with the ^{153}Eu evaluation is in the MF 6, MT 91 partial inelastic scattering cross section. The evaluation contains unphysical negative values for the PDF. The ACER routine in NJOY simply sets the negative values to very small positive values. `checkace` flags these abnormally small PDF values. On the multigroup side, the negatives are processed into Legendre polynomials and added into the other partial cross sections for scattering and lost in the shuffle. Therefore, this problem is not seen in `checkmg`.

2.1.4. ^{7}Be

The ^{7}Be evaluation file in ENDF/B-VII.1 only included energies up to 8 MeV. This file was inadvertently included in the final version of ENDF/B-VII.1 when a better evaluation was available. For MT71x, we have used a file created by Hale and Seamon [9, 10] and updated by White [11]. The improved evaluation file has energies up to 20 MeV. This is the same evaluation used in the MENDF71x library.

2.1.5. ^{239}U

The ^{239}U evaluation file in ENDF/B-VII.1 has some undesirable features. The resonances reach in to energy regions that are too low and the scattering cross section seems too

large. For MT71x, we have used an evaluation produced by Phil Young from T-2. This evaluation begins with the ENDF/B-VII.0 evaluation and makes some corrections to the obviously wrong data.

2.2. Identifying Data Tables in MT71x

Identifying NDI data tables in MT71x follows the convention established by the Nuclear Data Team in previous releases. NDI data tables are identified by a unique ZAID which has the format

$$\texttt{SSSZZZAAA.dddCC} \tag{1}$$

where

- `SSS` the excited state,
- `ZZZ` the atomic number,
- `AAA` the atomic mass,
- `ddd` the library identifier,
- `CC` class of data.

The combination of the library identifier and the class of data, `dddCC`, is called the extension. The `SZA` can be constructed using the formula

$$\texttt{ZAID} = \texttt{S} * 1\,000\,000 + \texttt{Z} * 1000 + \texttt{A}. \tag{2}$$

Table 1: List of `SZA`s for light-weight isotopes (i.e., $Z < 26$) in MT71x. `SZA`s marked with a dagger (†) indicate evaluations that have been modified from ENDF/B-VII.1 in MT71x.

1001	1002	1003	2003	2004	3006	3007	4007†
4009	5010	5011	6000	7014	7015	8016	8017
9019	11022	11023	12024	12025	12026	13027	14028
14029	14030	15031	16032	16033	16034	16036	17035
17037	18036	18038	18040	19039	19040	19041	20040
20042	20043	20044	20046	20048	21045	22046	22047
22048	22049	22050	23050	23051	24050	24052	24053
24054	25055						

2.2.1. Historical Exception to Naming Convention—^{242}Am

A historical exception to the above mentioned naming convention is made for the ground state and meta-stable state of ^{242}Am. This exception is made because the meta-stable state was the only evaluation available for many years. Beginning with ENDF/B-VII.0, an evaluation for the ground state was made available. NB the meta-stable isotope has a half-life of 141 year while the ground state isotope has a half-life of 16 hour.

Table 2: List of SZAs for mid-weight isotopes (i.e., $25 < Z \leq 88$) in MT71x. SZAs marked with a dagger (†) indicate evaluations that have been modified from ENDF/B-VII.1 in MT71x.

26054	26056†	26057	26058	27058	1027058	27059	28058
28059	28060	28061†	28062	28064	29063	29065	30064
30065	30066	30067	30068	30070	31069	31071	32070
32072	32073	32074	32076	33074	33075	34074	34076
34077	34078	34079	34080	34082	35079	35081	36078
36080	36082	36083	36084	36085	36086	37085	37086
37087	38084	38086	38087	38088	38089	38090	39089
39090	39091	40090	40091	40092	40093	40094	40095
40096	41093	41094	41095	42092	42094	42095	42096
42097	42098	42099	42100	43099	44096	44098	44099
44100	44101	44102	44103	44104	44105	44106	45103
45105	46102	46104	46105	46106	46107	46108	46110
47107	47109	1047110	47111	48106	48108	48110	48111
48112	48113	48114	1048115	48116	49113	49115	50112
50113	50114	50115	50116	50117	50118	50119	50120
50122	50123	50124	50125	50126	51121	51123	51124
51125	51126	52120	52122	52123	52124	52125	52126
1052127	52128	1052129	52130	52132	53127	53129	53130
53131	53135	54123	54124	54126	54128	54129	54130
54131	54132	54133	54134	54135	54136	55133	55134
55135	55136	55137	56130	56132	56133	56134	56135
56136	56137	56138	56140	57138	57139	57140	58136
58138	58139	58140	58141	58142	58143	58144	59141
59142	59143	60142	60143	60144	60145	60146	60147
60148	60150	61147	61148	1061148	61149	61151	62144
62147	62148	62149	62150	62151	62152	62153	62154
63151	63152	63153†	63154	63155	63156	63157	64152
64153	64154	64155	64156	64157	64158	64160	65159
65160	66156	66158	66160	66161	66162	66163	66164
67165	1067166	68162	68164	68166	68167	68168	68170
69168†	69169	69170	71175	71176	72174	72176	72177
72178	72179	72180	73180	73181	73182	74180	74182
74183	74184	74186	75185	75187	77191	77193	79197
80196	80198	80199	80200	80201	80202	80204	81203
81205	82204	82206	82207	82208	83209	88223	88224
88225	88226						

Table 3: List of SZAs for actinides (i.e., $Z > 88$) in MT71x. SZAs marked with a dagger (†) indicate evaluations that have been modified from ENDF/B-VII.1 in MT71x.

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	93237
93238	93239	94236	94237	94238	94239	94240	94241
94242	94243	94244	94246	95240	95241	95242	95042
1095242	95243	95244	1095244	96240	96241	96242	96243
96244	96245	96246	96247	96248	96249	96250	97245
97246	97247	97248	97249	97250	98246	98248	98249
98250	98251	98252	98253	98254	99251	99252	99253
99254	1099254	99255	100255				

Because the meta-stable evaluation was the only one available for decades, it was given the ZA of 95242. When ^{242m1}Am became available, the Nuclear Data Team decided not to change the ZA for the meta-stable evaluation and so the evaluation for ^{242m1}Am got 95042 as a ZA(1095242 with the new convention from Equation (2)).

Now, the ZAs for the two ^{242}Am evaluations (meta-stable and ground state) are switched compared to the decided convention.

2.3. Temperatures

The MT in MT71x stands for Multi-Temperature. MT71x is being made available in 23 temperatures shown in Table 4. The temperatures include the 15 temperatures in the mtmg01 and mtmg08 libraries, and adds 8 new temperatures based on a study by Parsons [12].

2.4. Additions to ENDF/B-VII.1 in MT71x

Due to frequent usage by users of our data, we have included additional data tables in MT71x that are not originally a part of ENDF/B-VII.1. The additions are of two varieties: regular evaluations and elementals; *the elementals are only available in multigroup energy MT71x.*

The non-elemental additions that were made are:

6012 an exact copy of the elemental carbon evaluation;
45117 lumped uranium fission product;
46119 lumped plutonium fission product; and
33073 evaluation for ^{73}As.

The lumped uranium fission product uses the same evaluation as 45117.905nm and the lumped plutonium fission product uses the same evaluation as 46119.905nm [13].

Table 4: SZA library identifiers and temperatures available in the MT71x library.

ID	Temperature	ID	Temperature
200	293.6 K	212	178 eV/k_B
201	1160 K	213	310 eV/k_B
202	2500 K	214	562 eV/k_B
203	1 eV/k_B	215	1 keV/k_B
204	1.78 eV/k_B	216	1.78 keV/k_B
205	3.1 eV/k_B	217	3.1 keV/k_B
206	5.36 eV/k_B	218	5.62 keV/k_B
207	10 eV/k_B	219	10 keV/k_B
208	1.78 eV/k_B	220	31 keV/k_B
209	31 eV/k_B	221	100 keV/k_B
210	56.2 eV/k_B	222	310 keV/k_B
211	100 eV/k_B		

The ^{73}As evaluation is from Toshihiko Kawano in T-2. This is a change from the ^{73}As evaluation that has been included in previous libraries. Additional information regarding the data from this library, please see *New As-73 Evaluation for MT71x Available with NDI Version 2.1.2* [14].

3. Multigroup MT71x

The multigroup energy MT71x ($MT71x_{MG}$) library is available in 618 groups and is collapse compatible with frequently used group structures as well as the new group structures recently developed [15], namely the `301_lanl`, `141_lanl`, `75_lanl`, and `47_lanl` group structures.

The "class of Data" (`CC` in Equation 1) for $MT71x_{MG}$ is `nm`, which indicates an incident neutron and multigroup energy representation. A fully qualified `ZAID` for ^{235}U at room temperature and multigroup energy representation would be `92235.200nm`.

There are 25 elemental data tables that have been calculated from the isotopic data tables. These elementals are not part of ENDF/B-VII.1, but have been created for the convenience of the users of the data. The list of elemental ZAIDs is given here:

- 12000
- 14000
- 17000
- 18000
- 19000
- 20000
- 22000
- 23000
- 24000
- 26000
- 28000
- 29000
- 31000
- 40000
- 42000
- 47000
- 48000
- 49000
- 54000
- 63000
- 64000
- 72000
- 74000
- 77000
- 82000

The general features of multigroup mt71x include:

- neutron transport data:

    - `618_lanl` neutron energy group structure.
    - temperature dependent td weight function.
    - temperature broadened cross sections.
    - upscatter data for elastic reaction.
    - scattering matrices for the first five Legendre moments.
    - infinitely dilute media (no self-shielding).
- gamma transport data:
    - `103_phot` gamma energy group structure; collapses to `48_phot`, `24_phot`, and `12_phot` group structures.
    - $1/e$ + roll-off gamma weight function
    - gamma production data (if present in the original evaluation).
- edit data:
    - reaction cross sections for production-depletion
    - reaction q-values.
    - kerma values.
    - kerma from gammas.
- actinide data (for fissionable materials):
    - total, prompt, and delayed nubar ($\overline{\nu}$).
    - incident energy dependent fission emission distributions (χ).
    - fission energy split to fragments, prompt, and delayed particles.

3.1. Verification

The initial testing of any new multi-group neutron cross section library at Los Alamos is carried out with the utility code `checkmg` [1]—a C code (originally written by Joann Campbell and now maintained by the nuclear data team) which reads NDI neutron cross section tables and applies various common sense rules to the data. The rules include neutron cross section balance, partial and total fission cross section consistency, chi normalization checks, Legendre Polynomial cross section balance and coefficient consistency checks, kerma, heating, and Q value checks. Recently, some additional rules have been added for checking typical ranges for cross section and gamma production values.

`checkmg` has proven very effective at finding problems in multi-group NDI formatted neutron cross section tables. Although `checkmg` does not explicitly fix any problems, its errors, warnings, and informative messages are very useful in identifying cross section problems.

For example, we used `checkmg` to identify negative elastic scattering (due to the truncated series of Legendre polynomials) in ^{11}B at 20 MeV [16]. Most recently, it helped us find an "LR=40" flag problem in the higher energy inelastic scattering levels of ^{10}B [17].

Another finding from `checkmg` is that the gamma production for neutron energies greater than 549 keV are very small for the ENDF/B-VII.0 and ENDF/B-VII.1 evaluations of ^{237}Np. Below 549 keV, inelastic, capture, and fission reactions all produce gammas (see MF 12) with reasonable multiplicities. Above 549 keV, however, the gamma

production is lumped into MF 13, MT 3. And the values are quite small—fractions of 1.0 up to about 2.0. Much more typical values would be numbers in the range of 10–15 and going up with respect to incident energy.

Currently, the MT71x library simply uses the official evaluation, though this ^{237}Np gamma production problem has been reported to and acknowledged by the NNDC.

The nuclear data team does not release any multi-group data without first running `checkmg`.

In addition to the checks performed by `checkmg`, acceptance tests have been performed for every data table in MT71x. These acceptance tests consist of a sphere that contains a single isotope and a point source of neutrons at the center. The spectrum of the source was logarithmically spaced from 1×10^{-11} MeV to 20 MeV. (A sample input deck for these acceptance input decks can be found in Appendix A.) Acceptance tests were performed with Partisn for each of the 427 isotopic data tables and each of the 25 elementals, for each of the 23 temperatures for a total of 10 396 calculations. None of the calculations performed caused fatal errors for Partisn.

Note, these tests were not designed to validate—test the physics—of the data tables. They were performed as mechanical tests—testing if the data tables are malformed in some manner.

3.2. Validation

A series of 91 critical assembly benchmarks were modeled using Partisn to validate the data tables. The benchmarks come from *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (ICSBEP) [18] and were performed experimentally at room temperature which is why we performed the benchmarks using the room temperature data. A detailed discussion of the results of the benchmark models can be found in *(U) Validation of MT71x-Multigroup with Upscatter Using Criticality Benchmark Calculations* [19]. A brief discussion of the benchmarks is given here.

The suite of 91 critical benchmarks have been used in the past by the Nuclear Data Team as a way to validate multigroup neutron transport libraries [20, 21, 22, 23]. The 91 benchmarks fall under eight classes of benchmarks based on the material of the critical assembly and the energy spectrum of the neutrons. In this document, the different classes will be identified and marked—in tables and figures—by the colors shown here:

HEU-MET-FAST	highly enriched uranium metal with a fast spectrum;
HEU-SOL-THERM	highly enriched uranium in solution with a thermal spectrum;
IEU-MET-FAST	intermediate enriched uranium metal with a fast spectrum;
MIX-MET-FAST	mixed uranium and plutonium metal with a fast spectrum;
PU-MET-FAST	plutonium metal with fast spectrum;
PU-SOL-THERM	plutonium in solution with thermal spectrum;
U233-MET-FAST	^{233}U metal with fast spectrum; and
U233-SOL-THERM	^{233}U in solution with thermal spectrum.

Since these are critical benchmarks, the primary calculated quantity is k_{eff}, the k-eigenvalue. Figure 1 shows the results of the Partisn calculations using the MT71x

library as well as the same models, but with different data libraries for comparison. Figure 2 shows the ratio of k_{eff} calculated with multigroup energy cross sections to those calculated with continuous energy cross sections (Monte Carlo) using different libraries for comparison. Monte Carlo does not suffer from spatial or energy discretization errors and is generally considered to be more accurate for calculating k_{eff} values so the k_{eff} comparison between the multigroup and continuous energy calculations helps give an indication of how well the multigroup energy data is.

We can see that for the most part the MT71x library is not very different than other recent libraries released at LANL. The dozen or so benchmarks which are rather different are those that have a lot of low-Z material which has a significant upscatter effect. For more information, see the related validation paper [19].

4. Continuous Energy MT71x

Along with the multigroup energy library, a continuous energy library (MT71x_{CE}) is available. It is available in the same 23 temperatures as MT71x_{GM}. MT71x_{CE} will be released using version 2.0.0 of the ACE data format [24].

The "class of Data" (`CC` in Equation 1) for MT71x_{CE} is `nc`, which indicates an incident neutron and continuous energy representation. A fully qualified `ZAID` for ^{235}U at room temperature and continuous energy representation would be `92235.200nc`.

4.1. Verification

The initial testing of any new continuous-energy neutron cross section library at Los Alamos is carried out with the utility code `checkace` [2]. `checkace` is a collection of Fortran and Perl routines which originally grew out of the CONSIS module of NJOY and have since been developed over many years. `checkace` has evolved into a very useful stand-alone checking tool for ACE formatted neutron cross section files. `checkace` applies a series of common sense rules to: check the consistency of partial and total cross sections for neutrons and photons, watch for negative cross sections, assure reasonable values for $\overline{\nu}$—the average number of neutrons released in fission—and other neutron producing reactions, verify outgoing energies of secondary neutrons, and check threshold energy values. All PDF/CDF distribution data is checked for CDF monotonicity, PDF non-negativity, and CDF normalization. Like `checkmg`, `checkace`'s error, warning, and informative messages are very helpful in identifying problems. Unlike `checkmg` though, `checkace` can fix some problems and produce a corrected ACE formatted file.

The nuclear data team does not release any continuous-energy data without first running `checkace`.

`checkace` has recently helped us identify a PDF/CDF problem in ^{1}H—which traced back to an NJOY bug (since fixed). `checkace` also reported finding negative PDF values in MF=6,MT=91 for ^{153}Eu. The negative values date back to at least the ENDF/B-VII.0 evaluation. `checkace` set the negative values to zero, renormalized the PDFs and CDFs and wrote a new corrected ACE formatted file. The corrected file is used in the MT71x library. `checkace` also identified two other reactions (MF=3,MT=22 or MT=28)

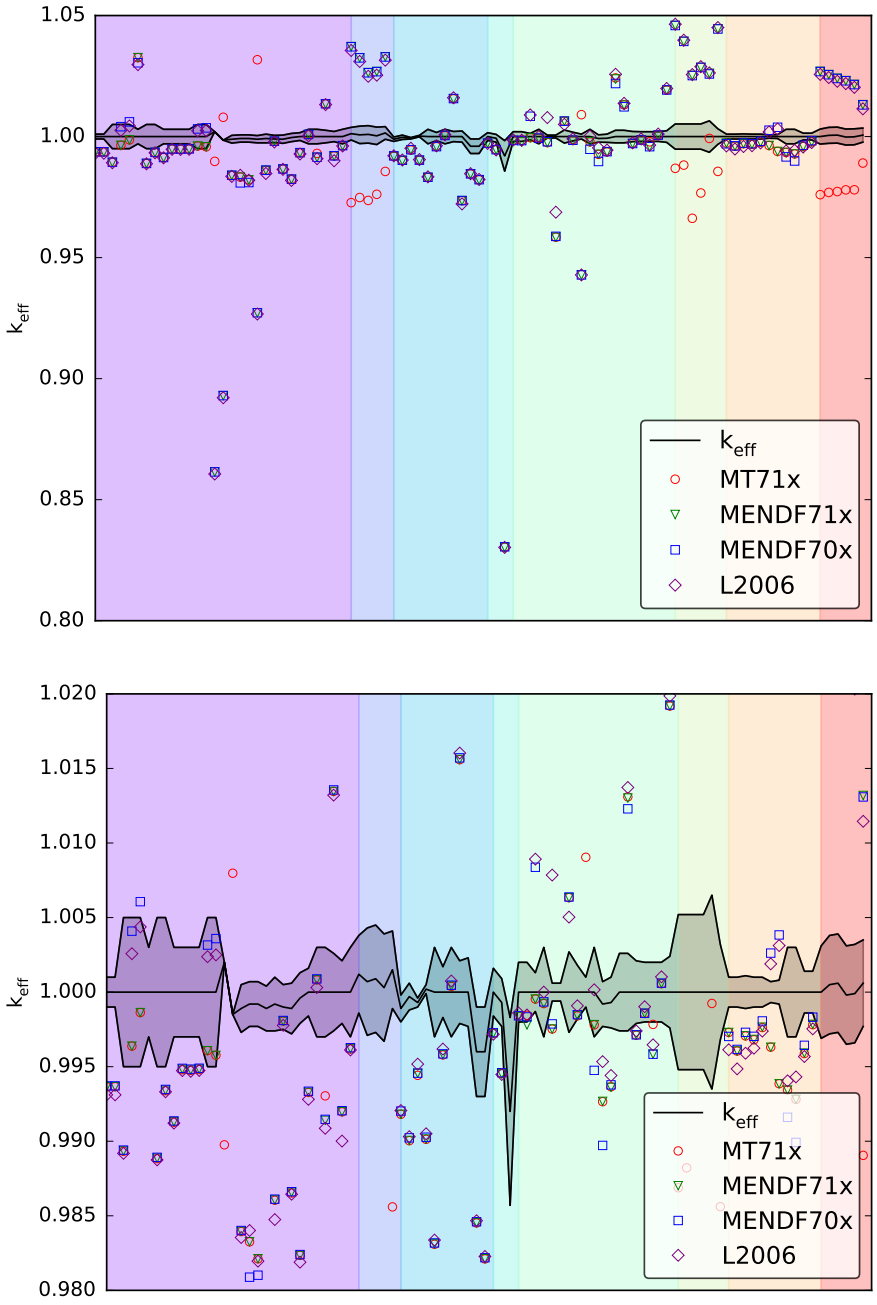

Figure 1: Plot of calculated/modeled k_{eff} for 91 critical assembly benchmarks. The two plots show the same data; the bottom figure shows in expanded detail, results in the vicinity of $k_{\text{eff}} = 1$. The experimental k_{eff} value and uncertainty is shown in the grey shaded region.

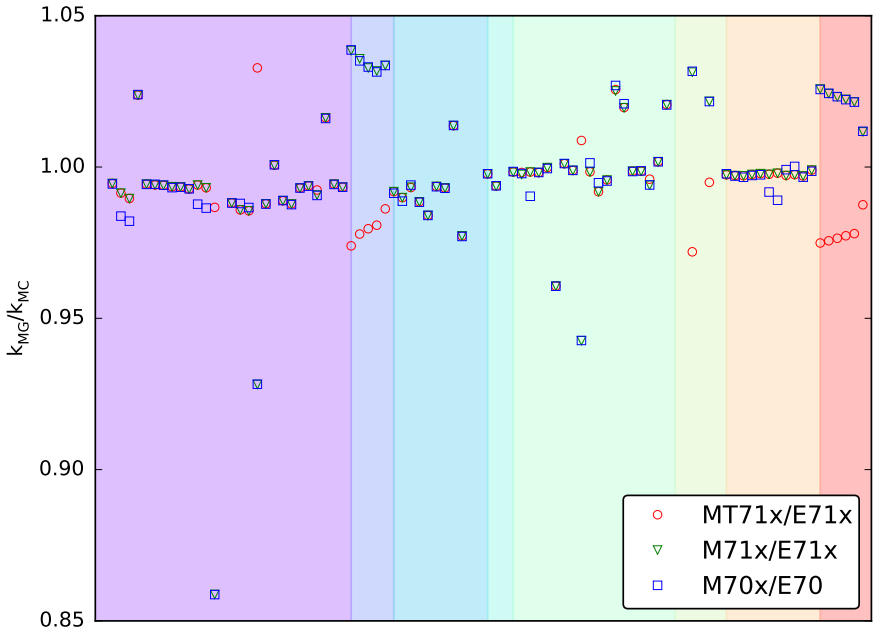

Figure 2: Ratio of multigroup energy to continuous energy k_{eff} values.

in ^{153}Eu where NJOY corrected negative PDF values into very small (i.e., 1×10^{-12}) positive values.

In addition to the checks performed by `checkace`, acceptance test have been performed for every data table in MT71x$_{\text{CE}}$. Like for the multigroup energy library, the acceptance tests consist of a sphere that contains a single isotope. (A sample input deck for these acceptance input decks can be found in Appendix B.) The acceptance tests were performed with MCNP6 for each of the 427 isotopic data tables, for each of the 23 temperatures for a total of 9821 calculations. None of the calculations performed caused fatal errors for MCNP6.

4.2. Validation

The validation of MT71x$_{\text{CE}}$ is much more extensive than the validation for MT71x$_{\text{MG}}$ as we have many more critical benchmark models. We have run a suite of more than 1000 critical benchmark models provided by Skip Kahler (T-2). The calculations were performed using the room temperature data from MT71x. (Benchmarks are not available at elevated temperatures.) The benchmarks are separated into 20 classes:

HEU-MET-FAST	highly enriched uranium metal with a fast spectrum;
HEU-MET-INTER	highly enriched uranium metal with an intermediate spectrum;
HEU-MET-MIXED	highly enriched uranium metal with a mixed spectrum;
HEU-MET-THERM	highly enriched uranium metal with a thermal spectrum;
HEU-SOL-THERM	highly enriched uranium in solution with a thermal spectrum;
IEU-COMP-FAST	intermediate enriched uranium in a compound system with a fast spectrum;
IEU-MET-FAST	intermediate enriched uranium metal with a fast spectrum;
LEU-COMP-THERM	low enriched uranium metal system with a fast spectrum;
LEU-SOL-THERM	low enriched uranium in solution with a thermal spectrum;
MIX-COMP-FAST	mixed plutonium/uranium metal in compound system with a fast spectrum;
MIX-MET-FAST	mixed uranium and plutonium metal with a fast spectrum;
MIX-MET-INTER	mixed uranium and plutonium metal with an intermediate spectrum;
MIX-MET-MIXED	mixed uranium and plutonium metal with a mixed spectrum;
PU-MET-FAST	plutonium metal with fast spectrum;
PU-MET-INTER	plutonium metal with an intermediate spectrum;
PU-SOL-THERM	plutonium in solution with thermal spectrum;
U233-COMP-THERM	^{233}U in a compound system with a thermal spectrum;
U233-MET-FAST	^{233}U metal with fast a spectrum;
U233-SOL-INTER	^{233}U in solution with an intermediate spectrum; and
U233-SOL-THERM	^{233}U in solution with a thermal spectrum.

The colors above are used to identify the classes of benchmarks in the following plots.

Figure 3 shows the k_{eff} values calculated using MCNP6 for MT71x. Included in Figure 3 are the k_{eff} values calculated using the ENDF71x [4] and ENDF70 [25] libraries. A comparison between MT71x and ENDF71x, and ENDF70 and ENDF71x is also given. We can see that the differences in k_{eff} between the the libraries is on the order of 0.5 % to 1.0 %.

5. Conclusion

The Nuclear Data Team in XCP-5 has produced the MT71x library from ENDF/B-VII.1. It has been produced into NDI files for use with NDI version 2.1.2 for deterministic applications and into ACE files for use with NDATK for Monte Carlo applications.

MT71x is suitable for all applications requiring neutron transport—particularly for those with sensitive temperature dependencies.

Please address any questions and problems to the Nuclear Data Team at: nucldata@lanl.gov.

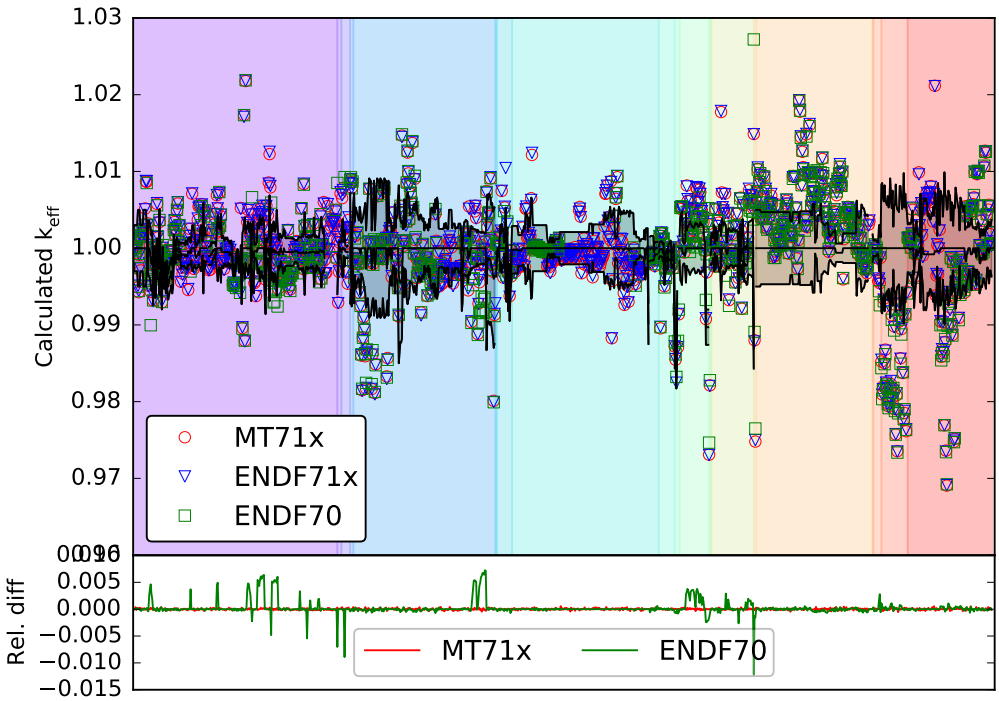

Figure 3: Comparison of k_{eff} values from 1000+ Monte Carlo benchmark calculations. The relative difference plotted is $(k_{\text{ref}} - k)/k_{\text{ref}}$ where k_{ref} is the k_{eff} value from the ENDF71x library.

References

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A. Sample Input Deck for Acceptance Test of Multigroup Energy Data

1001.i

```
2     0     1
1D SPHERE OF TEST MATERIAL
ndi xs
/ block 1
  igeom=sph ngroup=618 isn=8 niso=0 mt=1
 gendir= "/usr/projects/data/nuclear/ndi/devel/share/sn/mt71x/gendir.mt71x.t00"
  nzone=1 im=1 it=100  iquad=1 t
/ block 2
  xmesh=0.0 4.0
  xints=100
  zones=1   t
/ block 3
  lib=ndilib libname=mt71x t
/ block 4
  matls= mat1    "1001.200nm" 1.00000;
  assign=zone1 mat1 10.00;
  matspec= atfrac   t
/ block 5
  source=f1; sourcx=1,f0;
  ievt=0 isct=3 ith=0 ibl=1 ibr=0
  cellsol=1 nthread=16 initaf=1
  epsi=0.0001 trcor=diag norm=1.0 t
/ block 6
  massed=1  zned=1 pted=1
  igrped=0 rsfe=f1; t
```

B. Sample Input Deck for Acceptance Test of Continuous Energy Data

1001.20c_r4_sph_log

```
Hydrogen-1 Sphere at the Origin
C
C
C *** Block 1: Cells ***
1 1 -1.00 -1 imp:n,p=1 $ Sphere of hydrogen-1 centered at the origin
2 0  1 imp:n,p=0 $ The world outside of the hydrogen-1 sphere doesn't matter

C *** Block 2: Surfaces ***
1 so 4 $ Sphere centered at the origin (4 cm radius)

C *** Block 3: Data ***
C
MODE n p $ Track neutrons and photons
C
C
M1 1001.20c 1.0000  $ Hydrogen-1 at room temperature (use density = 1.00 g/cm^3)
C
TMP 2.5301e-8 2.5301e-8 $ The entire universe is at room temperature
C
SDEF pos=0 0 0 erg=d1 rad=d2  $ Isotropic source that emits neutrons uniformly within
C                             $ the volume of the sphere centered at the origin.
C
SI1  H  1.000e-11  1498ilog  2.000e1  $ The source emits neutrons with energies given by a log-u
C                                       $ distribution over the interval [1.000e-11 MeV, 2.0
C                                       $ This distribution is approximated by a histogram w
C                                       $ equally-probable logarithmically-spaced bins.
C
SP1  D   0   1   1498r                  $ All the bins are equally probable. Note that MCNP
C                                       $ enough to normalize this properly, so we can just
C                                       $ as the probability for each bin.
C
SI2 0  4  $ Spherical volumetric source centered at the origin and extending
C                     $ out to a radius of 4 (i.e., source is distributed
C                     $ throughout the volume of the sphere centered at the origin)
C
SP2 -21  2  $ Sample the starting locations of the neutrons
C           $ uniformly throughout the volume of the sphere
C
C
F1:N  1 $ Surface current tally for neutrons leaving the sphere.
E1 1.000e-11  498ilog  2.000e1  $ Use 500 logarithmically-spaced energy bins for this tally
FC1 Surface current of neutrons leaving the Hydrogen-1 sphere
C
F11:P  1 $ Surface current tally for photons leaving the sphere.
E11 1.000e-3  498ilog  2.000e1  $ Use 500 logarithmically-spaced energy bins for this tally
FC11 Surface current of photons leaving the Hydrogen-1 sphere
```

```
C
F2:N  1 $ Surface flux tally for neutrons leaving the sphere.
E2 1.000e-11  498ilog  2.000e1  $ Use 500 logarithmically-spaced energy bins for this tally
FC2 Surface flux of neutrons leaving the Hydrogen-1 sphere
C
F12:P  1 $ Surface flux tally for photons leaving the sphere.
E12 1.000e-3  498ilog  2.000e1  $ Use 500 logarithmically-spaced energy bins for this tally
FC12 Surface flux of photons leaving the Hydrogen-1 sphere
C
F4:N  1 $ Volume flux tally for neutrons inside the sphere.
E4  1.000e-11  498ilog 2.000e1  $ Use 500 logarithmically-spaced energy bins for this tally
FC4 Average flux of neutrons within the Hydrogen-1 sphere
C
F14:P  1 $ Volume flux tally for photons inside the sphere.
E14 1.000e-3  498ilog  2.000e1  $ Use 500 logarithmically-spaced energy bins for this tally
FC14 Average flux of photons within the Hydrogen-1 sphere
C
C
PHYS:N  1.000e2  6j  2.000e2  $ Use a maximum energy (Emax) equal to 5x the maximum energy
C                              $ on the ACE file energy grid for this isotope. Also turn
C                              $ all physics models off (only ACE data will be used).
C
C
PRDMP 1.000e9 1.000e9 1 J 1.000e8 $ Perform a dump to the output file,
C                                  $ the runtpe file, and the mctal file  after every 1.000e9  hi
C                                  $ and use the default mctal format. Also have the multiple pr
C                                  $ and write to the tally fluctuation chart every 1.000e8 parti
NPS 1.000e9     $ Maximum number of particle histories
C
C
PRINT $ Print a full output file
```