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On a formal ENDF format specification language

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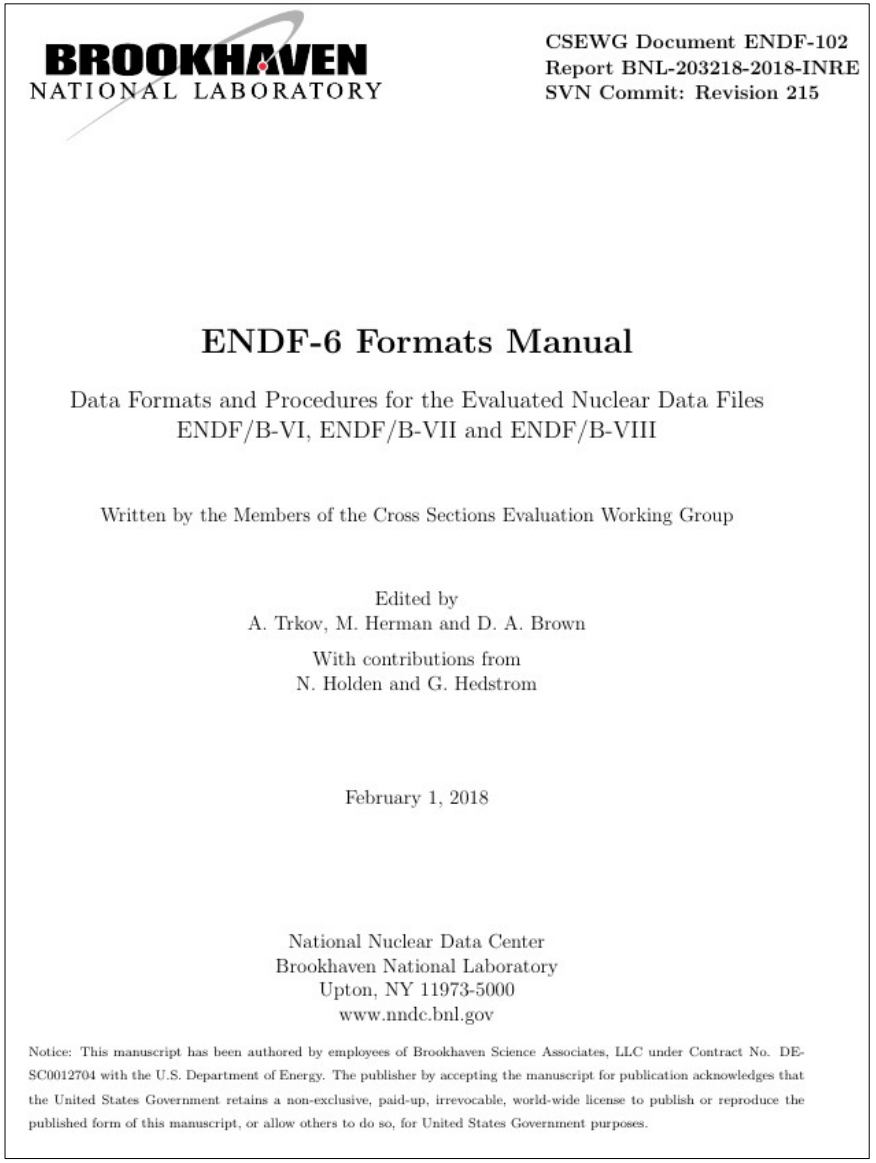
Wouldn’t it be great...



BROOKHAVEN NATIONAL LABORATORY

CSEWG Document ENDF-102
Report BNL-203218-2018-INRE
SVN Commit: Revision 215

ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data Files
ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
A. Trkov, M. Herman and D. A. Brown

With contributions from
N. Holden and G. Hedstrom

February 1, 2018

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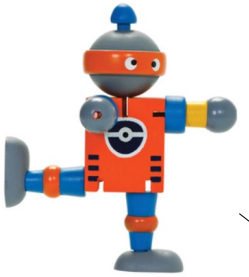
> 300 pages

n_2925_29-Cu-63.endf

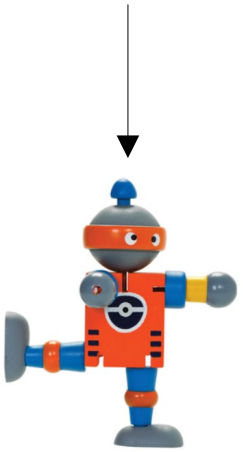


Something beautiful

This could be okay...

The structure of a section is:

```
[MAT, 3, MT/  ZA,  AWR,  0,  0,  0,  0] HEAD
[MAT, 3, MT/  QM,   QI,  0, LR, NR, NP/ E_int/ σ(E)]TAB1
[MAT, 3,  0/ 0.0,  0.0,  0,  0,  0,  0] SEND
```



n_2925_29-Cu-63.endf

JSON

Easy access to values, e.g.,

endf_file[‘ZA’]
endf_file[‘AWR’]

What about this one?

Case B

LFW=1 (fission widths given)

LRF=1 (only fission widths are energy-dependent; the rest are energy-independent).

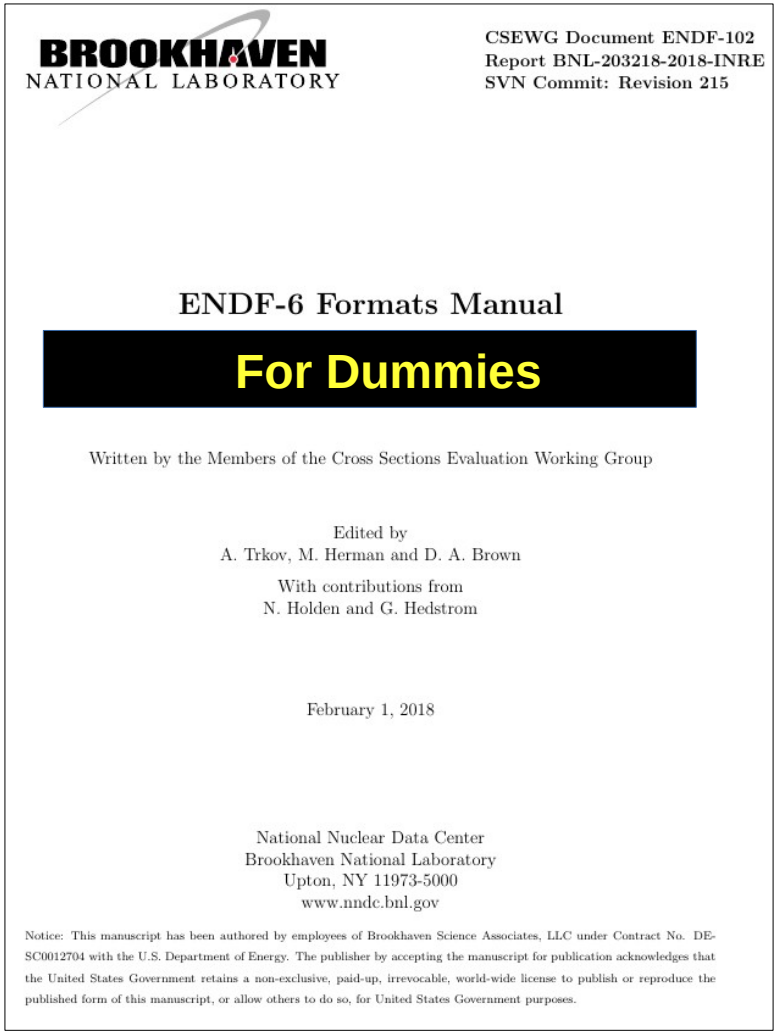
The structure of a subsection is:

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} /AP(E)]TAB1 (if NRO$\neq$ 0)
[MAT, 2,151/ SPI, AP, LSSF, 0, NE, NLS
ES_1, ES_2, ES_3, ----------
---------- ES_{NE}]LIST
[MAT, 2,151/AWRI, 0.0, L, 0, NJS, 0]CONT
[MAT, 2,151/ 0.0, 0.0, L, MUF, NE+6, 0/
D, AJ, AMUN, GNO, GG, 0.0,
GF_1, GF_2, GF_3,----------
---------- GF_{NE}]LIST

The last LIST record is repeated for each J-value (there will be NJS such LIST records). A new CONT(l) record will then be given which will be followed by its NJS LIST records until data for all l-values have been specified (there will be NLS sets of data).

In the above section, no provision was made for INT, and interpolation is assumed to be linear-linear. AMUG is assumed to be zero, AMUF equals MUF, and there is no competitive width.

ENDF manual for Dummies



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ENDF-6 Formats Manual

For Dummies

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So that even stupid computers can understand it.

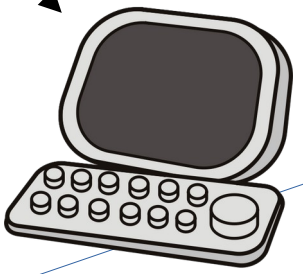
Example MF3 section

[MAT, 3, MT/ ZA, AWR, 0, 0, 0, 0] HEAD
[MAT, 3, MT/ QM, QI, 0, LR, NR, NP/ E_{int}/ $\sigma(E)$]TAB1
[MAT, 3, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND

Already fine for computers

Our first MF3 recipe

[MAT, 3, MT/ ZA, AWR, 0, 0, 0, 0] HEAD
[MAT, 3, MT/ QM, QI, 0, LR, NR, NP/ E_{int}/ $\sigma(E)$]TAB1
[MAT, 3, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND



ENDF format (MF3)

```
0.000000+0 0.000000+0          0          0          0          02925 0  0
2.906300+4 6.238900+1          0          0          0          02925 3  1
0.000000+0 0.000000+0          0          0          1       37492925 3  1
      3749          2                                          2925 3  1
1.000000-5-9.000000-1 2.530000-2-9.000000-1 1.000000+0-9.000000-12925 3  1
1.700000+2 0.000000+0 2.000000+3 0.000000+0 5.500000+4 0.000000+02925 3  1
5.500000+4 2.500000-2 8.500000+4 2.400000-2 9.950000+4 2.100000-22925 3  1
9.950000+4 3.822640+0 9.956090+4 3.531530+0 9.964990+4 3.380950+02925 3  1
9.973900+4 3.161780+0 9.982820+4 3.204480+0 9.991750+4 2.809990+02925 3  1
1.000070+5 2.820410+0 1.000970+5 2.819070+0 1.001860+5 2.856700+02925 3  1
```

JSON

- ZA
- AWR
- MF
- QM
- MT
- QI
- Eint (array)
- Sigma (array)

Out of loops

```
[MAT, 1,451/    ZA,    AWR,    LRP,     LFI,    NLIB,    NMOD]HEAD
[MAT, 1,451/  ELIS,    STA,    LIS,    LISO,       0,    NFOR]CONT
[MAT, 1,451/   AWI,   EMAX,   LREL,       0,    NSUB,    NVER]CONT
[MAT, 1,451/  TEMP,    0.0,   LDRV,       0,     NWD,     NXC]CONT
[MAT, 1,451/ZSYMAM,   ALAB, EDATE,  ...... AUTH ......    ]TEXT
[MAT, 1,451/ ... REF ... , DDATE,  RDATE, ENDATE, blank ]TEXT
[MAT, 1,451/  HSUB                                        ]TEXT
      -----------------------------------
      continue for the rest of the NWD descriptive records
      -----------------------------------
```

Out of loops

```
[MAT, 1,451/    ZA,    AWR,    LRP,     LFI,    NLIB,    NMOD]HEAD
[MAT, 1,451/  ELIS,    STA,    LIS,    LISO,       0,    NFOR]CONT
[MAT, 1,451/   AWI,   EMAX,   LREL,       0,    NSUB,    NVER]CONT
[MAT, 1,451/  TEMP,    0.0,   LDRV,       0,     NWD,     NXC]CONT
[MAT, 1,451/ZSYMAM,   ALAB, EDATE,  ...... AUTH ......    ]TEXT
[MAT, 1,451/ ... REF ... , DDATE,  RDATE, ENDATE, blank ]TEXT
[MAT, 1,451/  HSUB                                        ]TEXT
      ------------------------------------
      continue for the rest of the NWD descriptive records
      ------------------------------------
```

So we have a number of **NWD** TEXT records

Keep computers in the loop

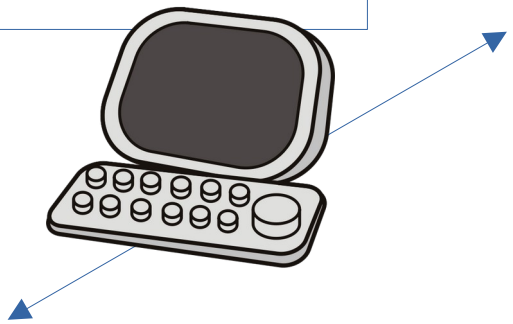
```
[MAT, 1,451/    ZA,    AWR,    LRP,     LFI,    NLIB,    NMOD]HEAD
[MAT, 1,451/  ELIS,    STA,    LIS,    LISO,       0,    NFOR]CONT
[MAT, 1,451/   AWI,   EMAX,   LREL,       0,    NSUB,    NVER]CONT
[MAT, 1,451/  TEMP,    0.0,   LDRV,       0,     NWD,     NXC]CONT
[MAT, 1,451/ZSYMAM,   ALAB, EDATE,  ...... AUTH ......    ]TEXT
[MAT, 1,451/ ... REF ... , DDATE,  RDATE, ENDATE, blank ]TEXT
[MAT, 1,451/  HSUB                                         ]TEXT
      ------------------------------------
      continue for the rest of the NWD descriptive records
      ------------------------------------
```

And here for stupid computers:

```
[MAT, 1,451/ ZA, AWR, LRP, LFI, NLIB, NMOD]HEAD
[MAT, 1,451/ ELIS, STA, LIS, LISO, 0, NFOR]CONT
[MAT, 1,451/ AWI, EMAX, LREL, 0, NSUB, NVER]CONT
[MAT, 1,451/ TEMP, 0.0, LDRV, 0, NWD, NXC]CONT
for i=1 to NWD:
    [MAT, 1,451/ DESCRIPTION[i]]TEXT
endfor
```

MF1/MT451 recipe

```
[MAT, 1,451/ ZA, AWR, LRP, LFI, NLIB, NMOD]HEAD
[MAT, 1,451/ ELIS, STA, LIS, LISO, 0, NFOR]CONT
[MAT, 1,451/ AWI, EMAX, LREL, 0, NSUB, NVER]CONT
[MAT, 1,451/ TEMP, 0.0, LDRV, 0, NWD, NXC]CONT
for i=1 to NWD:
    [MAT, 1,451/ DESCRIPTION[i]]TEXT
endfor
```



JSON

- ZA
- AWR
- MF
- ...
- MT
- DESCRIPTION (array)

```
 2.906300+4 6.238900+1          1          0          0          52925 1451
 0.000000+0 0.000000+0          0          0          0          62925 1451
 1.000000+0 1.500000+8          8          0         10          72925 1451
 0.000000+0 0.000000+0          0          0        481        1152925 1451
 29-Cu- 63 LANL,ORNL  EVAL-FEB98 A.Koning,M.Chadwick,Hetrick      2925 1451
 CH98,CH99            DIST-DEC06 REV4-                 20011108   2925 1451
----ENDF/B-VII        MATERIAL 2925         REVISION 4            2925 1451
-----INCIDENT NEUTRON DATA                                       2925 1451
------ENDF-6 FORMAT                                             2925 1451
```

A list as long as your arm

2.2.1.1 SLBW and MLBW (LRF=1 or 2)

$$
\begin{aligned}
&\texttt{[MAT, 2,151/ AWRI, QX, L, LRX, 6*NRS, NRS}\\
&\qquad \mathrm{ER}_1, \ \mathrm{AJ}_1, \ \mathrm{GT}_1, \ \mathrm{GN}_1, \ \mathrm{GG}_1, \ \mathrm{GF}_1,\\
&\qquad \mathrm{ER}_2, \ \mathrm{AJ}_2, \ \mathrm{GT}_2, \ \mathrm{GN}_2, \ \mathrm{GG}_2, \ \mathrm{GF}_2,\\
&\qquad \mathrm{ER}_{NRS}, \ \mathrm{AJ}_{NRS}, \ \mathrm{GT}_{NRS}, \ \mathrm{GN}_{NRS}, \ \mathrm{GG}_{NRS}, \ \mathrm{GF}_{NRS}\texttt{] LIST}
\end{aligned}
$$

A list as long as your arm

2.2.1.1 SLBW and MLBW (LRF=1 or 2)

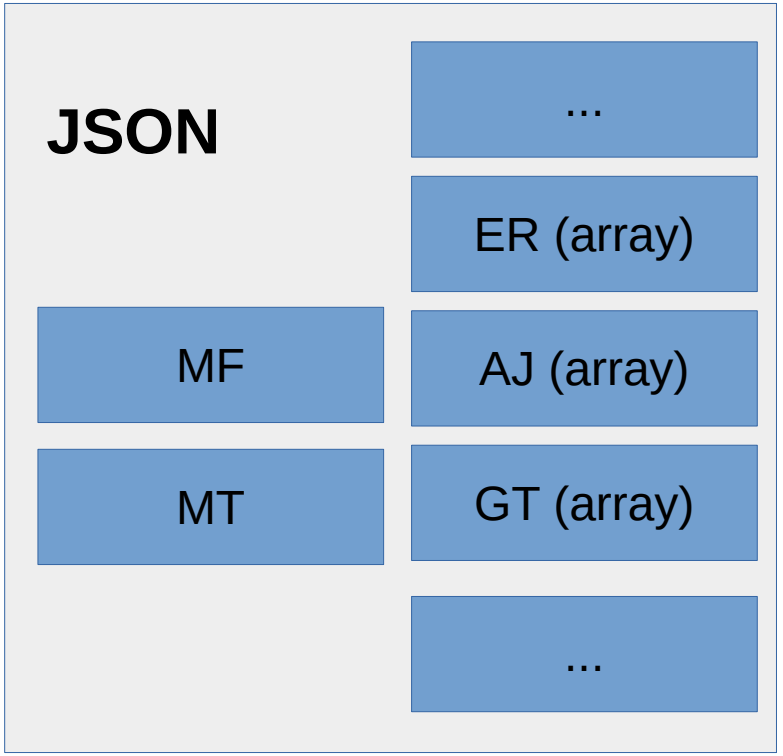
$$
\begin{aligned}
&\texttt{[MAT, 2,151/ AWRI, QX, L, LRX, 6*NRS, NRS}\\
&\qquad \mathrm{ER}_1, \mathrm{AJ}_1, \mathrm{GT}_1, \mathrm{GN}_1, \mathrm{GG}_1, \mathrm{GF}_1,\\
&\qquad \mathrm{ER}_2, \mathrm{AJ}_2, \mathrm{GT}_2, \mathrm{GN}_2, \mathrm{GG}_2, \mathrm{GF}_2,\\
&\qquad \mathrm{ER}_{NRS}, \mathrm{AJ}_{NRS}, \mathrm{GT}_{NRS}, \mathrm{GN}_{NRS}, \mathrm{GG}_{NRS}, \mathrm{GF}_{NRS}\texttt{] LIST}
\end{aligned}
$$

Simplified for our dense computer:

```
[MAT, 2,151/ AWRI, QX, L, LRX, 6*NRS, NRS /
{ER[k], AJ[k], GT[k], GN[k], GG[k], GF[k]}{k=1 to NRS} ]LIST
```

And again JSON...

```
[MAT, 2,151/ AWRI, QX, L, LRX, 6*NRS, NRS /
{ER[k], AJ[k], GT[k], GN[k], GG[k], GF[k]}{k=1 to NRS} ]LIST
```



What if...

4.2.1 Legendre Polynomial Coefficients (LTT=1, LI=0)

When LTT=1 (angular distributions given in terms of Legendre polynomial coefficients), the structure of the section is:

```
[MAT, 4, MT/  ZA, AWR,  0, LTT,  0,  0]HEAD     (LTT=1)
[MAT, 4, MT/ 0.0, AWR, LI, LCT,  0,  0]CONT     (LI=0)
[MAT, 4, MT/ 0.0, 0.0,  0,   0, NR, NE/ E_int]TAB2
[MAT, 4, MT/   T,  E_1, LT,   0, NL,  0/ a_l(E_1)]LIST
[MAT, 4, MT/   T,  E_2, LT,   0, NL,  0/ a_l(E_2)]LIST
   ----------------------------------------
   ----------------------------------------
[MAT, 4, MT/   T,E_NE, LT,   0, NL,  0/ a_l(E_NE)]LIST
[MAT, 4,  0/ 0.0, 0.0,  0,   0,  0,  0]SEND
```

What if… we could use if

4.2.1 Legendre Polynomial Coefficients (LTT=1, LI=0)

When LTT=1 (angular distributions given in terms of Legendre polynomial coefficients), the structure of the section is:

```
[MAT, 4, MT/  ZA, AWR,  0, LTT,  0,  0]HEAD     (LTT=1)
[MAT, 4, MT/ 0.0, AWR, LI, LCT,  0,  0]CONT     (LI=0)
[MAT, 4, MT/ 0.0, 0.0,  0,   0, NR, NE/ E_int]TAB2
[MAT, 4, MT/   T,  E_1, LT,   0, NL,  0/ a_l(E_1)]LIST
[MAT, 4, MT/   T,  E_2, LT,   0, NL,  0/ a_l(E_2)]LIST
   ----------------------------------------
   ----------------------------------------
[MAT, 4, MT/   T,E_NE, LT,   0, NL,  0/ a_l(E_NE)]LIST
[MAT, 4,  0/ 0.0, 0.0,  0,   0,  0,  0]SEND
```

```
# Legendre coefficients
if LTT == 1 and LI == 0:
    [MAT, 4, MT/ 0.0, 0.0, 0, 0, NR, NE/ Eint ]TAB2
    for i=1 to NE:
        [MAT, 4, MT/ T, E[i] , LT, 0, NL[i], 0/ {a[i,l]}{l=1 to NL[i]} ]LIST
    endfor
```

Summary

- The ENDF format description in the manual can be formalized so that even computers can understand it
- By introducing loops, if statements and sections (latter item was not discussed)
- Computers can rely on this “ENDF manual for dummies” to translate ENDF files to JSON and back
- Such a “simplified ENDF manual” that covers most of the ENDF-6 format is available on the IAEA-NDS GitHub account bundled together with a Python package to read and use it:
  - github.com/iaea-nds/endf-parserpy

How can it help in the future?

- Every ENDF format extension that is described in such a simplified ENDF format specification language can be leveraged immediately by ENDF parsers to read, write and verify ENDF files
- All numbers in an ENDF file can be associated with the variable names used in the ENDF manual → The format description at the level of sequence of records becomes irrelevant and all downstream processing can already rely on meaningful variable names
- New processing, verification and data analysis codes (e.g., ML) can have a head start by directly having the variable names available in a well-defined hierarchical structure
- Creating ENDF files becomes easier by creating a JSON file of appropriate structure and converting it to an ENDF file