IAEA

60 Years

Atoms for Peace and Development

Lowering the ENDF-6 entrance barrier for evaluators

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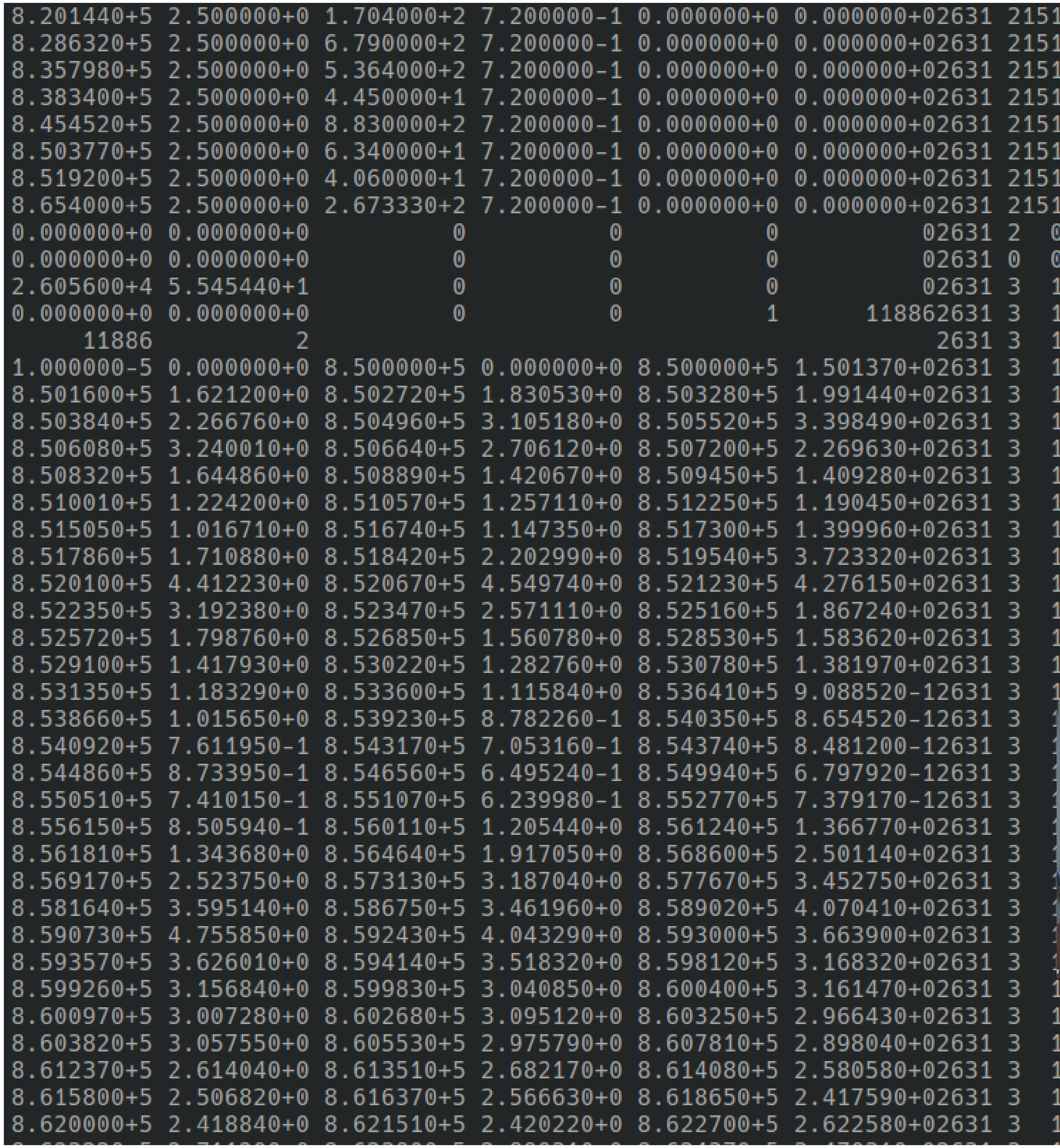
INDEN CM on Structural Materials

18 December 2022

Acknowledgment



```
8.201440+5 2.500000+0 1.704000+2 7.200000-1 0.000000+0 0.000000+02631 2151   320
8.286320+5 2.500000+0 6.790000+2 7.200000-1 0.000000+0 0.000000+02631 2151   321
8.357980+5 2.500000+0 5.364000+2 7.200000-1 0.000000+0 0.000000+02631 2151   322
8.383400+5 2.500000+0 4.450000+1 7.200000-1 0.000000+0 0.000000+02631 2151   323
8.454520+5 2.500000+0 8.830000+2 7.200000-1 0.000000+0 0.000000+02631 2151   324
8.503770+5 2.500000+0 6.340000+1 7.200000-1 0.000000+0 0.000000+02631 2151   325
8.519200+5 2.500000+0 4.060000+1 7.200000-1 0.000000+0 0.000000+02631 2151   326
8.654000+5 2.500000+0 2.673330+2 7.200000-1 0.000000+0 0.000000+02631 2151   327
0.000000+0 0.000000+0          0          0          0          02631 2  099999
0.000000+0 0.000000+0          0          0          0          02631 0  0     0
2.605600+4 5.545440+1          0          0          0          02631 3  1     1
0.000000+0 0.000000+0          0          0          1      118862631 3  1     2
     11886          2                                         2631 3  1     3
1.000000-5 0.000000+0 8.500000+5 0.000000+0 8.500000+5 1.501370+02631 3  1     4
8.501600+5 1.621200+0 8.502720+5 1.830530+0 8.503280+5 1.991440+02631 3  1     5
8.503840+5 2.266760+0 8.504960+5 3.105180+0 8.505520+5 3.398490+02631 3  1     6
8.506080+5 3.240010+0 8.506640+5 2.706120+0 8.507200+5 2.269630+02631 3  1     7
8.508320+5 1.644860+0 8.508890+5 1.420670+0 8.509450+5 1.409280+02631 3  1     8
8.510010+5 1.224200+0 8.510570+5 1.257110+0 8.512250+5 1.190450+02631 3  1     9
8.515050+5 1.016710+0 8.516740+5 1.147350+0 8.517300+5 1.399960+02631 3  1    10
8.517860+5 1.710880+0 8.518420+5 2.202990+0 8.519540+5 3.723320+02631 3  1    11
8.520100+5 4.412230+0 8.520670+5 4.549740+0 8.521230+5 4.276150+02631 3  1    12
8.522350+5 3.192380+0 8.523470+5 2.571110+0 8.525160+5 1.867240+02631 3  1    13
8.525720+5 1.798760+0 8.526850+5 1.560780+0 8.528530+5 1.583620+02631 3  1    14
8.529100+5 1.417930+0 8.530220+5 1.282760+0 8.530780+5 1.381970+02631 3  1    15
8.531350+5 1.183290+0 8.533600+5 1.115840+0 8.536410+5 9.088520-12631 3  1    16
8.538660+5 1.015650+0 8.539230+5 8.782260-1 8.540350+5 8.654520-12631 3
8.540920+5 7.611950-1 8.543170+5 7.053160-1 8.543740+5 8.481200-12631 3
8.544860+5 8.733950-1 8.546560+5 6.495240-1 8.549940+5 6.797920-12631 3
8.550510+5 7.410150-1 8.551070+5 6.239980-1 8.552770+5 7.379170-12631 3
8.556150+5 8.505940-1 8.560110+5 1.205440+0 8.561240+5 1.366770+02631 3
8.561810+5 1.343680+0 8.564640+5 1.917050+0 8.568600+5 2.501140+02631 3
8.569170+5 2.523750+0 8.573130+5 3.187040+0 8.577670+5 3.452750+02631 3
8.581640+5 3.595140+0 8.586750+5 3.461960+0 8.589020+5 4.070410+02631 3
8.590730+5 4.755850+0 8.592430+5 4.043290+0 8.593000+5 3.663900+02631 3
8.593570+5 3.626010+0 8.594140+5 3.518320+0 8.598120+5 3.168320+02631 3
8.599260+5 3.156840+0 8.599830+5 3.040850+0 8.600400+5 3.161470+02631 3  1    27
8.600970+5 3.007280+0 8.602680+5 3.095120+0 8.603250+5 2.966430+02631 3  1    28
8.603820+5 3.057550+0 8.605530+5 2.975790+0 8.607810+5 2.898040+02631 3  1    29
8.612370+5 2.614040+0 8.613510+5 2.682170+0 8.614080+5 2.580580+02631 3  1    30
8.615800+5 2.506820+0 8.616370+5 2.566630+0 8.618650+5 2.417590+02631 3  1    31
8.620000+5 2.418840+0 8.621510+5 2.420220+0 8.622700+5 2.622580+02631 3  1    32
```

Daniel Lopez Aldama
(IAEA Consultant)

https://github.com/iaea-nds/acemaker

How to put nuclear data into an ENDF-6 formatted file?

Paths to ENDF-6 file creation

- Model code systems (e.g. Talys and Empire)
- Statistical evaluation systems (e.g. GANDR)
- Packages to interact with ENDF-6 formatted files

Popular and recent packages

Reading & Writing

- SANDY
- DeCE
- ENDFtk?

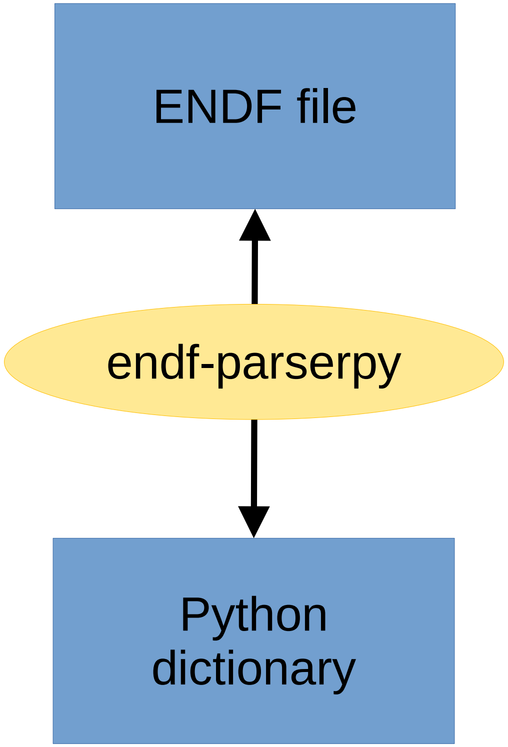
Only reading

- Endf-parser
- PyNE

Two (+one) requirements

- Support reading and writing of entire ENDF-6 format
- Convenient use from a data science language (e.g. Python)
- *Provably correct*

Basic design

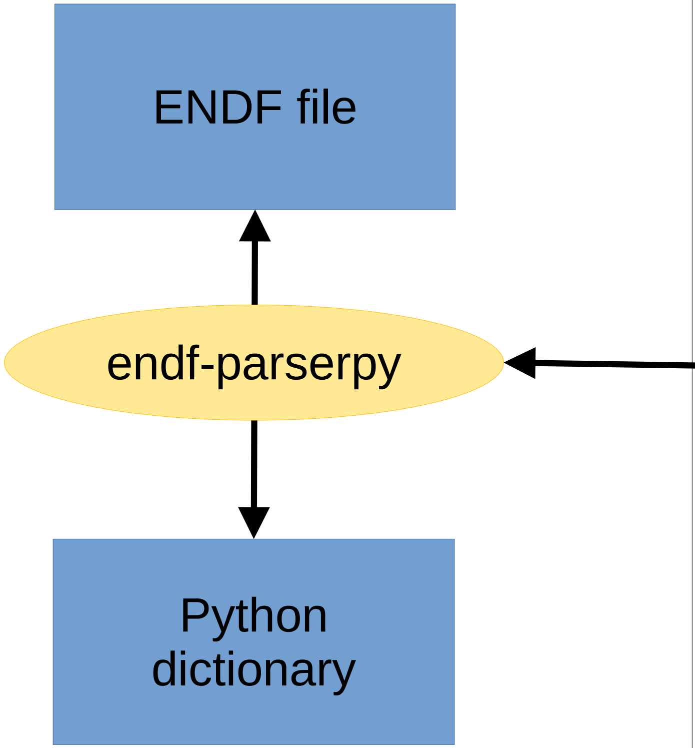


ENDF file

endf-parserpy

Python dictionary

Basic design

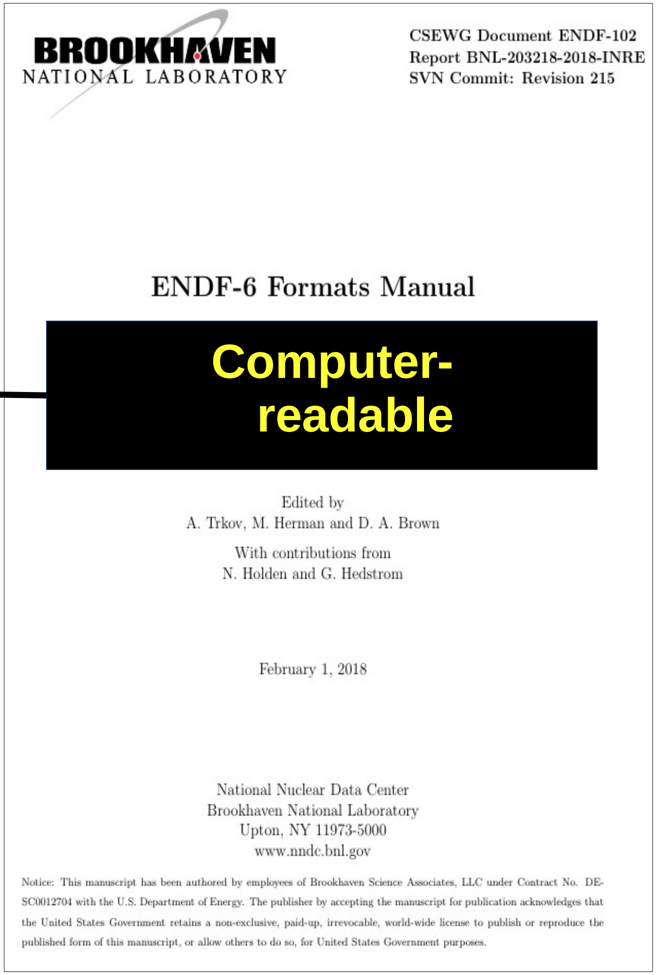


ENDF file

endf-parserpy

Python dictionary

Computer-readable



BROOKHAVEN
NATIONAL LABORATORY

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

ENDF-6 Formats Manual

Edited by
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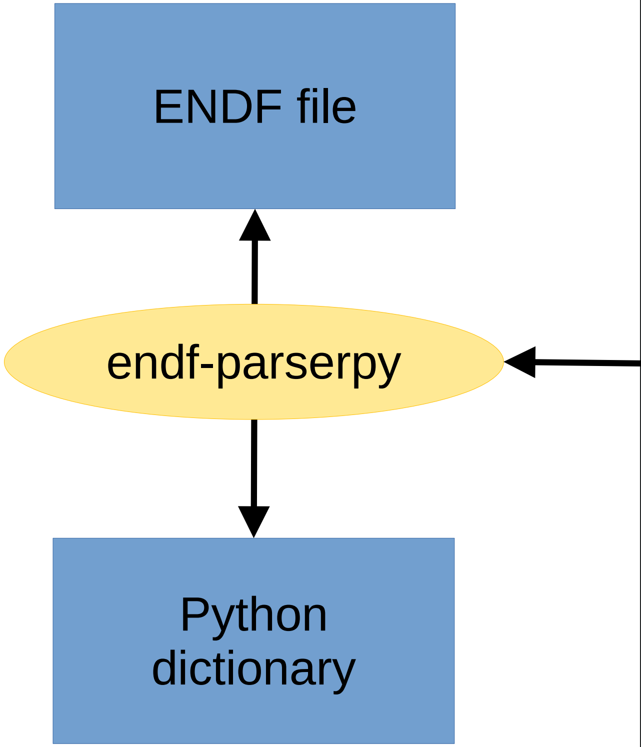
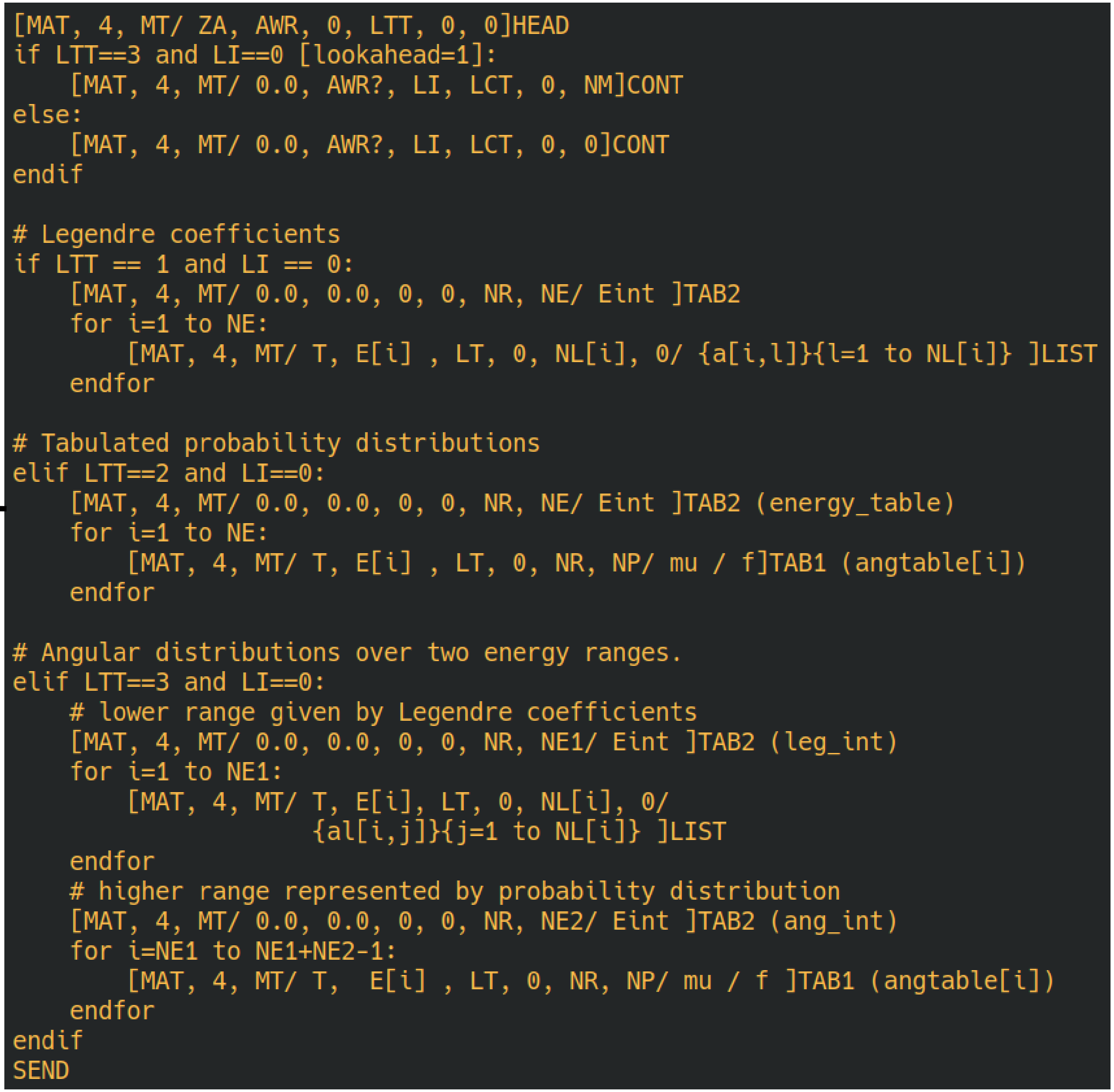
Formal ENDF format description



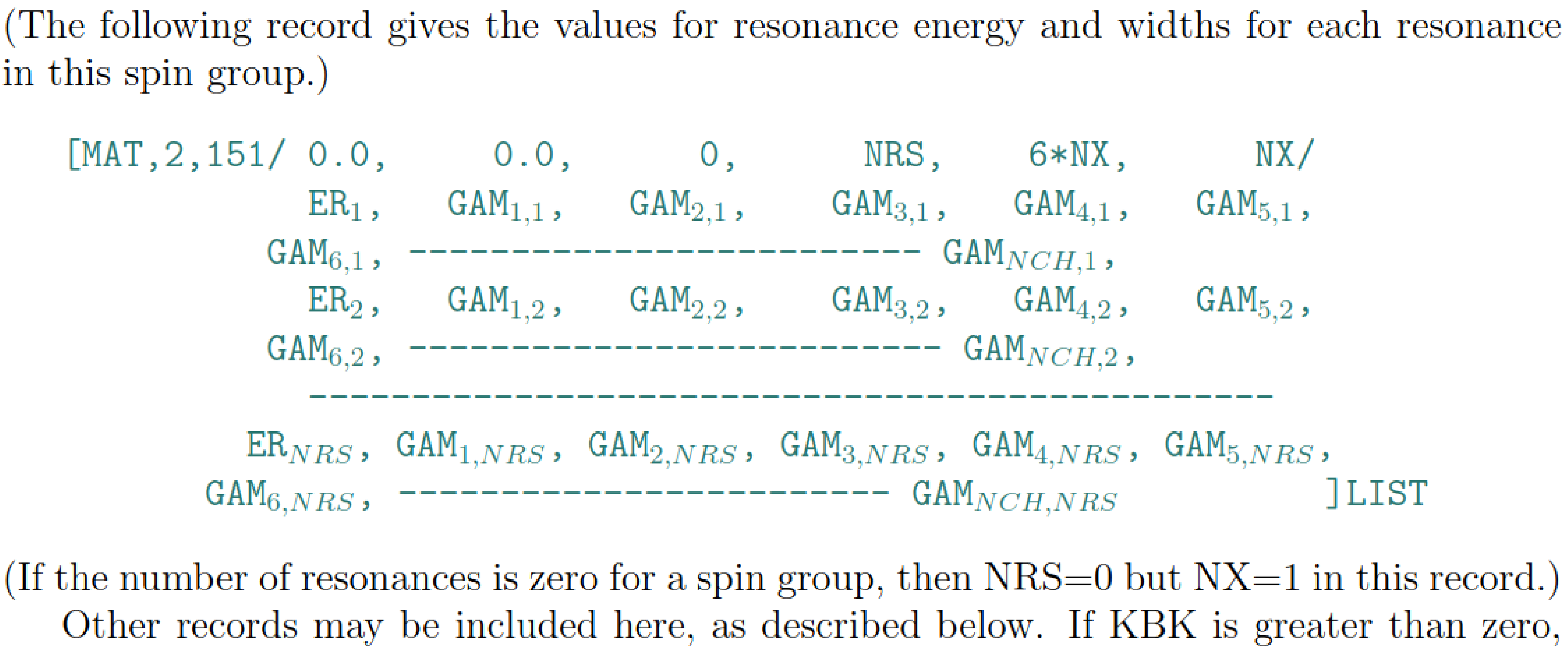


```
[MAT, 4, MT/ ZA, AWR, 0, LTT, 0, 0]HEAD
if LTT==3 and LI==0 [lookahead=1]:
    [MAT, 4, MT/ 0.0, AWR?, LI, LCT, 0, NM]CONT
else:
    [MAT, 4, MT/ 0.0, AWR?, LI, LCT, 0, 0]CONT
endif

# 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

# Tabulated probability distributions
elif LTT==2 and LI==0:
    [MAT, 4, MT/ 0.0, 0.0, 0, 0, NR, NE/ Eint ]TAB2 (energy_table)
    for i=1 to NE:
        [MAT, 4, MT/ T, E[i] , LT, 0, NR, NP/ mu / f]TAB1 (angtable[i])
    endfor

# Angular distributions over two energy ranges.
elif LTT==3 and LI==0:
    # lower range given by Legendre coefficients
    [MAT, 4, MT/ 0.0, 0.0, 0, 0, NR, NE1/ Eint ]TAB2 (leg_int)
    for i=1 to NE1:
        [MAT, 4, MT/ T, E[i], LT, 0, NL[i], 0/
                     {al[i,j]}{j=1 to NL[i]} ]LIST
    endfor
    # higher range represented by probability distribution
    [MAT, 4, MT/ 0.0, 0.0, 0, 0, NR, NE2/ Eint ]TAB2 (ang_int)
    for i=NE1 to NE1+NE2-1:
        [MAT, 4, MT/ T,  E[i] , LT, 0, NR, NP/ mu / f ]TAB1 (angtable[i])
    endfor
endif
SEND
```

“How to explain ENDF-6 to computers: A formal ENDF description language”, arXiv:2312.08249

Provably correct

- The ENDF-6 format manual is incomplete/misleading* for LRF=7
- Result: some divergence between packages



(The following record gives the values for resonance energy and widths for each resonance in this spin group.)

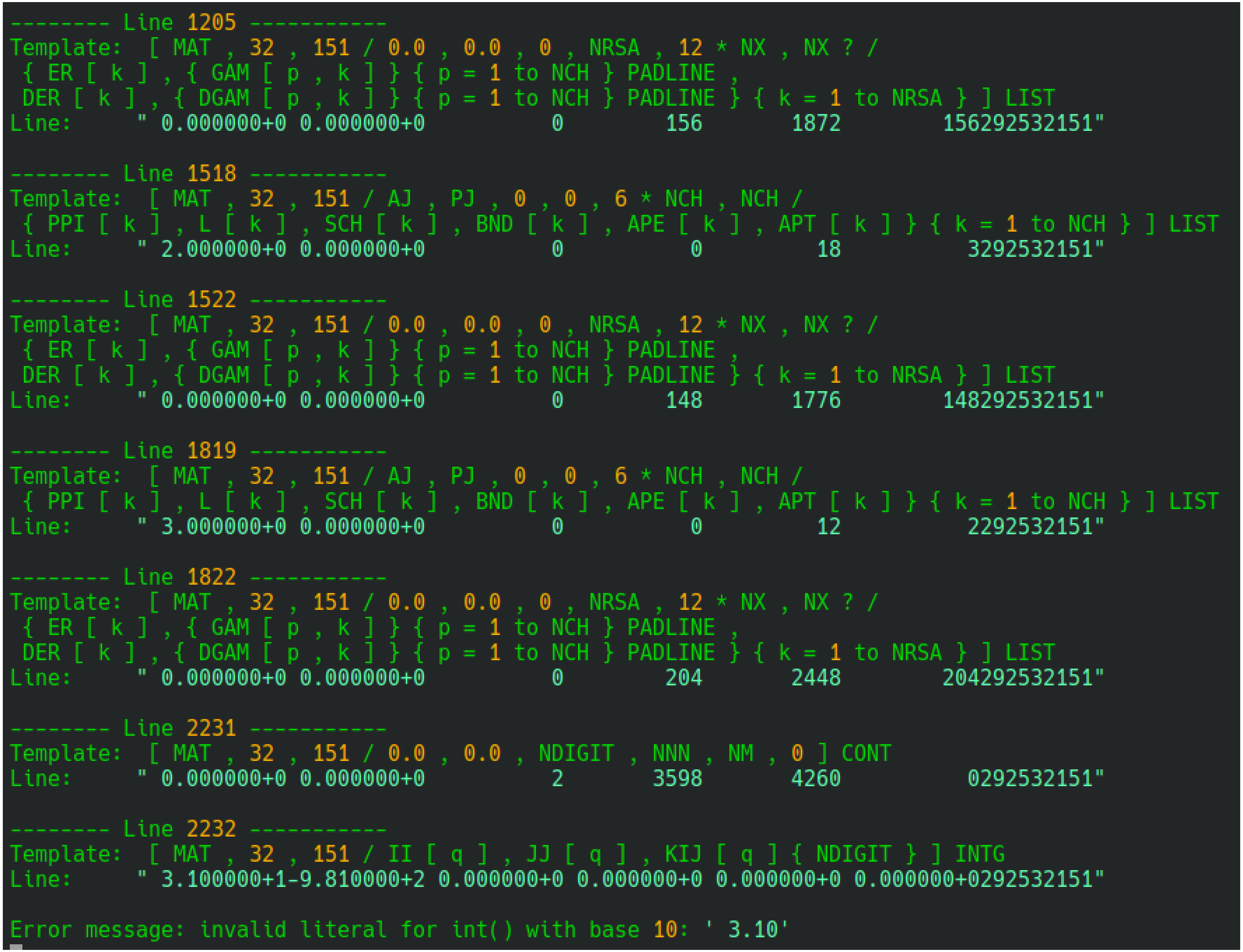
[MAT,2,151/ 0.0, 0.0, 0, NRS, 6*NX, NX/
ER_1, $\mathrm{GAM}_{1,1}$, $\mathrm{GAM}_{2,1}$, $\mathrm{GAM}_{3,1}$, $\mathrm{GAM}_{4,1}$, $\mathrm{GAM}_{5,1}$,
$\mathrm{GAM}_{6,1}$, -------------------------- $\mathrm{GAM}_{NCH,1}$,
ER_2, $\mathrm{GAM}_{1,2}$, $\mathrm{GAM}_{2,2}$, $\mathrm{GAM}_{3,2}$, $\mathrm{GAM}_{4,2}$, $\mathrm{GAM}_{5,2}$,
$\mathrm{GAM}_{6,2}$, --------------------------- $\mathrm{GAM}_{NCH,2}$,
----
ER_{NRS}, $\mathrm{GAM}_{1,NRS}$, $\mathrm{GAM}_{2,NRS}$, $\mathrm{GAM}_{3,NRS}$, $\mathrm{GAM}_{4,NRS}$, $\mathrm{GAM}_{5,NRS}$,
$\mathrm{GAM}_{6,NRS}$, ------------------------- $\mathrm{GAM}_{NCH,NRS}$]LIST

(If the number of resonances is zero for a spin group, then NRS=0 but NX=1 in this record.)

Other records may be included here, as described below. If KBK is greater than zero,

* or at the very least inconsistent with ENDF/B-VIII.0

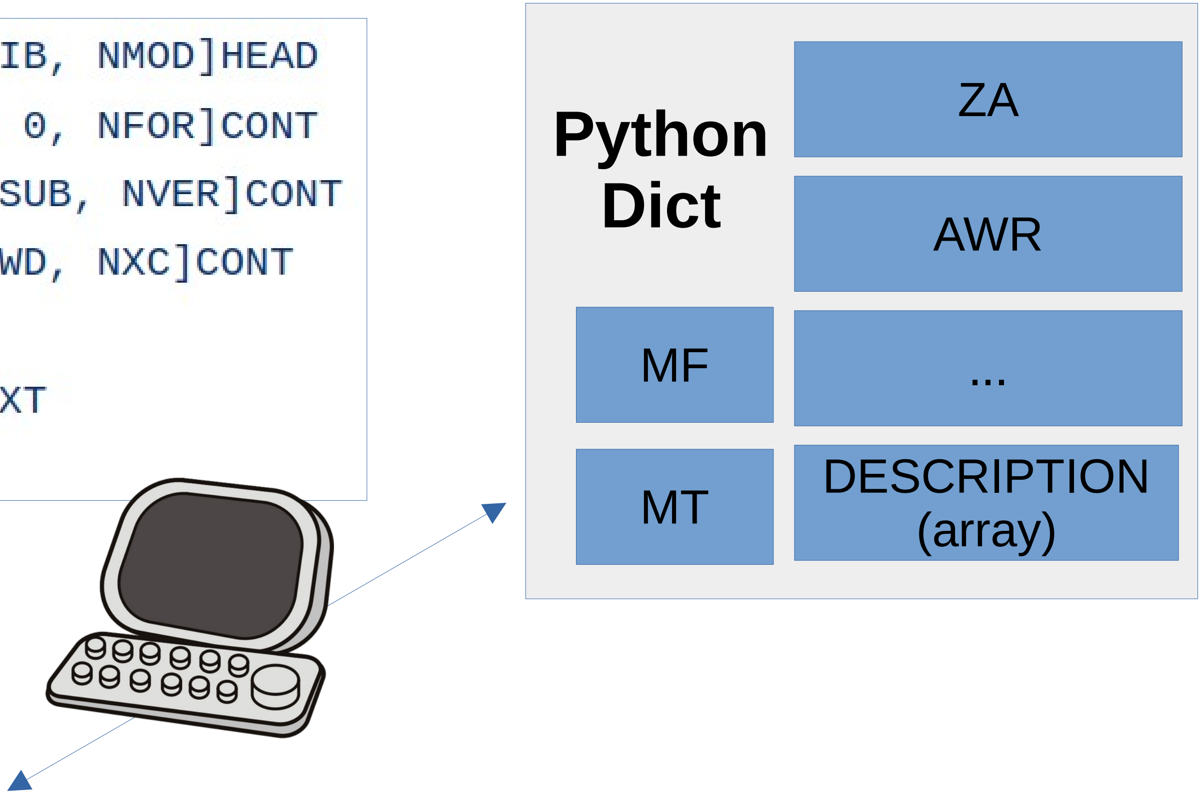
Example of format checking: Cu-63

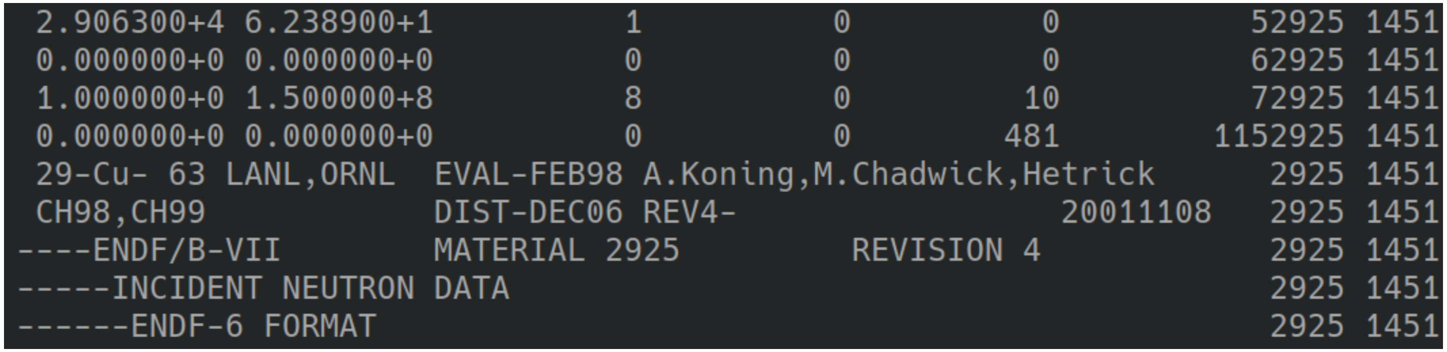


```
-------- Line 1205 -----------
Template:  [ MAT , 32 , 151 / 0.0 , 0.0 , 0 , NRSA , 12 * NX , NX ? /
 { ER [ k ] , { GAM [ p , k ] } { p = 1 to NCH } PADLINE ,
 DER [ k ] , { DGAM [ p , k ] } { p = 1 to NCH } PADLINE } { k = 1 to NRSA } ] LIST
Line:     " 0.000000+0 0.000000+0          0        156       1872        156292532151"

-------- Line 1518 -----------
Template:  [ MAT , 32 , 151 / AJ , PJ , 0 , 0 , 6 * NCH , NCH /
 { PPI [ k ] , L [ k ] , SCH [ k ] , BND [ k ] , APE [ k ] , APT [ k ] } { k = 1 to NCH } ] LIST
Line:     " 2.000000+0 0.000000+0          0          0         18          3292532151"

-------- Line 1522 -----------
Template:  [ MAT , 32 , 151 / 0.0 , 0.0 , 0 , NRSA , 12 * NX , NX ? /
 { ER [ k ] , { GAM [ p , k ] } { p = 1 to NCH } PADLINE ,
 DER [ k ] , { DGAM [ p , k ] } { p = 1 to NCH } PADLINE } { k = 1 to NRSA } ] LIST
Line:     " 0.000000+0 0.000000+0          0        148       1776        148292532151"

-------- Line 1819 -----------
Template:  [ MAT , 32 , 151 / AJ , PJ , 0 , 0 , 6 * NCH , NCH /
 { PPI [ k ] , L [ k ] , SCH [ k ] , BND [ k ] , APE [ k ] , APT [ k ] } { k = 1 to NCH } ] LIST
Line:     " 3.000000+0 0.000000+0          0          0         12          2292532151"

-------- Line 1822 -----------
Template:  [ MAT , 32 , 151 / 0.0 , 0.0 , 0 , NRSA , 12 * NX , NX ? /
 { ER [ k ] , { GAM [ p , k ] } { p = 1 to NCH } PADLINE ,
 DER [ k ] , { DGAM [ p , k ] } { p = 1 to NCH } PADLINE } { k = 1 to NRSA } ] LIST
Line:     " 0.000000+0 0.000000+0          0        204       2448        204292532151"

-------- Line 2231 -----------
Template:  [ MAT , 32 , 151 / 0.0 , 0.0 , NDIGIT , NNN , NM , 0 ] CONT
Line:     " 0.000000+0 0.000000+0          2       3598       4260          0292532151"

-------- Line 2232 -----------
Template:  [ MAT , 32 , 151 / II [ q ] , JJ [ q ] , KIJ [ q ] { NDIGIT } ] INTG
Line:     " 3.100000+1-9.810000+2 0.000000+0 0.000000+0 0.000000+0 0.000000+0292532151"

Error message: invalid literal for int() with base 10: ' 3.10'
```

Basic translation

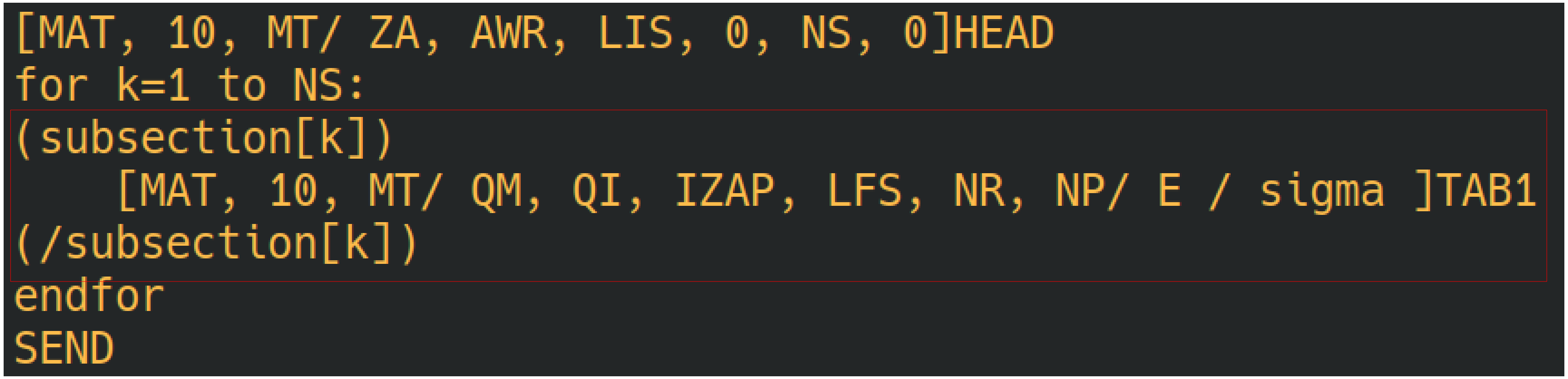
```
[MAT, 1,451/ ZA, AWR, LRP, LFI, NLIB, NMOD]HEAD
[MAT, 1,451/ ELIS, STA, LIS, LISO, 0, NFOR]CONT
[MAT, 1,451/ AWI, EMAX, LREL, 0, NSUB, NVER]CONT
[MAT, 1,451/ TEMP, 0.0, LDRV, 0, NWD, NXC]CONT
for i=1 to NWD:
    [MAT, 1,451/ DESCRIPTION[i]]TEXT
endfor
```



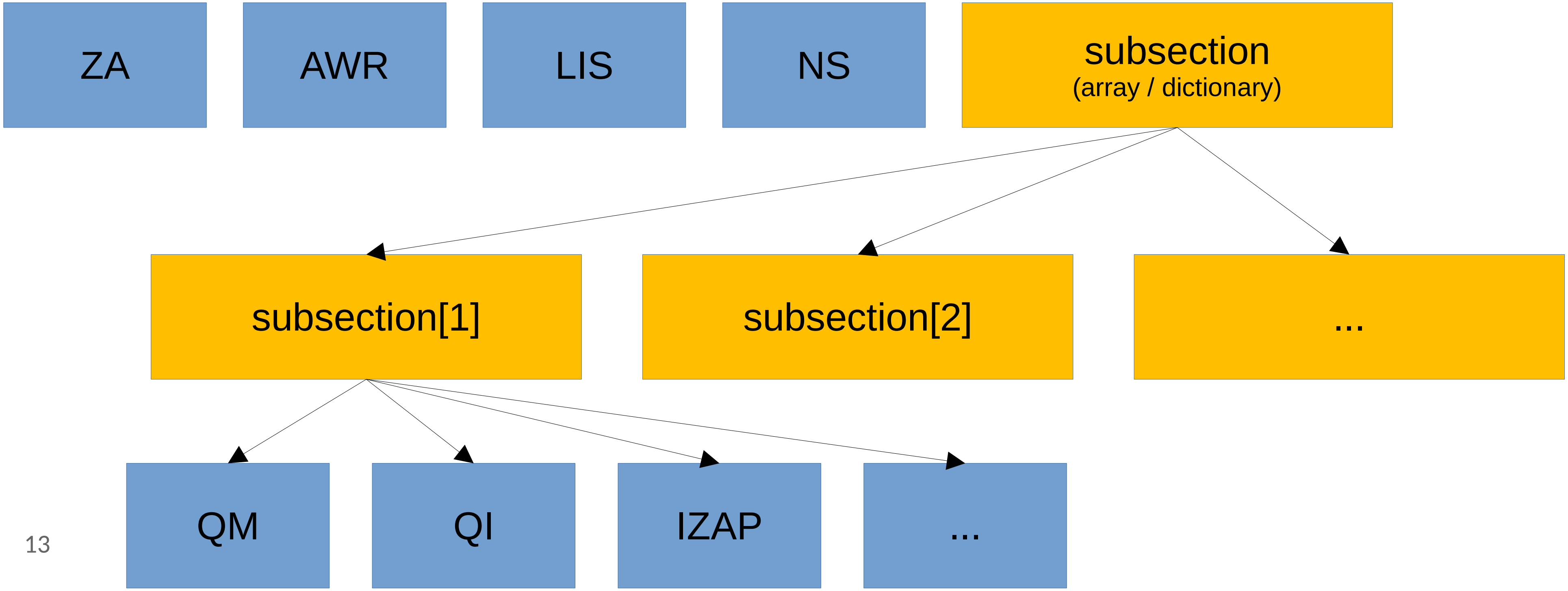


```
 2.906300+4 6.238900+1          1          0          0          52925 1451
 0.000000+0 0.000000+0          0          0          0          62925 1451
 1.000000+0 1.500000+8          8          0         10          72925 1451
 0.000000+0 0.000000+0          0          0        481       1152925 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
```

Allowing for nesting: Sections



```
[MAT, 10, MT/ ZA, AWR, LIS, 0, NS, 0]HEAD
for k=1 to NS:
(subsection[k])
    [MAT, 10, MT/ QM, QI, IZAP, LFS, NR, NP/ E / sigma ]TAB1
(/subsection[k])
endfor
SEND
```



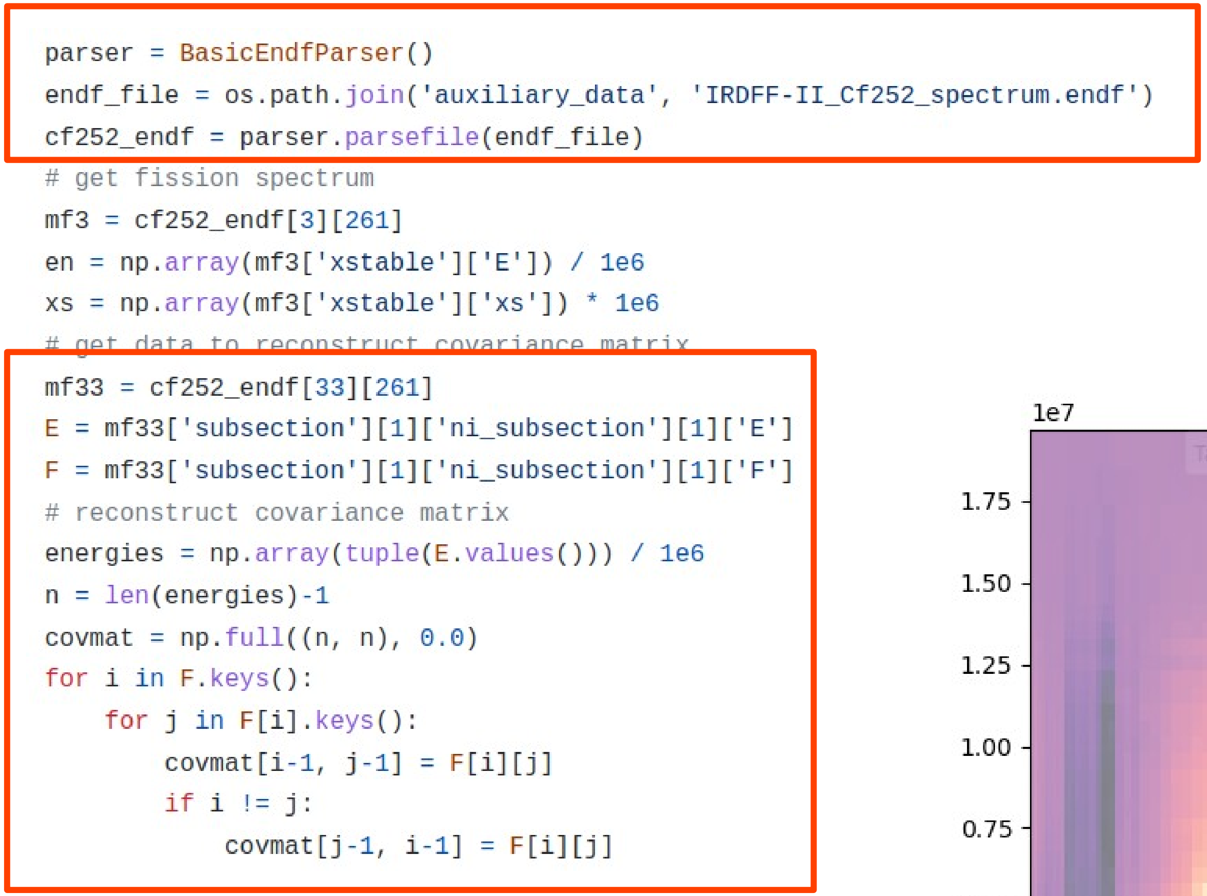
Example of use: Changing (n,tot) cross section

```
from endf_parserpy import ExtEndfParser

parser = ExtEndfParser()
endf_dict = parser.parsefile("input.endf")




parser.writefile("output.endf", endf_dict)
```

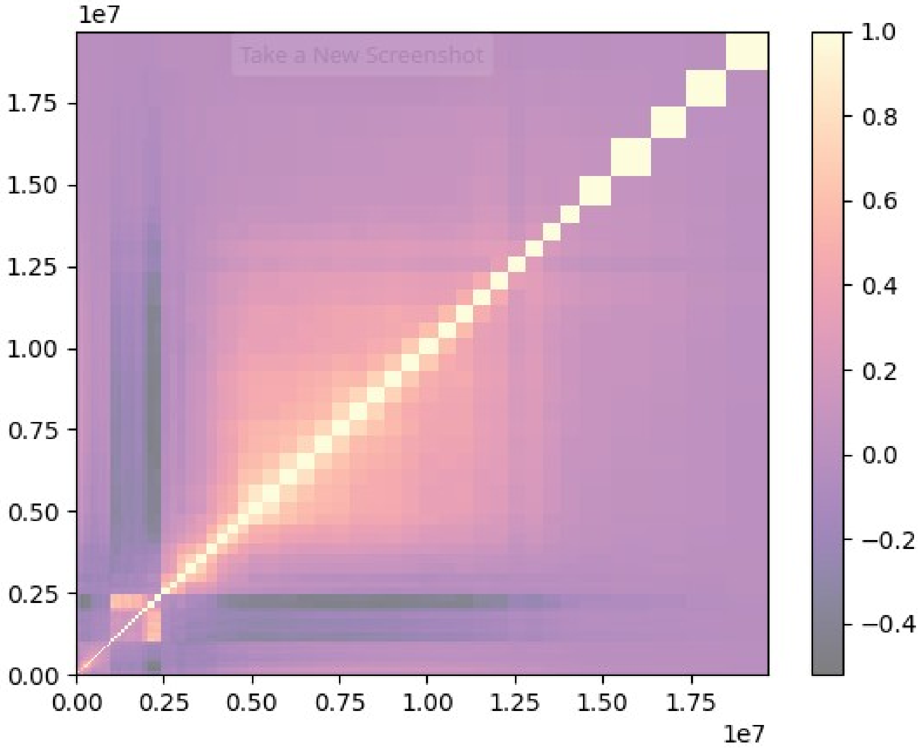
Example of use:
Changing (n,tot) cross section

```
from endf_parserpy import ExtEndfParser

parser = ExtEndfParser()
endf_dict = parser.parsefile("input.endf")

updated_energies = np.linspace(1e6, 1e8, 100)

endf_dict[3][1]['xstable']['E'] = updated_energies
endf_dict[3][1]['xstable']['xs'] = np.sin(updated_energies) + 2

endf_dict[3][1]['xstable']['NBT'] = [len(updated_energies)]
endf_dict[3][1]['xstable']['INT'] = [2]

parser.writefile("output.endf”, endf_dict)
```

Covariance retrieval example



```
parser = BasicEndfParser()
endf_file = os.path.join('auxiliary_data', 'IRDFF-II_Cf252_spectrum.endf')
cf252_endf = parser.parsefile(endf_file)
# get fission spectrum
mf3 = cf252_endf[3][261]
en = np.array(mf3['xstable']['E']) / 1e6
xs = np.array(mf3['xstable']['xs']) * 1e6
# get data to reconstruct covariance matrix
mf33 = cf252_endf[33][261]
E = mf33['subsection'][1]['ni_subsection'][1]['E']
F = mf33['subsection'][1]['ni_subsection'][1]['F']
# reconstruct covariance matrix
energies = np.array(tuple(E.values())) / 1e6
n = len(energies)-1
covmat = np.full((n, n), 0.0)
for i in F.keys():
    for j in F[i].keys():
        covmat[i-1, j-1] = F[i][j]
        if i != j:
            covmat[j-1, i-1] = F[i][j]
```



https://github.com/IAEA-NDS/neutron-standards-database/blob/main/codes/database_modifications/use_irdff_cf252_spectrum.py

Translation between representations

Translation between representations

endf-parserpy

ENDF-6

Python dictionary

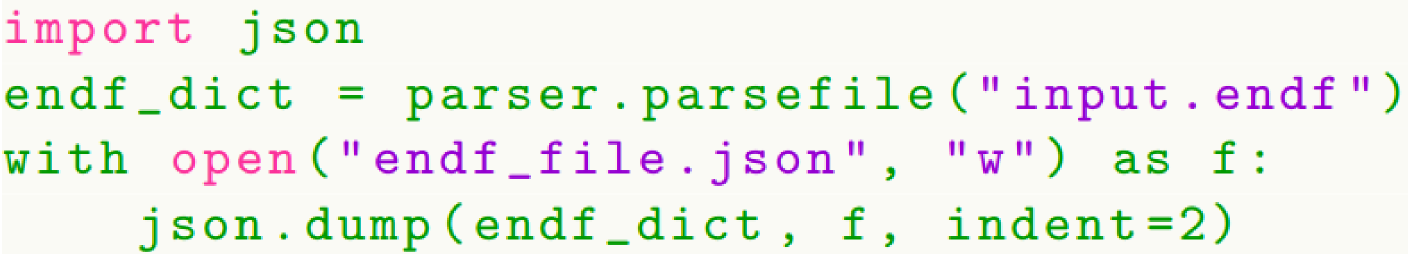
Translation between representations

FUDGE

ENDF-6

GNDS

Translation between representations

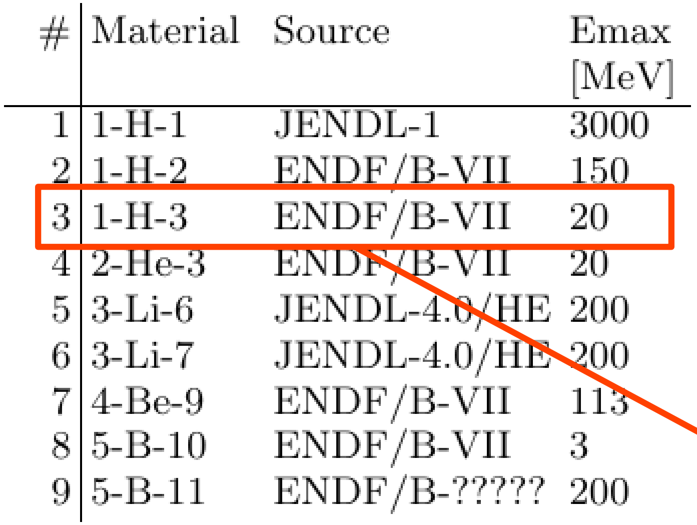


```
import json
endf_dict = parser.parsefile("input.endf")
with open("endf_file.json", "w") as f:
    json.dump(endf_dict, f, indent=2)
```

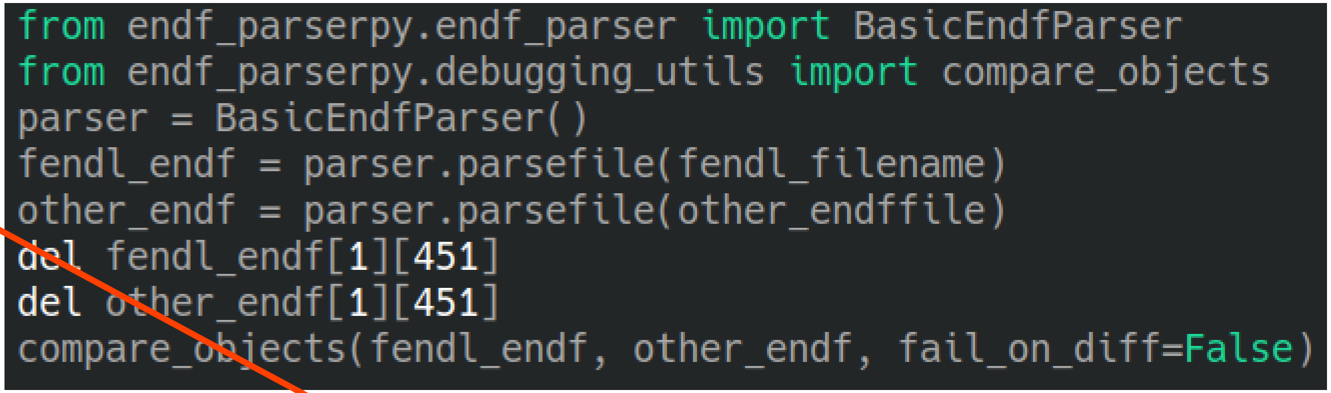
Python dictionary

JSON

Advanced diff functionality (Provenance checking in FENDL)

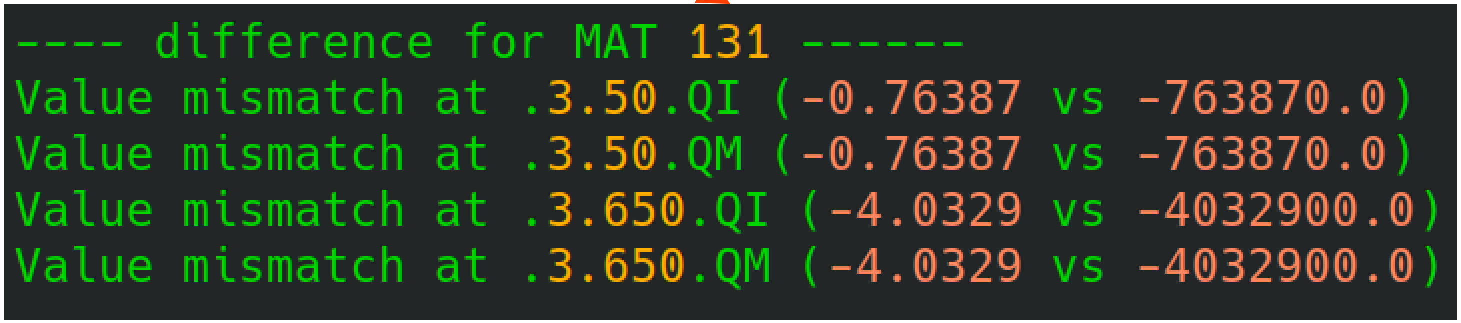


#	Material	Source	Emax [MeV]
1	1-H-1	JENDL-1	3000
2	1-H-2	ENDF/B-VII	150
3	1-H-3	ENDF/B-VII	20
4	2-He-3	ENDF/B-VII	20
5	3-Li-6	JENDL-4.0/HE	200
6	3-Li-7	JENDL-4.0/HE	200
7	4-Be-9	ENDF/B-VII	113
8	5-B-10	ENDF/B-VII	3
9	5-B-11	ENDF/B-?????	200



```
from endf_parserpy.endf_parser import BasicEndfParser
from endf_parserpy.debugging_utils import compare_objects
parser = BasicEndfParser()
fendl_endf = parser.parsefile(fendl_filename)
other_endf = parser.parsefile(other_endffile)
del fendl_endf[1][451]
del other_endf[1][451]
compare_objects(fendl_endf, other_endf, fail_on_diff=False)
```

FENDL 3.2b = ENDF/B.VII.0



```
---- difference for MAT 131 ------
Value mismatch at .3.50.QI (-0.76387 vs -763870.0)
Value mismatch at .3.50.QM (-0.76387 vs -763870.0)
Value mismatch at .3.650.QI (-4.0329 vs -4032900.0)
Value mismatch at .3.650.QM (-4.0329 vs -4032900.0)
```

Comparison with ENDF/B-VII.1

Summary

- New Python package for ENDF-6 formatted files enabling:
  - Reading
  - Writing
  - Translating
  - Verifying
- Supports (nearly) the entire ENDF-6 format
- Provably correct implementation
- Assembling an ENDF-6 file becomes much easier:
  - Working with symbol names instead of locations
  - Leveraging powerful data science capabilities of Python