IAEA 60 Years
Atoms for Peace and Development

YANDF: Yet another Nuclear Data Format
or
YANDF: YANDL Ain't Nuclear Data Format

Arjan Koning, IAEA

IAEA Meeting, January 15-19 2024

Introduction

- TALYS: plan to make output (even) more consistent
- Some data formats: GNDS, TALYS, ENDF, EXFOR
- Attempt to unify, at least, EXFOR, TALYS and ENDF, with a “light” format
- Your opinion, please

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Review

TALYS: modeling of nuclear reactions

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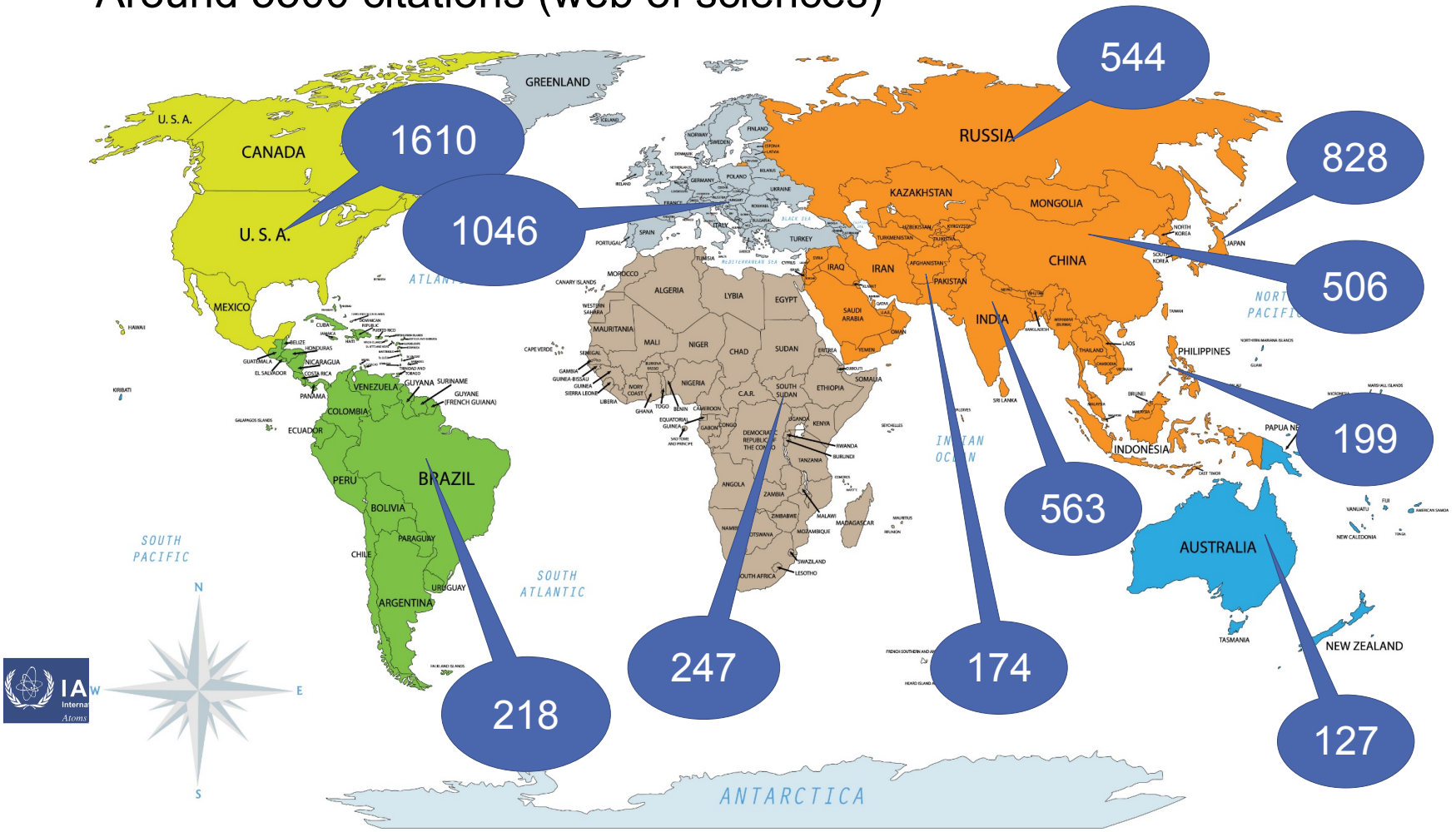
Communicated by Nicolas Alamanos

Abstract TALYS is a software package for the simulation of nuclear reactions below 200 MeV. It is used worldwide for the analysis and prediction of nuclear reactions and is based on state-of-art nuclear structure and nuclear reaction models. A general overview of the implemented physics and capabilities of TALYS is given. The general nuclear reaction mechanisms described are the optical model, direct reactions, compound nucleus model, pre-equilibrium reactions and fission. The most important nuclear structure models are those for masses, discrete levels, level densities, photon strength

TALYS around the World

- Around 5500 citations (web of sciences)



Never ending question: Is the input and output interfacing still up to date?

TALYS

TALYS-Related Software and Databases

TALYS and the TALYS-related packages are open source software and datasets (MIT License) for the simulation of nuclear reactions.

TALYS

Arjan Koning, Stephane Hilaire, Stephane Goriely

Nuclear reaction model code.

- Download TALYS-2.0 or TALYS-1.97
- Download previous versions
- Read Tutorial
- Cite Reference
- Use TALYSworld
- Access on GitHub

Created at NRG CEA ULB IAEA

TASMAN

Arjan Koning

Statistical software for TALYS: Uncertainties, sensitivities and optimization.

- Download TASMAN-2.0
- Read Tutorial
- Access on GitHub

TEFAL

Arjan Koning

Code to make ENDF-6 nuclear data libraries from TALYS.

- Download TEFAL-2.0
- Read Tutorial
- Access on GitHub

EXFORTABLES

Arjan Koning

ENDFTABLES

Arjan Koning

Arjan Koning

arjankoning1

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2 followers · **0** following

Popular repositories

Customize your pins

endftables — Public
Code to translate ENDF-6 file into x-y tables
Fortran

talys — Public
The nuclear reaction model code
Fortran

tefal — Public
Making ENDF-6 nuclear data libraries with TALYS
Fortran

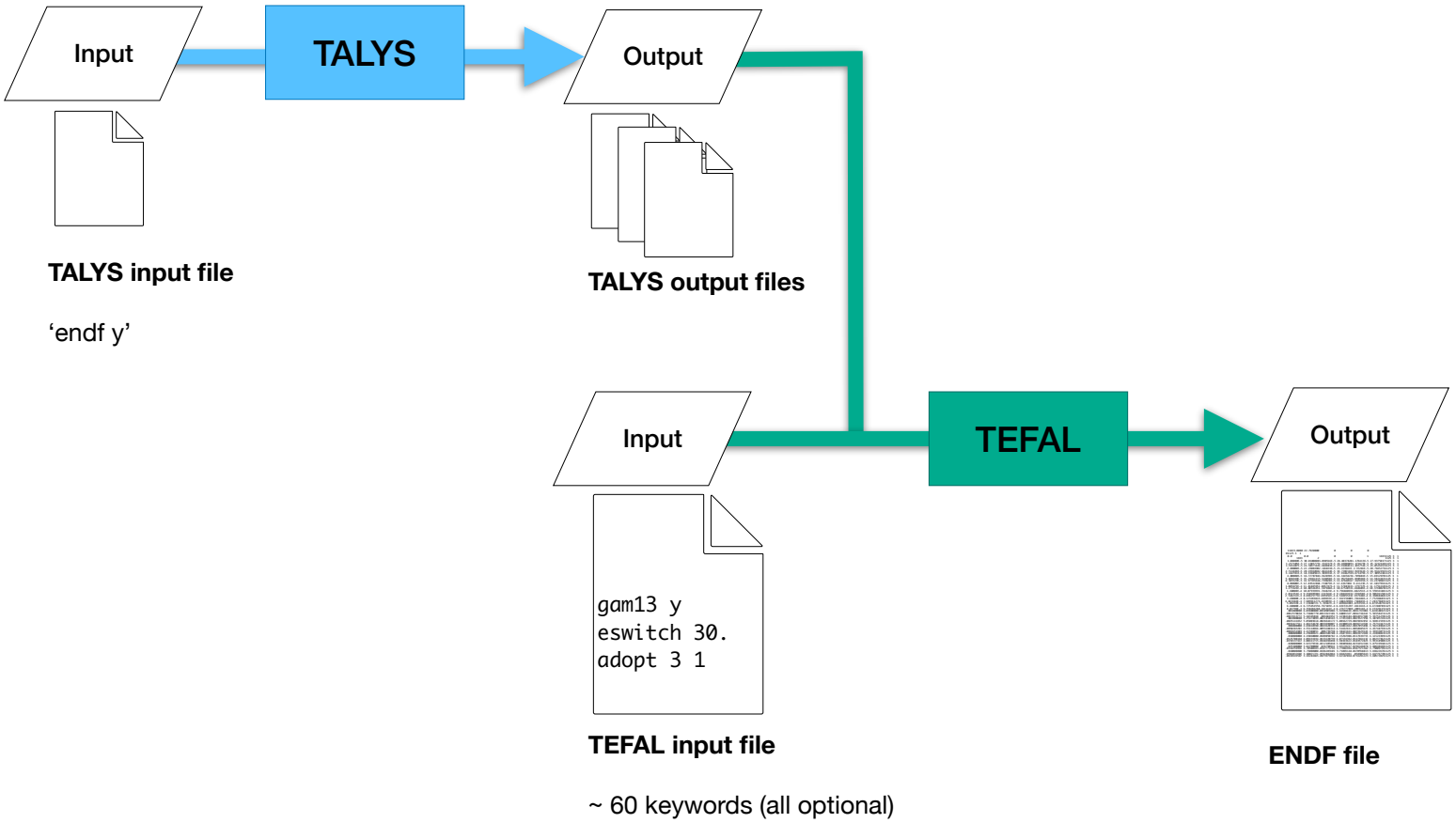
tasman — Public
Statistical software for TALYS: Uncertainties, sensitivities and optimization
Fortran

exfortables — Public
An experimental nuclear reaction database based on EXFOR

resonancetables — Public
Database for thermal cross sections, MACS and average resonance parameters
Fortran

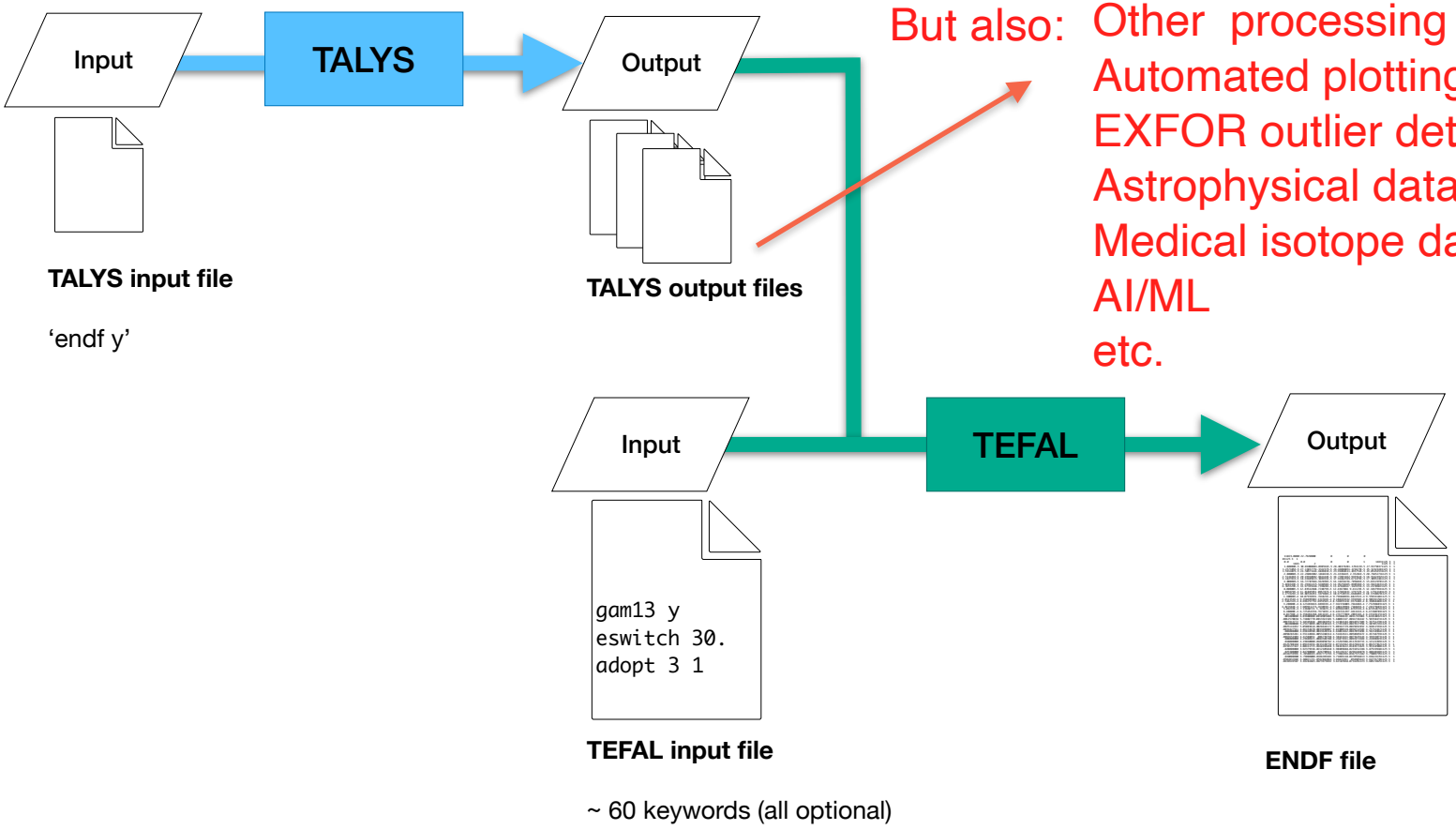
TEFAL + TALYS

- TEFAL processes the output of TALYS, and data from other sources, into an ENDF-6 data library



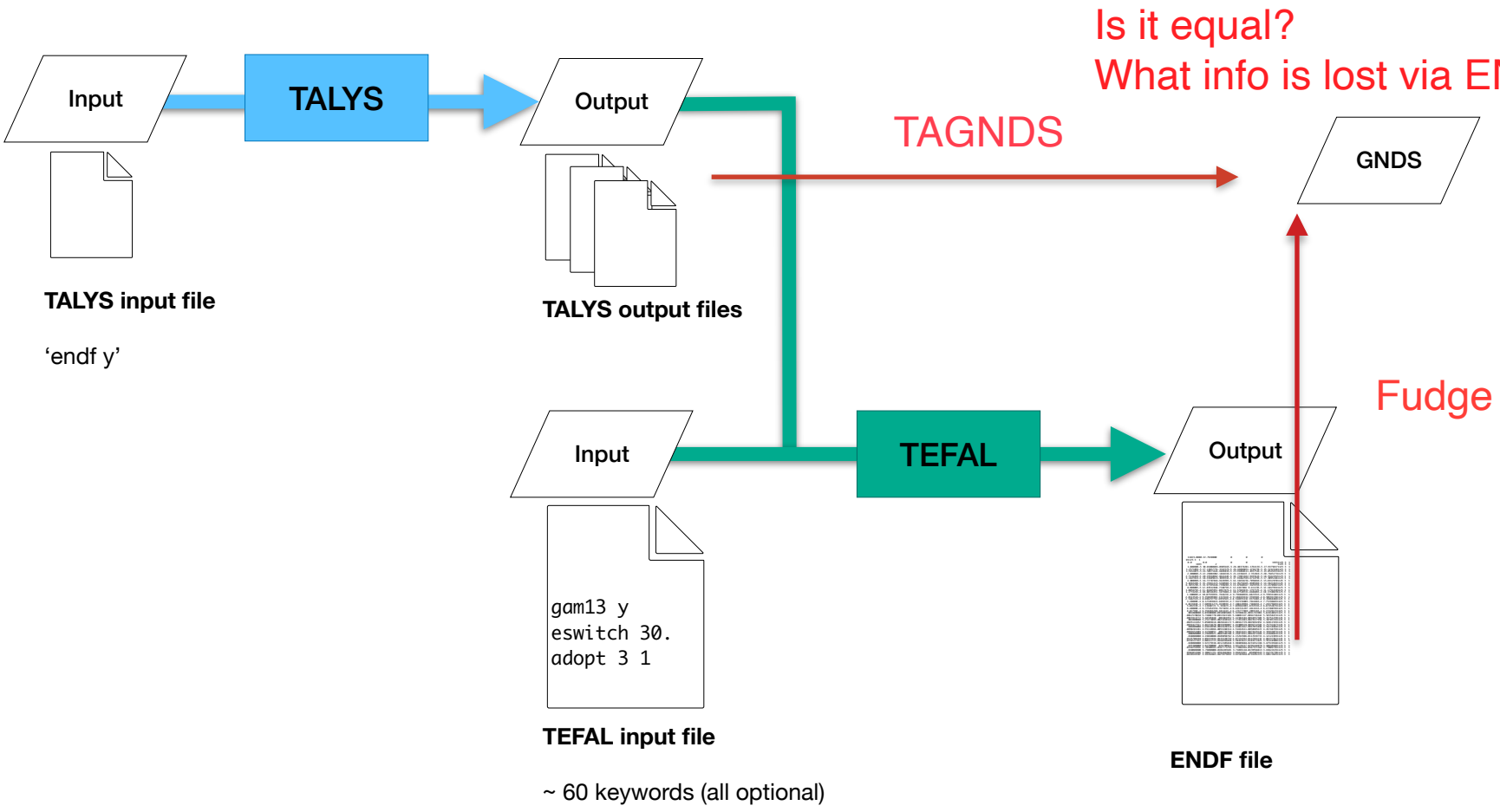
TEFAL + TALYS

- TEFAL processes the output of TALYS, and data from other sources, into an ENDF-6 data library



TEFAL + TALYS

- TEFAL processes the output of TALYS, and data from other sources, into an ENDF-6 data library



GNDS

```
<reaction label="U236 + photon" ENDF_MT="102">
  <crossSection>
    <resonancesWithBackground label="eval">
      <resonances href="/reactionSuite/resonances"/>
      <background>
        <resolvedRegion>
          <XYs1d>
            <axes>
              <axis index="1" label="energy_in" unit="eV"/>
              <axis index="0" label="crossSection" unit="b"/></axes>
            <values>
              1.00000000e-05 0.00000000e+00 2.25000000e+03 0.00000000e+00</values><
        <fastRegion>
          <XYs1d>
            <axes>
              <axis index="1" label="energy_in" unit="eV"/>
              <axis index="0" label="crossSection" unit="b"/></axes>
            <values>
              2.25000000e+03 2.32822500e+00 2.50000000e+03 2.20619000e+00 3.00000000e+03 2
```

EXFOR

```
TITLE       New precision measurements of the 235U(n,g) cross
             section
AUTHOR      (M.Jandel, T.A.Bredeweg, E.M.Bond, M.B.Chadwick,
             A.Couture, J.M.O'Donnell, M.Fowler, R.C.Haight,
             T.Kawano, R.Reifarth, R.S.Rundberg, J.L.Ullmann,
             D.J.Vieira, J.M.Wouters, J.B.Wilhelmy, C.Y.Wu,
             J.A.Becker)
INSTITUTE   (1USALAS,1USALRL)
REFERENCE   (J,PRL,109,202506,2012) Final (n,g) and alpha
            (J,NIM/B,261,986,2007)  Prelim. (n,g) and (n,f) in figs
            (C,2007NICE,1,607,2008) Prelim. (n,g) and (n,f) in figs
FACILITY    (LINAC,1USALAS) Lujan Neutron Scattering Center of
```

TALYS-1.97

```
# n + 235U     : (n,g)              Total
# Q-value      = 6.54552E+00
# E-threshold= 0.00000E+00
# # energies =     24
#      E            xs          gamma xs   xs/res.prod.xs
 1.00000E-02 2.07936E+03 1.13814E+04 1.00000E+00
 2.00000E-02 1.43254E+03 7.88163E+03 1.00000E+00
 4.00000E-02 1.17702E+03 6.52455E+03 1.00000E+00
 7.00000E-02 9.83417E+02 5.49190E+03 1.00000E+00
 1.00000E-01 8.45338E+02 4.74815E+03 1.00000E+00
 2.00000E-01 5.62366E+02 3.19982E+03 1.00000E+00
```

EXFORtables

```
# Target Z    :  92
# Target A    : 235
# Target state:
# Projectile  : n
# Reaction    : (n,g)
# Final state :
# Quantity    : Cross section
# Frame       : L
# MF          :   3
# MT          : 102
# X4 Subentry : 141490072
# X4 Reaction : 92-U-235(N,G)92-U-236,,SIG
# Author      : Jandel
# Year        : 2012
# Data points :    66
#    E(MeV)        xs(mb)       dxs(mb)      dE(MeV)
  5.00036E-04  2.61329E+03  5.78510E+02  1.15100E-06
  5.07024E-04  3.55298E+03  3.12190E+02  5.83701E-06
  5.18834E-04  4.99961E+03  3.47930E+02  5.97351E-06
  5.30919E-04  5.00055E+03  3.10070E+02  6.11151E-06
```

ENDF

```
 9.223500+4 2.330248+2          0          0          0          09228 3102
 6.544430+6 6.544430+6          0          0          1       1119228 3102
        111          2                                             9228 3102
1.000000-5 0.000000+0 2.250000+3 0.000000+0 2.250000+3 2.047808+09228 3102
2.370000+3 1.711010+0 2.650000+3 1.881410+0 3.000000+3 1.828870+09228 3102
3.350000+3 1.963650+0 3.750000+3 1.838280+0 4.000000+3 1.676190+09228 3102
4.200000+3 1.534880+0 4.700000+3 1.626720+0 5.300000+3 1.145940+09228 3102
```

YANDF

- Zen of Python: Explicit is better than implicit
- Key - value approach: allow ‘easy’ parsing into JSON, YAML, GNDS/XML etc.
- Not as non-descriptive as ENDF
- Not as heavy as GNDS
- Not as extensive and abbreviated as EXFOR
- More metadata than in the previous TALYS output files
- Human-readable
- Same schema for TALYS, EXFOR and ENDF
- From the point of view of a nuclear physicist, not from EXFOR or ENDF
- Would make ALL nuclear reaction data programmatically available at the same time: good for TENDL, other large data projects, AI/ML

Structure

- Inspired by YAML
- Multi-level
- Still using ‘#’ for metadata
- A relative small number of main attributes
- Use of defaults: if not relevant for particular reaction then metadata is not given
- Consistent, clean and parsable (I hope)

TALYS output file: rp039090.L02

```
# header:
#   title: Nb93(n,x)Y90m cross section
#   source: TALYS-2.0
#   user: Arjan Koning
#   date: 2024-01-11
#   format: YANDF-0.1
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,x)
#   Q-value [MeV]:  4.248473E+00
#   E-threshold [MeV]:  0.000000E+00
#   ENDF_MF: 6
#   ENDF_MT: 5
# residual:
#   Z: 39
#   A: 90
#   nuclide: Y90m
#   mass [amu]:  8.990714E+01
#   level:
#     number: 2
#     energy [MeV]:  6.820100E-01
#     spin:  7.000000E+00
#     parity: 1
#     isomer: 1
#     half-life [sec]:  1.148000E+04
# datablock:
#   quantity: cross section
#   columns: 3
#   entries: 25
##       E              xs       Isomeric ratio
##     [MeV]           [mb]             []
   2.000000E-01   0.000000E+00   0.000000E+00
   4.000000E-01   0.000000E+00   0.000000E+00
   6.000000E-01   0.000000E+00   0.000000E+00
   8.000000E-01   0.000000E+00   0.000000E+00
   1.000000E+00   0.000000E+00   0.000000E+00
   1.200000E+00   0.000000E+00   0.000000E+00
   1.400000E+00   8.135896E-05   0.000000E+00
   1.600000E+00   1.296808E-04   1.266436E-01
   1.800000E+00   2.699952E-04   1.644318E-01
   2.000000E+00   5.832345E-04   2.057970E-01
```

‘#’ for direct use in various software, e.g. Gnuplot

Without ‘#’: YAMLesque 2 space indentation per level

Parsing to JSON should be easy

Only 5 main attributes for nuclear reactions

TALYS: 2 more main attributes: ‘parameters’ and ‘observables’

EXFOR: All specific metadata may follow after the datablock

TALYS

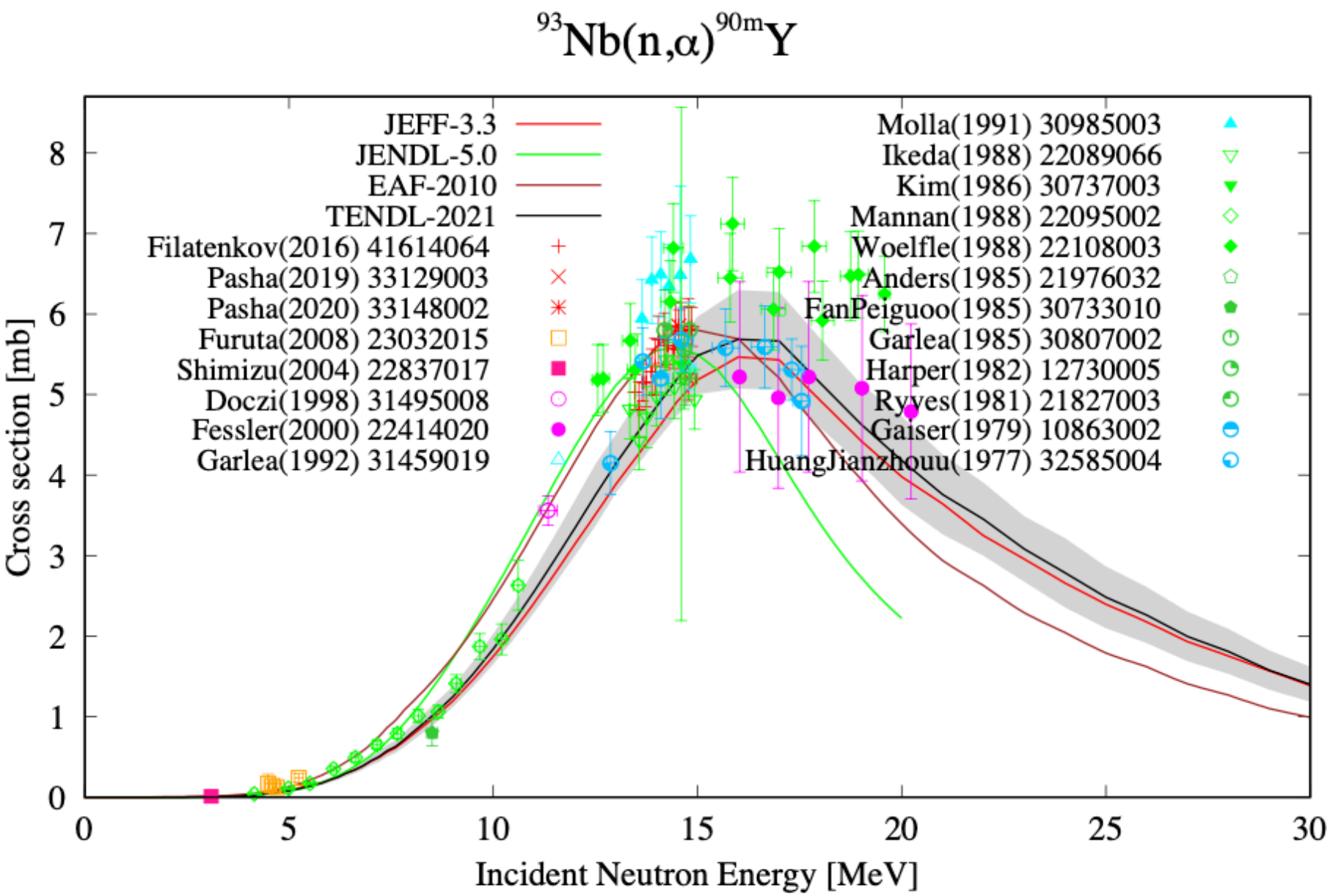
```
# header:
#   title: Nb93(n,a)Y90m cross section
#   source: TALYS-2.0
#   user: Arjan Koning
#   date: 2024-01-16
#   format: YANDF-0.1
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,a)
#   Q-value [MeV]:  4.248473E+00
#   E-threshold [MeV]:  0.000000E+00
#   ENDF_MF: 10
#   ENDF_MT: 107
# residual:
#   Z: 39
#   A: 90
#   nuclide: Y90m
#   level:
#     number: 2
#     energy [MeV]:  6.820100E-01
#     spin:  7.000000E+00
#     parity: 1
#     isomer: 1
#     half-life [sec]:  1.148000E+04
# datablock:
#   quantity: cross section
#   columns: 3
#   entries: 25
##       E              xs        Isomer
##     [MeV]           [mb]
   2.000000E-01   5.000000E-08   5.000
   4.000000E-01   5.000000E-08   5.000
   6.000000E-01   0.000000E+00   0.000
   8.000000E-01   0.000000E+00   0.000
   1.000000E+00   0.000000E+00   0.000
   1.200000E+00   0.000000E+00   0.000
```

JENDL5.0

```
# header:
#   title: Nb93(n,a)Y90m cross section
#   source: ENDF
#   user: Arjan Koning
#   date: 2024-01-02
#   format: YANDF-0.1
# endf:
#   library: jendl5.0
#   author: A.Ichihara
#   year: 2018
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,a)
#   Q-value [MeV]:  4.246250E+00
#   E-threshold [MeV]:  1.000000
#   ENDF_MF: 10
#   ENDF_MT: 107
# residual:
#   Z: 39
#   A: 90
#   nuclide: Y90m
#   level:
#     isomer: 1
# datablock:
#   quantity: cross section
#   columns: 2
#   entries: 802
##       E              xs
##     [MeV]           [mb]
   1.000000E-11   4.231872E-04
   1.032229E-11   4.165287E-04
   1.065491E-11   4.099758E-04
   1.099830E-11   4.035247E-04
   1.135271E-11   3.971754E-04
   1.171859E-11   3.909265E-04
```

EXFOR
(One file per data set)

```
# header:
#   title: Nb93(n,a)Y90m cross section
#   source: EXFOR
#   user: Arjan Koning
#   date: 2023-12-30
#   format: YANDF-0.1
# exfor:
#   author: Fessler
#   year: 2000
#   subentry: 22414020
#   X4 reaction: 41-NB-93(N,A)39-Y-90-M,,SIG
#   X4 source: IAEA-NDS C5 file, database version 2023-08-08
#   X4 link: https://nds.iaea.org/EXFOR/22414020
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,a)
#   ENDF_MF: 3
#   ENDF_MT: 107
# residual:
#   Z: 39
#   A: 90
#   nuclide: Y90m
#   level:
#     number: 0
#     energy [MeV]:  0.000000E+00
#     spin:  0.000000E+00
#     parity: 0
# datablock:
#   quantity: cross section
#   columns: 5
#   entries: 5
##       E              dE             xs             dxs        Normali
##     [MeV]          [MeV]          [mb]           [mb]           []
   1.603300E+01   6.200000E-02   5.220000E+00   3.100000E-01   1.00000
   1.698100E+01   4.000000E-02   4.960000E+00   3.100000E-01   1.00000
   1.772300E+01   3.200000E-02   5.220000E+00   3.100000E-01   1.00000
```


^{93}Nb(n,α)^{90m}Y
JEFF-3.3
JENDL-5.0
EAF-2010
TENDL-2021
Filatenkov(2016) 41614064
Pasha(2019) 33129003
Pasha(2020) 33148002
Furuta(2008) 23032015
Shimizu(2004) 22837017
Doczi(1998) 31495008
Fessler(2000) 22414020
Garlea(1992) 31459019
Molla(1991) 30985003
Ikeda(1988) 22089066
Kim(1986) 30737003
Mannan(1988) 22095002
Woelfle(1988) 22108003
Anders(1985) 21976032
FanPeiguoo(1985) 30733010
Garlea(1985) 30807002
Harper(1982) 12730005
Ryves(1981) 21827003
Gaiser(1979) 10863002
HuangJianzhouu(1977) 32585004
Cross section [mb]
Incident Neutron Energy [MeV]
0
1
2
3
4
5
6
7
8
0
5
10
15
20
25
30

TALYS output file: nn0011.000ang.L00


```
# header:
#   title: Pb208(n,el) angular distribution at  1.100000E+01 MeV
#   source: TALYS-2.0
#   user: Arjan Koning
#   date: 2024-01-11
#   format: YANDF-0.1
# target:
#   Z: 82
#   A: 208
#   nuclide: Pb208
# reaction:
#   type: (n,el)
#   ENDF_MF: 4
#   ENDF_MT: 2
#   E-incident [MeV]:  1.100000E+01
# datablock:
#   quantity: angular distribution
#   columns: 4
#   entries: 91
##      Angle            xs            Direct          Compound
##      [deg]          [mb/sr]         [mb/sr]          [mb/sr]
   0.000000E+00   8.526230E+03   8.526230E+03   0.000000E+00
   2.000000E+00   8.380680E+03   8.380680E+03   0.000000E+00
   4.000000E+00   7.956300E+03   7.956300E+03   0.000000E+00
   6.000000E+00   7.288450E+03   7.288450E+03   0.000000E+00
   8.000000E+00   6.431510E+03   6.431510E+03   0.000000E+00
   1.000000E+01   5.452650E+03   5.452650E+03   0.000000E+00
   1.200000E+01   4.424430E+03   4.424430E+03   0.000000E+00
   1.400000E+01   3.417150E+03   3.417150E+03   0.000000E+00
   1.600000E+01   2.492000E+03   2.492000E+03   0.000000E+00
   1.800000E+01   1.695680E+03   1.695680E+03   0.000000E+00
```

TALYS output file: gam082207L09L03.tot


```
# header:
#   title: Pb208(n,xg_9-3)Pb207 gamma-ray production cross section
#   source: TALYS-2.0
#   user: Arjan Koning
#   date: 2024-01-11
#   format: YANDF-0.1
# target:
#   Z: 82
#   A: 208
#   nuclide: Pb208
# reaction:
#   type: (n,xg_9-3)
#   Q-value [MeV]: -1.026987E+01
#   E-threshold [MeV]:  1.031968E+01
#   level:
#     number: 9
#     energy [MeV]:  2.902000E+00
#     spin:  5.500000E+00
#     parity: -1
#     level:
#       number: 3
#       energy [MeV]:  1.633356E+00
#       spin:  6.500000E+00
#       parity: 1
#   gamma energy [MeV]:  1.268644E+00
# residual:
#   Z: 82
#   A: 207
#   nuclide: Pb207
# datablock:
#   quantity: gamma-ray production cross section
#   columns: 2
#   entries: 67
##       E             xs
##     [MeV]          [mb]
   1.000000E-11   0.000000E+00
   2.530000E-08   0.000000E+00
   2.000000E-07   0.000000E+00
```

Uncertainties: Variance, in-channel covariance, cross-channel covariance


```
# header:
#   title: Nb93(n,tot) cross section covariance matrix
#   source: TASMAN
#   user: Arjan Koning
#   date: 2024-01-11
#   format: YANDF-0.1
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,tot)
#   ENDF_MF: 3
#   ENDF_MT: 1
# covariance:
#   class: cross-channel covariance
#   reaction: (n,el)
#   ENDF_MF: 3
#   ENDF_MT: 2
# datablock:
#   quantity: cross section covariance matrix
#   columns: 5
#   entries: 100
##       E_a             E_b             Rcov            Ccov            Vcov
##     [MeV]           [MeV]             []              []              []
   1.000000E-01    1.000000E-01    7.522166E-03    1.000000E+00    6.941382E+05
   1.000000E-01    2.000000E-01    7.292479E-03    9.931619E-01    7.072012E+05
   1.000000E-01    5.000000E-01    5.171597E-03    9.666104E-01    4.456966E+05
   1.000000E-01    1.000000E+00    4.337216E-03    9.747387E-01    2.541089E+05
   1.000000E-01    2.000000E+00    5.513683E-03    9.930789E-01    1.526950E+05
   1.000000E-01    3.000000E+00    3.230189E-03    9.947272E-01    6.223200E+04
   1.000000E-01    4.000000E+00    6.676997E-05    5.188200E-01    1.170094E+03
   1.000000E-01    5.000000E+00   -1.492215E-03   -9.738176E-01   -2.651213E+04
   1.000000E-01    8.000000E+00   -5.710922E-04   -9.359357E-01   -1.261057E+04
```

Summary/discussion points

- Main purpose is TALYS output, EXFOR and NDL's taken along as a bonus.
- TALYS-2.0 now uses this output
- TALYS output: Should I go straight to JSON?
- TALYS output: GNDS/XML not preferred
- Unify the structure of all fundamental ND: RIPL (masses, discrete levels, photon strength functions etc. resonance parameters, average resonance parameters (sigma_0, D_0 etc databases): Add Metadata
- Do you foresee any trouble/regret?

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Thank you!