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, Consultancy meeting on GNDS/FUDGE/TAGNDS , May 22-25 2023

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

TALYS

Input

```
projectile n
element Fe
mass 56
energy 14.0
```

~ 400 keywords

Physical parameters

Nuclear Structure (RIPL-3)

- Masses
- Discrete levels
- Level densities
- Resonance parameters
- Photon strength functions
- Optical model parameters
- Fission barrier parameters

Other

- Fission fragment distributions
- 'Best' nuclear model parameters optimised to experimental reaction data

- Phenomenological parameters
- Microscopic tables

Reaction models

Optical model (ECIS)

- Local/global OMP
- Phenomenological
- Semi-microscopic (JLM)

Direct reaction

- Spherical OMP
- DWBA
- Coupled-channels
  - Rotational
  - Vibrational
- Giant resonances

Compound reactions

- Hauser-Feshbach
- Width fluctuations
- Blatt-Biedenharn ang. dis.
- Particle, photon and fission transmission coeff.

Pre-equilibrium reactions

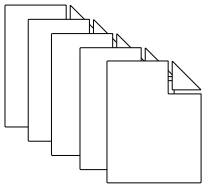
- Exciton model
- Particle hole level density
- Kalbach systematics
  - Angular distribution
  - Cluster emission
- γ-ray emission

Multiple emission

Multiple emission

- Hauser-Feshbach
- Multiple preeq. exciton
- Fission competition
- γ-ray cascade
- Exclusive channels
- Recoils
- Fission fragment de-excitation

Output



Output files per reaction channel

- Cross sections
  - Total
  - Exclusive: (n,γ), (n,f), (n,n'), (n,2n), (n,p) etc.
  - Per level
  - Residual production
  - Particle production
  - γ-ray production
- Emission spectra
  - Single-differential
  - Double differential
  - Recoils
- Angular distributions
  - Elastic
  - Per level
- Particle multiplicities
- Fission yields, neutron observables
- Astrophysical reaction rates, MACS
- …etc

European Physical Journal A
Accepted for publication, 108 pages

TALYS: Modeling of nuclear reactions

Arjan Koning[1*], Stephane Hilaire[2,3] and Stephane Goriely[4]

[1*]Nuclear Data Section, IAEA, Wagrammerstrasse 5, Vienna, 1400, Austria.
[2]DIF, CEA, CEA, Arpajon, F-91297, France.
[3]Université Paris-Saclay, CEA, LMCE, 91680, Bruyères-le-Châtel, France.
[4]Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, Campus de la Plaine, CP-226, Brussels, 1050, Belgium.

*Corresponding author(s). E-mail(s): A.Koning@iaea.org;
Contributing authors: Stephane.Hilaire@cea.fr; Stephane.Goriely@ulb.be;

Abstract

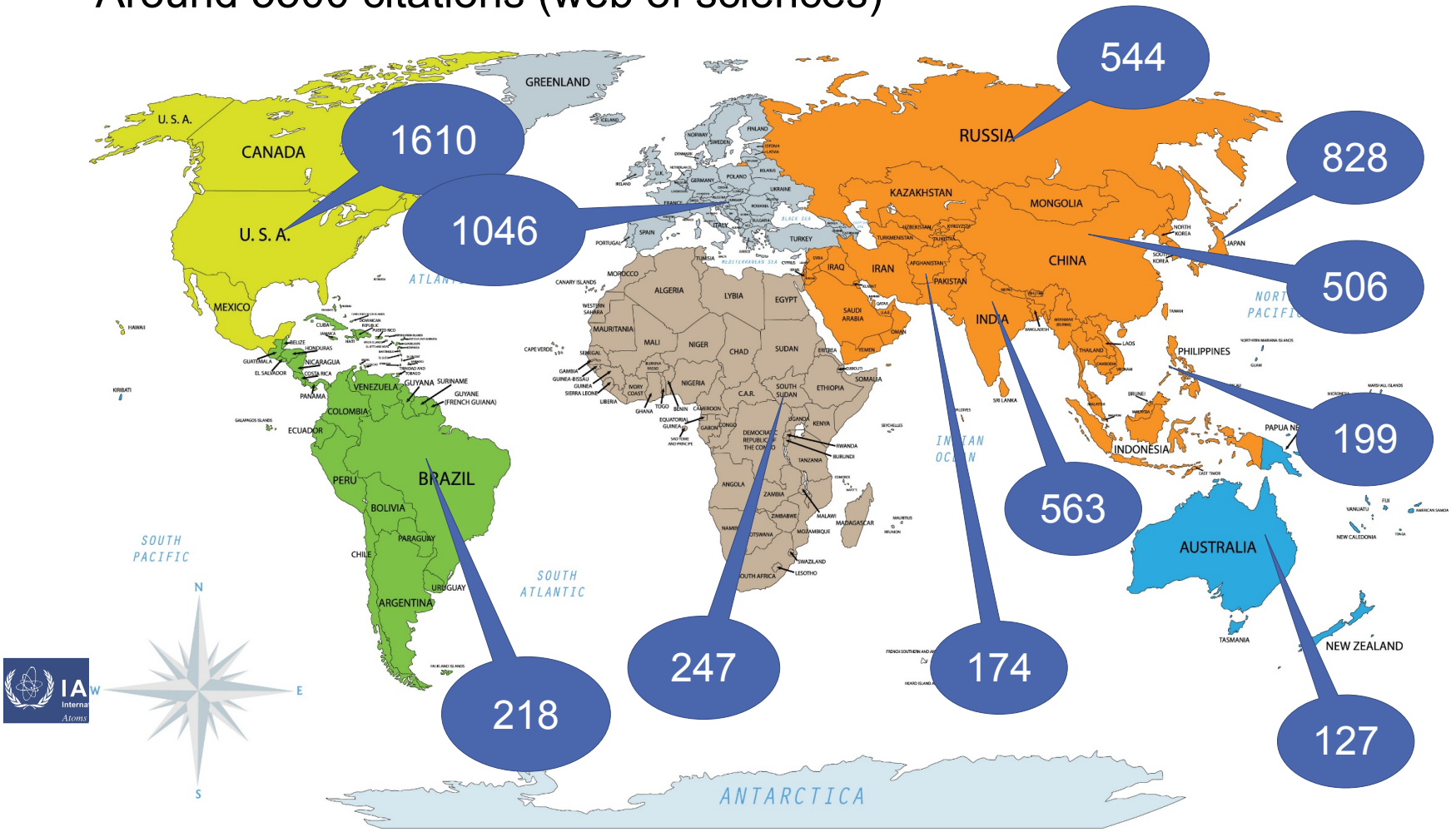
Purpose: TALYS is a software package for the simulation of nuclear reactions below 200 MeV. It is used worldwide for the analysis and prediction of nuclear reactions and is based on state-of-art nuclear structure and nuclear reaction models. **Methods:** A general overview of the implemented physics 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 functions and fission barriers. **Results:** A wide variety of nuclear reactions simulated with TALYS will be demonstrated, ranging from low-energy neutron cross sections, astrophysics, high-energy charged particle reactions and other reactions. **Conclusion:** TALYS is a nuclear reaction software which aims to give a complete description of nuclear reaction observables, and to be an important link between fundamental nuclear physics and applications.

Keywords: TALYS, nuclear reaction, nuclear structure, cross section, optical model, compound nucleus, pre-equilibrium, level density, photon strength function, fission, astrophysics

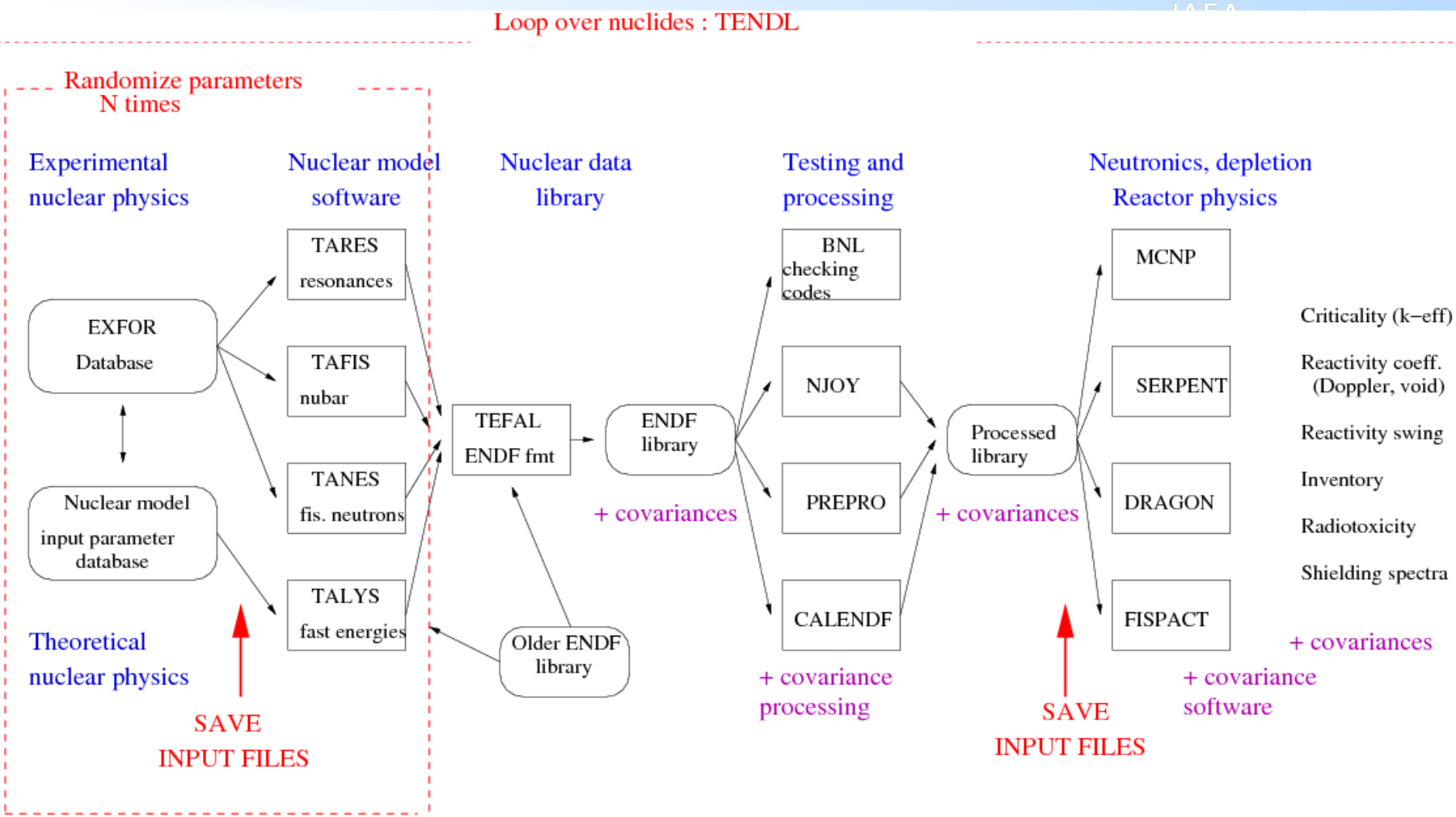
MSC Classification: 25.40.-h , 24.10.Ht , 24.60.Dr , 24.10.Pa

TALYS around the World

- Around 5500 citations (web of sciences)

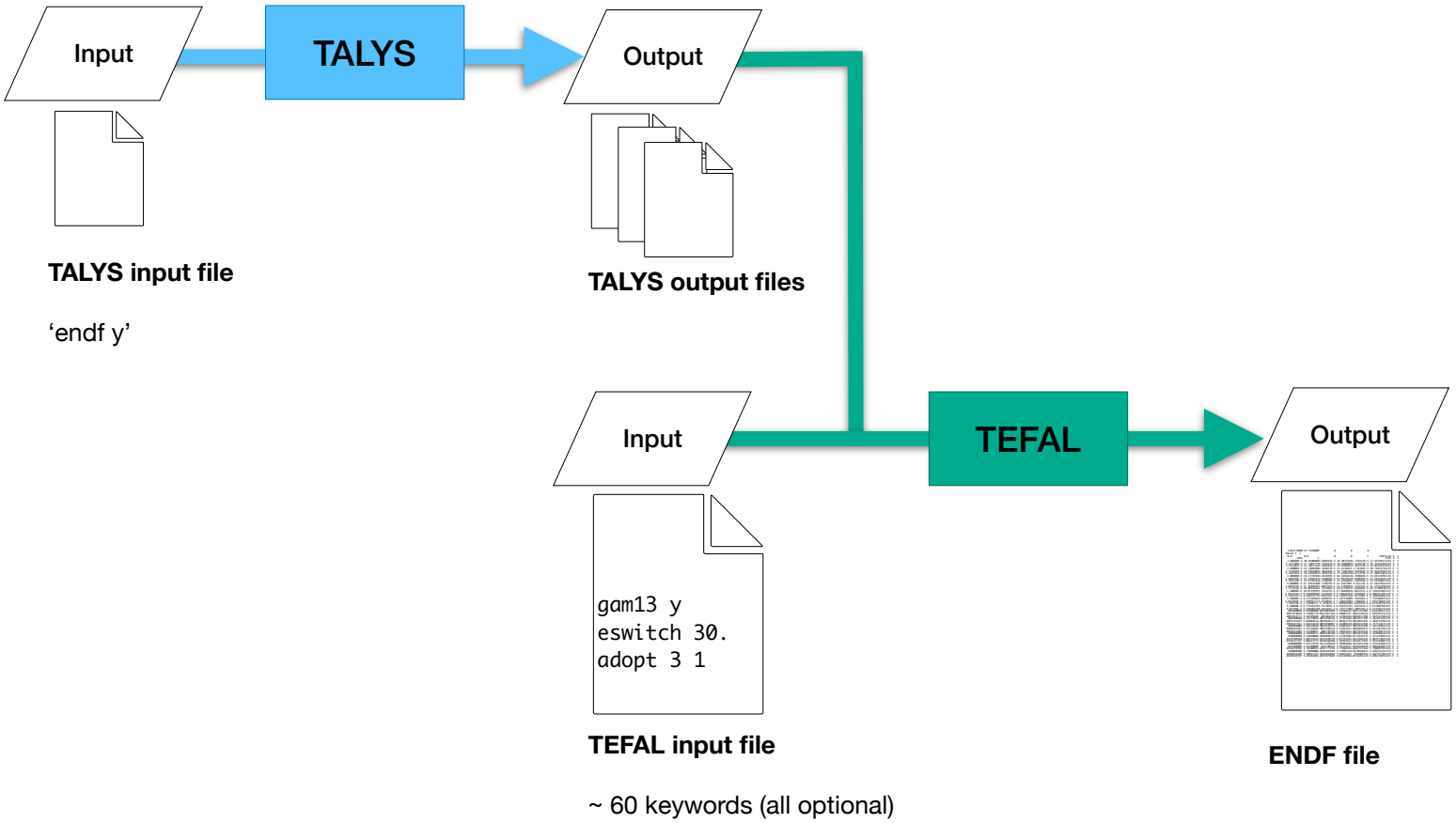


Never ending question: Is the input and output interfacing still up to date?


Loop over nuclides : TENDL
Randomize parameters
N times
Experimental
nuclear physics
Nuclear model
software
Nuclear data
library
Testing and
processing
Neutronics, depletion
Reactor physics
EXFOR
Database
Nuclear model
input parameter
database
Theoretical
nuclear physics
TARES
resonances
TAFIS
nubar
TANES
fis. neutrons
TALYS
fast energies
SAVE
INPUT FILES
TEFAL
ENDF fmt
Older ENDF
library
ENDF
library
+ covariances
BNL
checking
codes
NJOY
PREPRO
CALENDF
+ covariance
processing
Processed
library
+ covariances
SAVE
INPUT FILES
MCNP
SERPENT
DRAGON
FISPACT
+ covariance
software
Criticality (k−eff)
Reactivity coeff.
(Doppler, void)
Reactivity swing
Inventory
Radiotoxicity
Shielding spectra
+ covariances

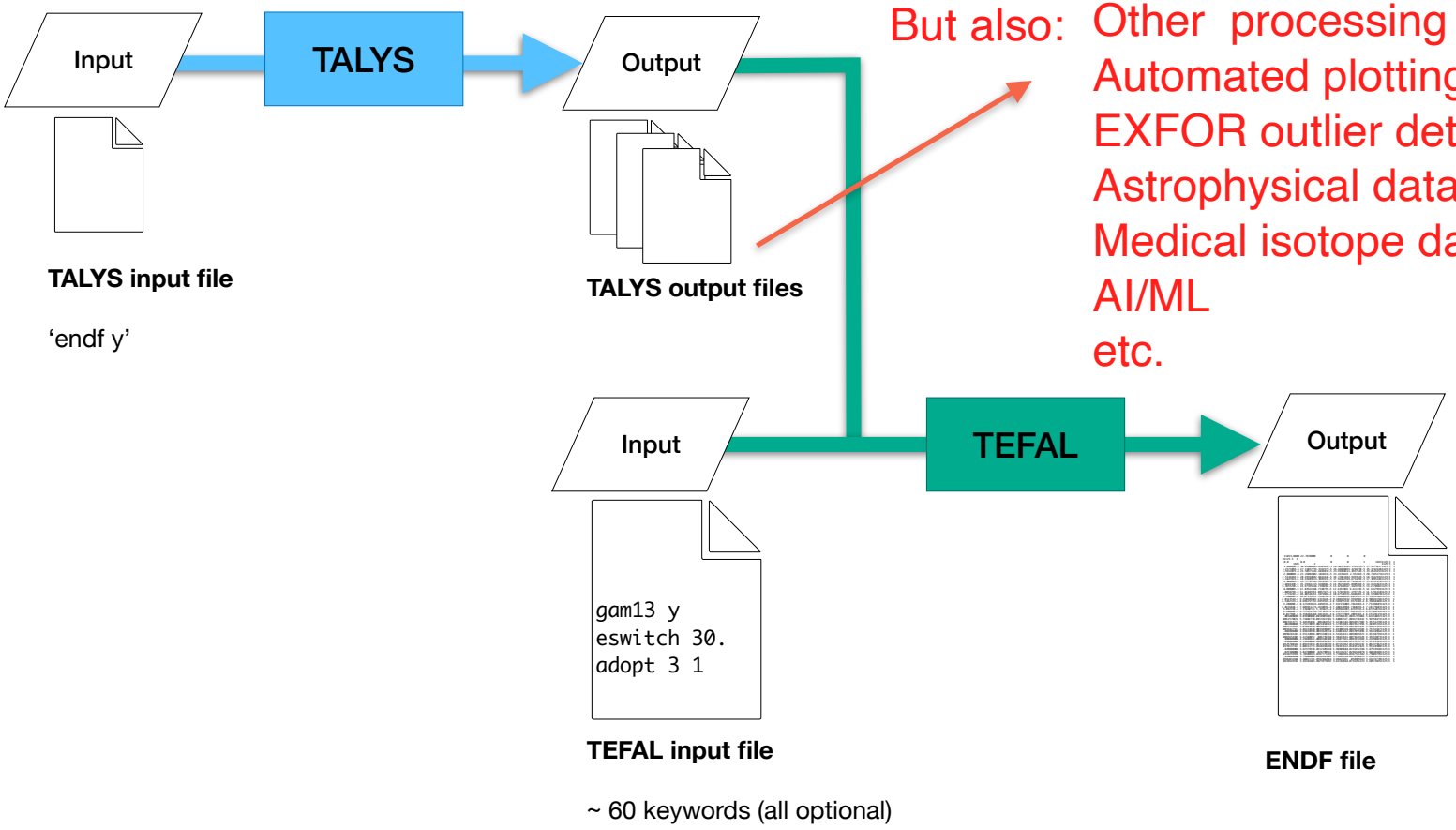
TEFAL + TALYS

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



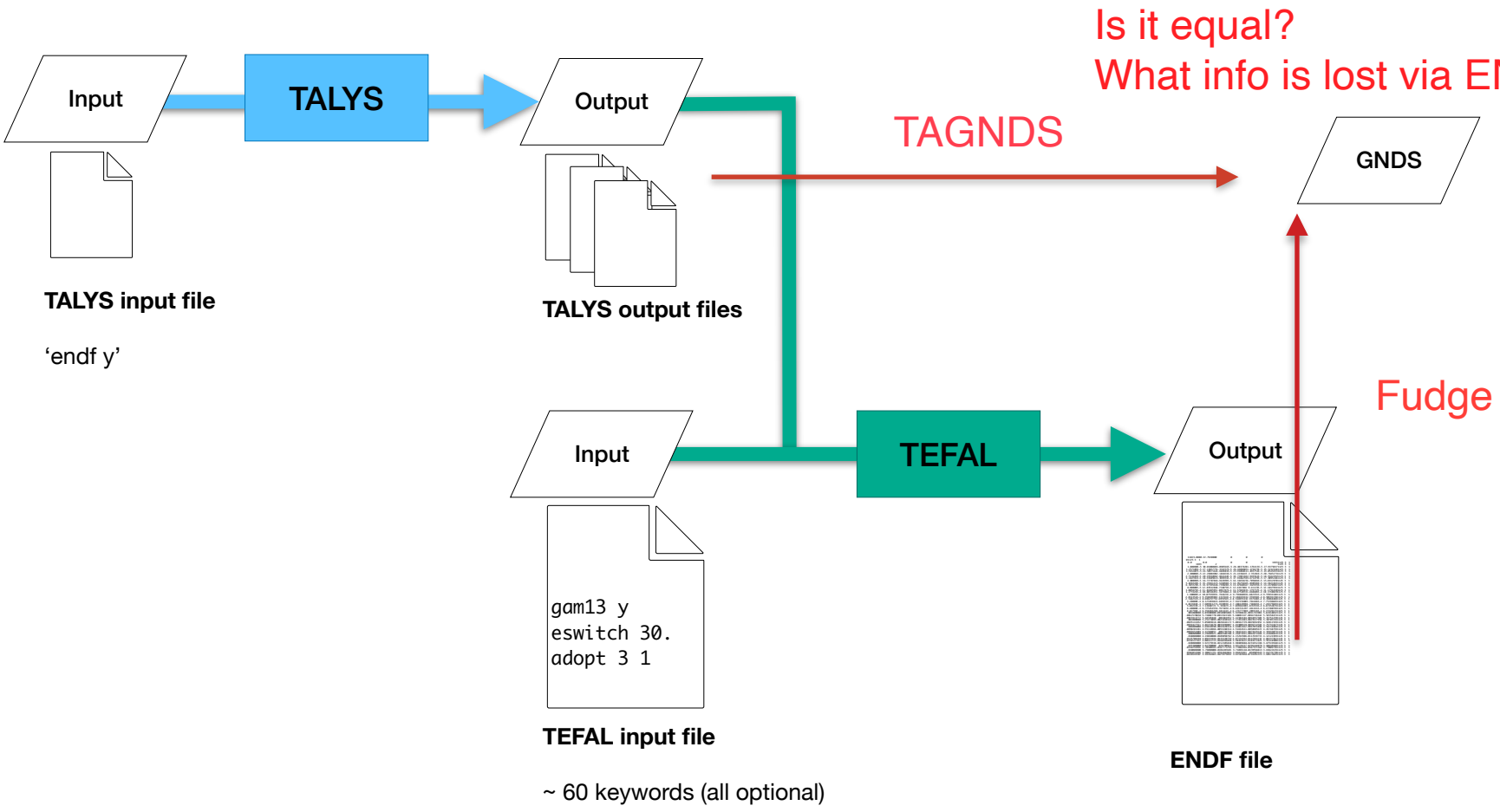
TEFAL + TALYS

- 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
```

Current TALYS

```
# 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 complicated and extensive as EXFOR
- More metadata than in the current 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

- Almost 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: xs000001.L02

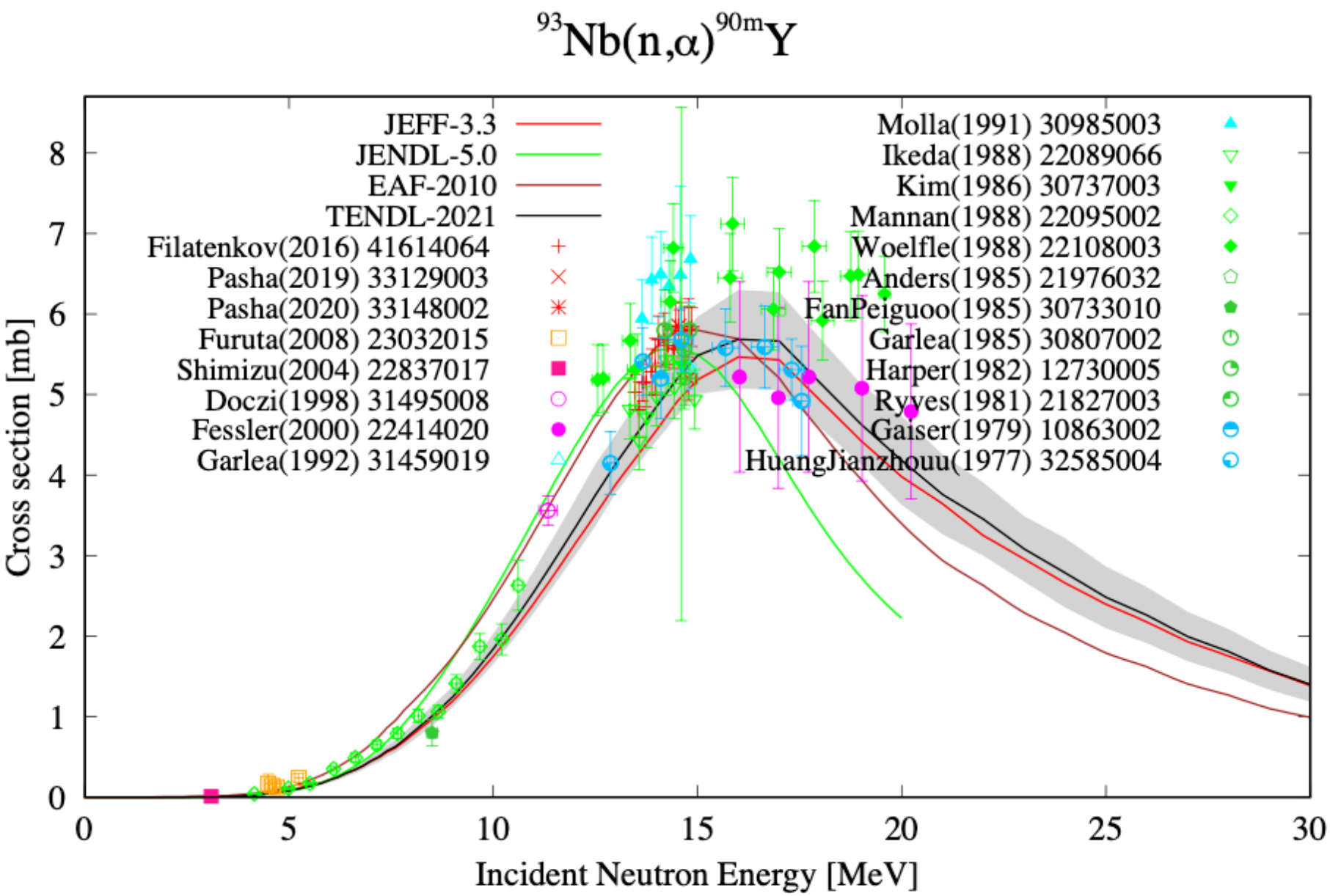
```
# header:
#   title:                              Nb93(n,a)Y90m Cross section
#   source:                             TALYS
# target:
#   Z:                                      41
#   A:                                      93
#   nuclide:                            Nb93
# reaction:
#   type:                               (n,a)
#   Q-value [MeV]:                       4.24847E+00
#   E-threshold [MeV]:                   0.00000E+00
# residual:
#   Z:                                      39
#   A:                                      90
#   nuclide:                            Y090m
#   level:
#     number:                                2
#     isomer:                                1
#     energy [MeV]:                     6.82010E-01
#     spin:                             7.00000E+00
#     parity:                                1
#     half-life [sec]:                  1.14800E+04
# datablock:
#   quantity:                           cross section
#   columns:                                3
#   entries:                               20
#     E [MeV]          xs [mb]     Isomeric ratio
    1.00000E+00    0.00000E+00     0.00000E+00
    2.00000E+00    3.58223E-04     8.61059E-02
    3.00000E+00    4.10306E-03     1.15148E-01
    4.00000E+00    2.84606E-02     2.26655E-01
    5.00000E+00    1.16184E-01     2.88622E-01
....
```

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

Without '#': YAML.
2 space indentation per level

Parsing to JSON should be easy

All values starting in column 41


^{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

IAEA 60 Years Atoms for Peace and Development

TALYS

```
# header:
#   title:                                Nb93(n,a)Y90m Cross section
#   source:                               TALYS
# target:
#   Z:                                       41
#   A:                                       93
#   nuclide:                              Nb93
# reaction:
#   type:                                 (n,a)
#   Q-value [MeV]:                         4.24847E+00
#   E-threshold [MeV]:                     0.00000E+00
# residual:
#   Z:                                       39
#   A:                                       90
#   nuclide:                              Y090m
#   level:
#     number:                                 2
#     isomer:                                 1
#     energy [MeV]:                      6.82010E-01
#     spin:                              7.00000E+00
#     parity:                                 1
#     half-life [sec]:                   1.14800E+04
# datablock:
#   quantity:                             cross section
#   columns:                                 3
#   entries:                                20
#     E [MeV]          xs [mb]     Isomeric ratio
    1.00000E+00     0.00000E+00     0.00000E+00
    2.00000E+00     3.58223E-04     8.61059E-02
    3.00000E+00     4.10306E-03     1.15148E-01
    4.00000E+00     2.84606E-02     2.26655E-01
    5.00000E+00     1.16184E-01     2.88622E-01
....
```

JENDL5.0

```
# header:
#   title:                                Nb93(n,a)Y90m Cross section
#   source:                               JENDL5.0
#   author:                               A.Ichihara
#   year:                                 2018
# target:
#   Z:                                       41
#   A:                                       93
#   nuclide:                              Nb93
# reaction:
#   type:                                 (n,a)
#   Q-value [MeV]:                         4.24625E+00
#   E-threshold [MeV]:                     0.00000E+00
# residual:
#   Z:                                       39
#   A:                                       90
#   nuclide:                              Y090m
#   level:
#     number:                                 2
#     isomer:                                 1
#     energy [MeV]:                      6.87000E-01
#     spin:                              7.00000E+00
#     parity:                                 1
#     half-life [sec]:                   1.14800E+04
# datablock:
#   quantity:                             cross section
#   columns:                                 2
#   entries:                               802
#     E [MeV]          xs [mb]
    1.00000E-11     4.23187E-04
    1.03223E-11     4.16529E-04
    1.06549E-11     4.09976E-04
    1.09983E-11     4.03525E-04
    1.13527E-11     3.97175E-04
    1.17186E-11     3.90926E-04
    1.20962E-11     3.84776E-04
.....
```

EXFOR
(One file per data set)

```
# header:
#   title:                                Nb93(n,a)Y90m Cross section
#   source:                               EXFOR
#   author:                               Fessler
#   year:                                 2000
#   subentry:                             22414020
# target:
#   Z:                                       41
#   A:                                       93
#   nuclide:                              Nb93
# reaction:
#   type:                                 (n,a)
#   Q-value [MeV]:                         4.24847E+00
#   E-threshold [MeV]:                     0.00000E+00
# residual:
#   Z:                                       39
#   A:                                       90
#   nuclide:                              Y090m
#   level:
#     number:                                 2
#     isomer:                                 1
#     energy [MeV]:                      6.82010E-01
#     spin:                              7.00000E+00
#     parity:                                 1
#     half-life [sec]:                   1.14800E+04
# datablock:
#   quantity:                             cross section
#   columns:                                 4
#   entries:                                 5
#     E [MeV]          dE [MeV]        xs [mb]          dxs [mb]
    1.60330E+01     6.20000E-02     5.22000E+00     1.18250E+00
    1.69810E+01     4.00000E-02     4.96000E+00     1.12360E+00
....
```

TALYS output file: xs000001.L02

```
# header:
#   title:                              Nb93(n,a)Y90m Cross section
#   source:                             TALYS
# target:
#   Z:                                      41
#   A:                                      93
#   nuclide:                            Nb93
# reaction:
#   type:                               (n,a)
#   Q-value [MeV]:                       4.24847E+00
#   E-threshold [MeV]:                   0.00000E+00
# residual:
#   Z:                                      39
#   A:                                      90
#   nuclide:                            Y090m
#   level:
#     number:                                2
#     isomer:                                1
#     energy [MeV]:                    6.82010E-01
#     spin:                            7.00000E+00
#     parity:                                1
#     half-life [sec]:                 1.14800E+04
# datablock:
#   quantity:                           cross section
#   columns:                                3
#   entries:                               20
#     E [MeV]          xs [mb]     Isomeric ratio
    1.00000E+00    0.00000E+00     0.00000E+00
    2.00000E+00    3.58223E-04     8.61059E-02
    3.00000E+00    4.10306E-03     1.15148E-01
    4.00000E+00    2.84606E-02     2.26655E-01
    5.00000E+00    1.16184E-01     2.88622E-01
....
```

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 output file: nnang.L00

```
# header:
#   title:                                Zr96(n,el) angular distribution
#   source:                               TALYS
# target:
#   Z:                                        40
#   A:                                        96
#   nuclide:                              Zr96
# reaction:
#   type:                                 (n,el)
#   E-incident [MeV]:                        1.300000E-02
# datablock:
#   quantity:                             angular distribution
#   columns:                                   4
#   entries:                                  91
#   Angle [deg]     xs [mb/sr]    Direct [mb/sr] Compound [mb/sr
    0.000000E+00   7.676554E+02   4.376280E+02   3.300274E+02
    2.000000E+00   7.675304E+02   4.376310E+02   3.298994E+02
    4.000000E+00   7.671560E+02   4.376400E+02   3.295160E+02
    6.000000E+00   7.665339E+02   4.376550E+02   3.288789E+02
    8.000000E+00   7.656674E+02   4.376760E+02   3.279914E+02
    1.000000E+01   7.645598E+02   4.377020E+02   3.268578E+02
    1.200000E+01   7.632186E+02   4.377350E+02   3.254836E+02
```

TALYS output file: gam040096L03L02.tot

```
# header:
#   title:                          Zr96(n,x)Zr96 gamma-ray production cross section - Level   3 --> Level   2
#   source:                         TALYS
# target:
#   Z:                                 40
#   A:                                 96
#   nuclide:                        Zr96
# reaction:
#   type:                           (n,x)
#   Q-value [MeV]:                   -1.897158E+00
#   E-threshold [MeV]:                1.917110E+00
#   level:
#     number:                            3
#     energy [MeV]:                   1.897158E+00
#     spin:                           3.000000E+00
#     parity:                          -1
#     level:
#       number:                          2
#       energy [MeV]:                 1.750497E+00
#       spin:                         2.000000E+00
#       parity:                          1
#   gamma energy [MeV]:               1.466610E-01
# datablock:
#   quantity:                       gamma-ray production cross section
#   columns:                           2
#   entries:                          44
#     E [MeV]          xs [mb]
   1.000000E-11   0.000000E+00
   2.530000E-08   0.000000E+00
   1.000000E-06   0.000000E+00
.........
   1.800000E+00   0.000000E+00
   2.000000E+00   1.373152E+02
   2.500000E+00   2.823970E+02
   3.000000E+00   4.165735E+02
   3.500000E+00   5.313192E+02
   4.000000E+00   5.755005E+02
   5.000000E+00   6.474636E+02
   6.000000E+00   7.208881E+02
```

TALYS-Related Software and Databases

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

Coming soon, still available here

TALYS

Arjan Koning, Stephane Hilaire, Stephane Goriely

Nuclear reaction model code.

Download TALYS-1.95
Download previous versions
Read Tutorial

Created at NRG CEA ULB UNIVERSITÉ LIBRE DE BRUXELLES IAEA

EXFORTABLES

Arjan Koning

Experimental nuclear reaction database based on EXFOR.

Download EXFORTABLES-1.0
Read Tutorial

RESONANCETABLES

Arjan Koning, Dimitri Rochman

Database for thermal cross sections, MACS and average resonance parameters.

Download RESONANCETABLES-1.0
Read Tutorial

Created at IAEA PSI

ENDFTABLES

Arjan Koning

Code to translate ENDF nuclear data libraries into tabular format.

Download ENDFTABLES-1.0
Read Tutorial (Chapter 2)

Libraries-2020

Arjan Koning

Evaluated nuclear data libraries and EXFOR in tabular format.

Libraries-2020 [15GB]
Read Tutorial (Chapter 3)

IAEA 60 Years Atoms for Peace and Development

nds.iaea.org/talys

Summary/discussion points

- Main purpose is TALYS output, EXFOR and NDL's taken along as a bonus.
- TALYS output: Should I go straight to JSON?
- TALYS output: GNDS/XML not preferred
- Do you foresee any trouble/regret?

IAEA 60 Years
Atoms for Peace and Development

Thank you!