IAEA 60 Years
Atoms for Peace and Development

Challenges in unifying nuclear data access

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Contents

- Some points to consider
- Some data formats: TALYS, ENDF, EXFOR, GNDS
- Attempt to unify, at least, EXFOR, TALYS and ENDF, with a “light” format: YANDF

Some points to consider

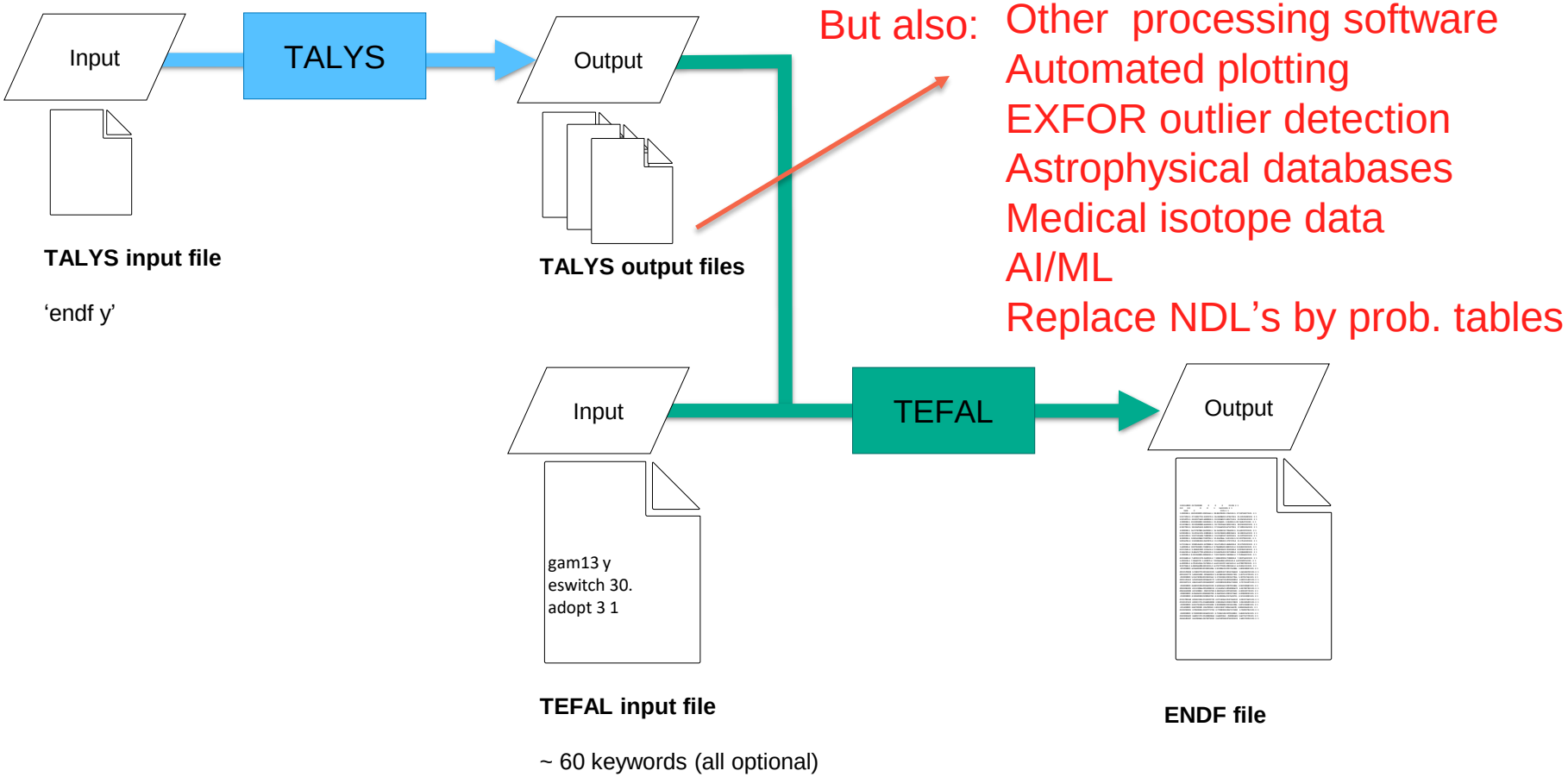
- General trend: Transition from web-GUI's to programmatic access (Web-API's)
- 3 dominant databases in nuclear data
  - ENSDF (evaluated nuclear structure)
  - ENDF (evaluated nuclear reactions)
  - EXFOR (experimental nuclear reactions)
  - ….all with > 50 year old formats
  - Parsers and entirely new formats underway, interpretation of the databases is the challenge to allow general use

Some points to consider

- IAEA Nuclear Data Section hosts many other basic nuclear databases of which many are in need of
  - Unified format (if possible)
  - Richer metadata
  - Programmatic access
  - …to allow for more automation and AI/ML applications
- Examples:
  - Nuclear model parameters - Reference Input Parameter Library (RIPL)
  - Essential experimental/evaluated databases
    - Thermal cross sections
    - Full resonance parameter collections
    - Resonance integrals
    - 30 keV Maxwellian-averaged cross sections
    - Average radiative widths
  - Evaluated Gamma-ray Activation file (EGAF)
  - Evaluated cross sections for medical isotopes
  - Reference database for beta-delayed neutron emission
  - Etc.
- A new website with emphasis on “Findable” of the FAIR principle.

TEFAL + TALYS

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



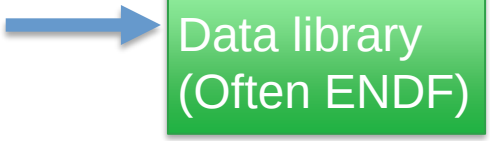
Nuclear data pipeline should flow in 2 directions!

EXFOR

Evaluated experiments
- -Resonance Atlas
- -thermal c.s.
- -MACS
- -etc.

TALYS, EMPIRE, etc.

Non-model evaluation
- -GLS
- -model defects
- - etc



Diagnosis
- - CHECKR
- - FIZCON
- - PSYCHE
- - PREPRO, etc.

Processing
- - NJOY
- - FRENDY
- - FUDGE
- - etc.

Manipulation
- - ENDFtk
- - DECE
- - Endfparser_py
- - etc.

Making observables
- - ENDVER
- - Endftables

Applications

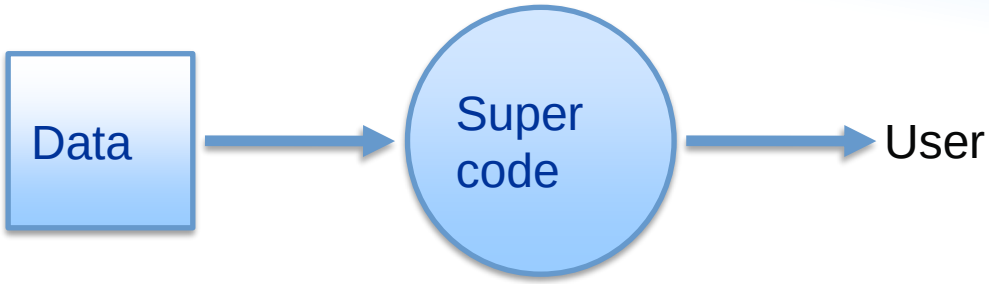
Apply ENDF multiplication rules!
Only observables in ENDF:
- - simple cross sections
- - nubar
The rest: relative distributions

Vertical nuclear data evaluation

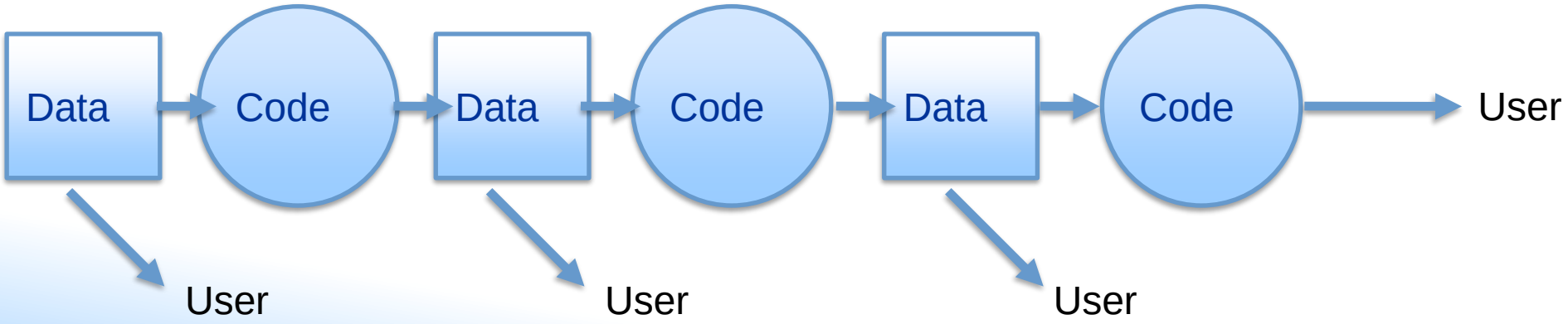
- Improve nuclear data evaluation of a particular projectile - target (- reaction) combination:
  - Sometimes driven by a sponsor
  - Sometimes driven by a new measurement
  - Sometimes driven by feedback from suboptimal integral validation
  - Hackatons needed
  - Frankenstein files
    - We should never throw away data which work well (although we may not remember why), often in the RR
    - If safe, add missing categories: emission spectra, gamma data, covariances, data above 20 MeV, etc.
  - Major ‘continental’ NDL’s, ENDF/B-VIII.1, JEFF-3.3, JENDL-5.0, CENDL-3.2, based on this.
  - Leads to currently the best nuclear data libraries for fission applications
  - IAEA-INDEN wish list a good example
  - No evaluators left

Horizontal nuclear data evaluation

- Ensure a reproducible nuclear data flow with all experimental, theoretical and evaluated data directly available. Requires:
  - a parsed and interpreted EXFOR database
  - evaluated experimental databases with rich metadata:
    - Thermal cross sections, resonance integrals
    - Full resonance databases
    - Maxwellian cross sections (MACS), average radiative widths etc.
  - Automated non-model evaluation software for low energies
  - Full control over evaluated nuclear data libraries for optimisation, ML, plotting etc.
  - Time spent on correct retrieval of all the above should be minimal
- Can go (far) beyond ENDF
- TALYS code system and TENDL is based on this
- Ideal situation: A Horizontal nuclear data approach in which vertical knowledge is inserted

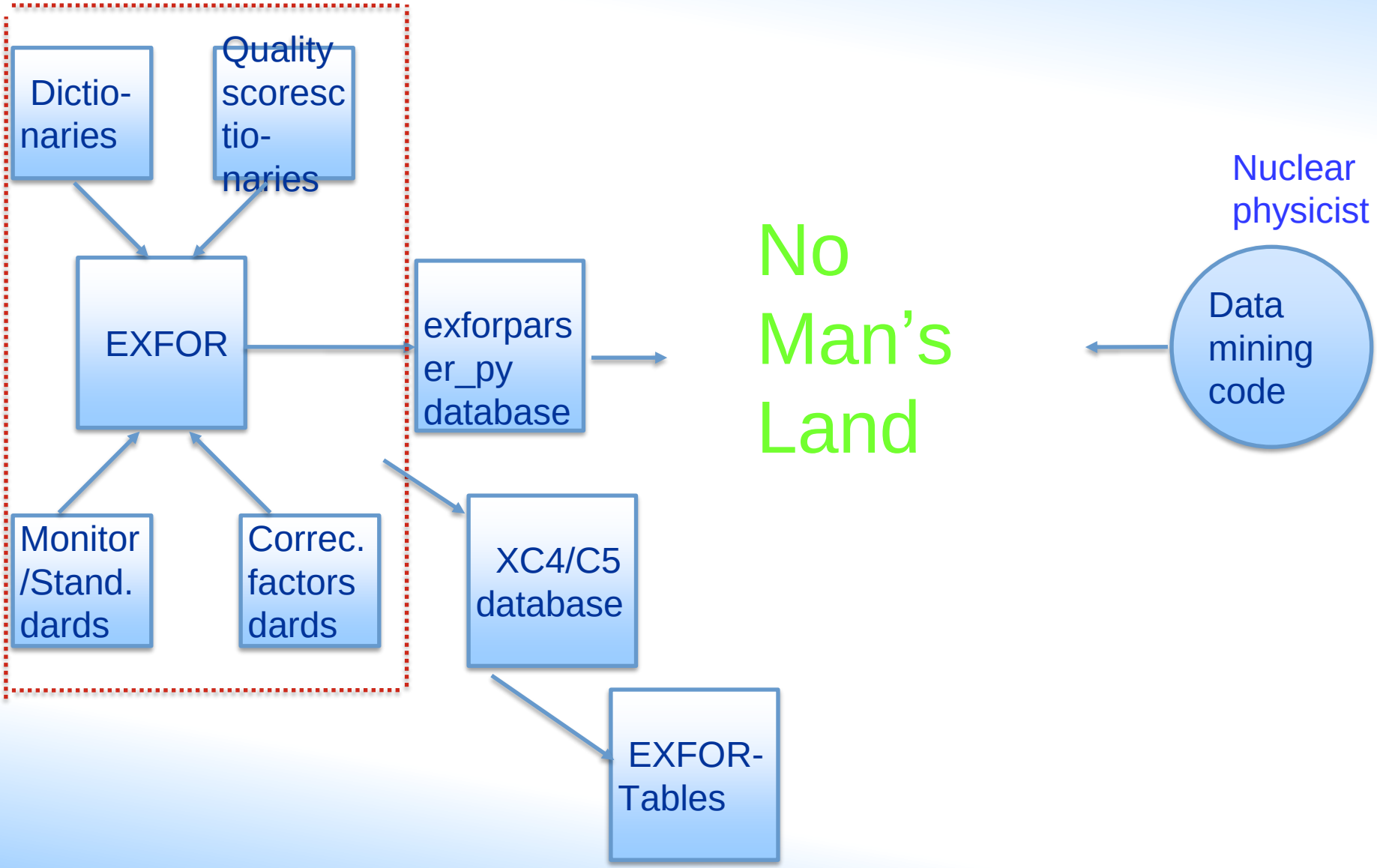

Data
Super code
User

Versus


Data
Code
Data
Code
Data
Code
User
User
User
User

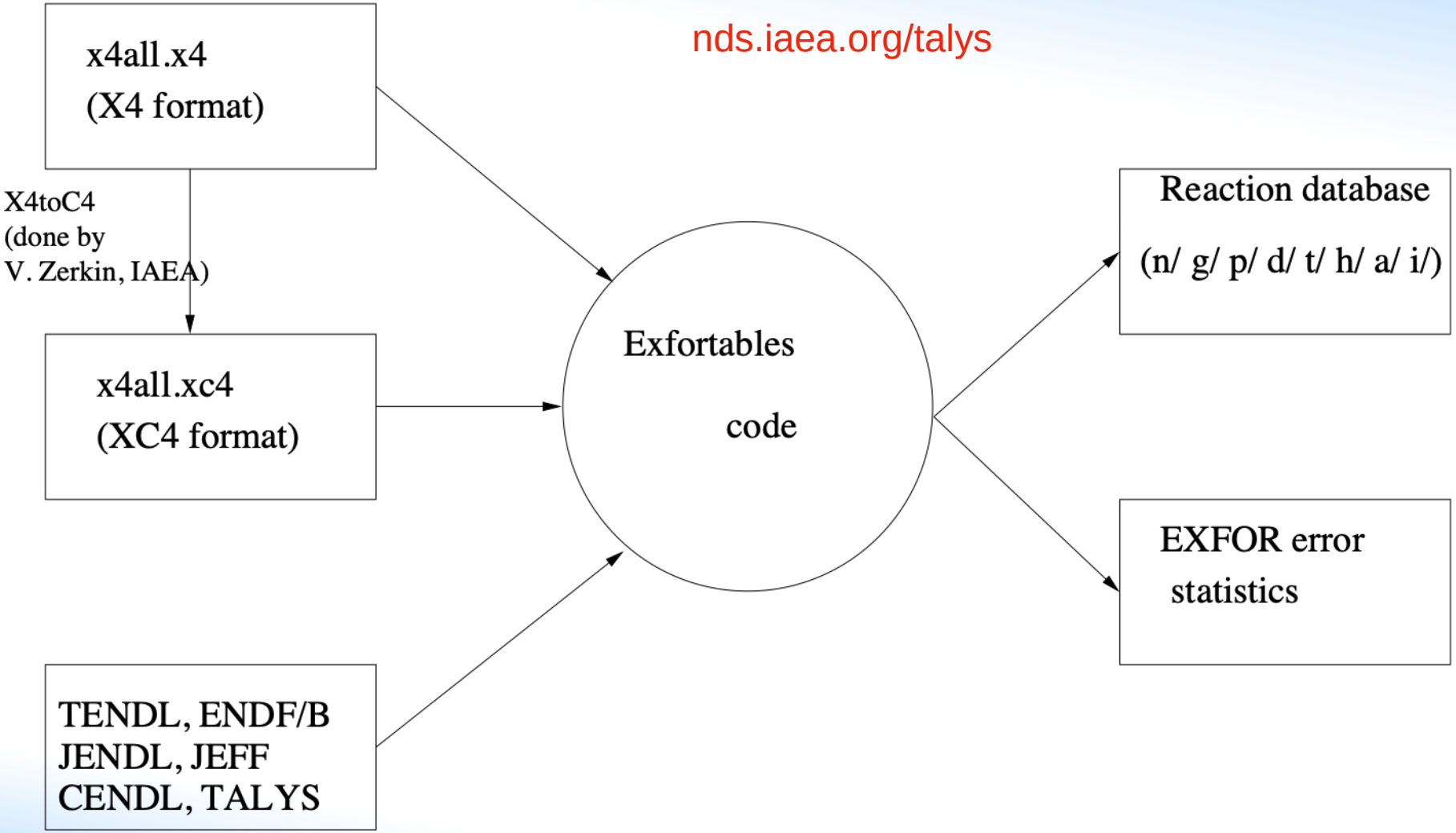
EXFOR parsing

Data mining

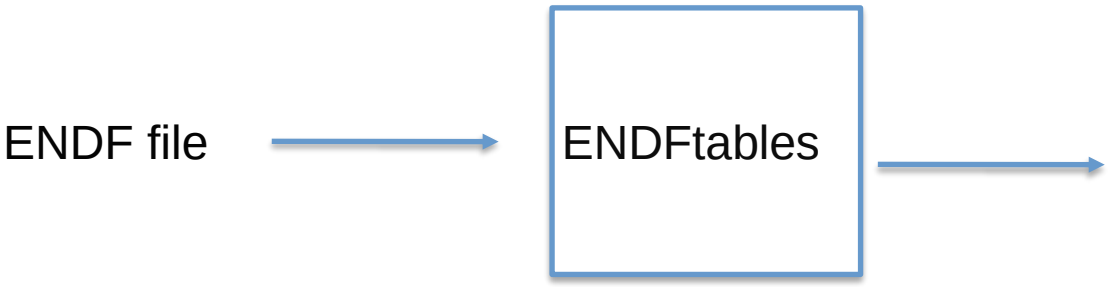


EXFORTABLES code and database

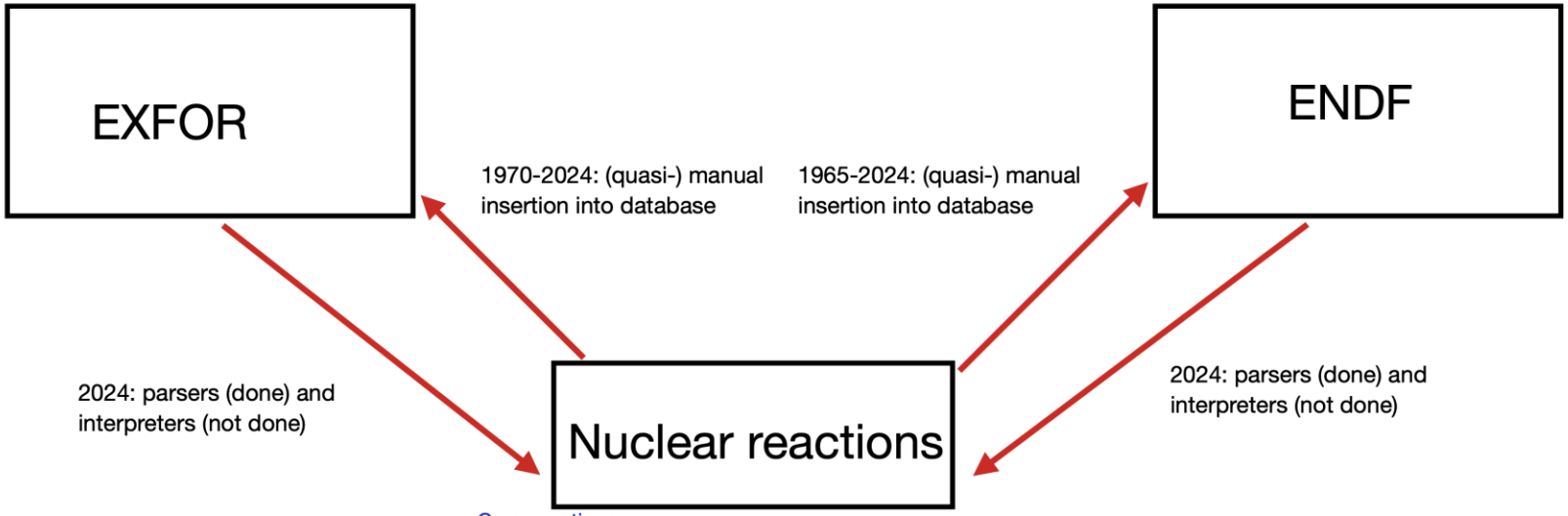
nds.iaea.org/talys



Very complete output of statistics of EXFOR entries: C/E of all data libraries for a large



Many output files of observables:
One x-y (-dy) table per reaction channel



Cross sections
- Cumulative: total, elastic, non-elastic
- Exclusive: (n,n'), (n,2n), (n,g), (n,f), n,p),….to ground state and isomer
- Discrete level: (n,n'_1), (n,n'_2),…(n,p_0),….
- Particle production: (n,xn), (n,xp),….
- Residual production: (n,x), (p,x),….to ground state and isomer

Angular distributions
- Elastic
- Inelastic

Single-differential emission spectra (energy)
Double-differential emission spectra (energy-angle)
Gamma-ray production cross sections
Fission yields
Fission neutron observables (nubar, nu(A), PFNS, etc.)
……

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: Yet Another Nuclear Data Format

- 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 previous output files
- Human-readable
- Same schema for TALYS, EXFOR and ENDF
- Data model from the point of view of a nuclear physicist, not from the specialised EXFOR or ENDF formats
- 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
- Using ‘#’ for attributes
- 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

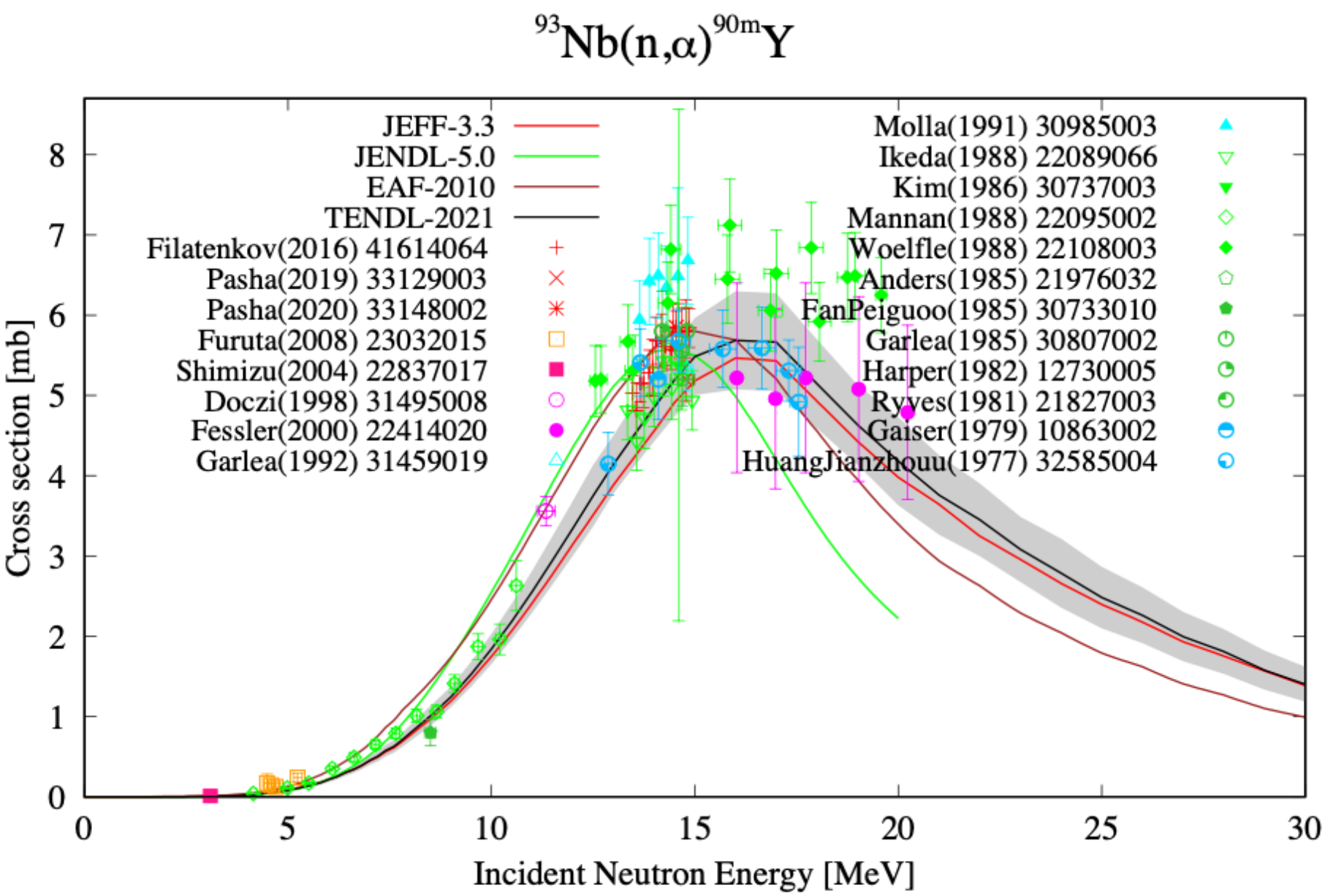
```
# header:
#   title: Nb93(n,a)Y90m cross section
#   source: TALYS-2.0
#   user: Arjan Koning
#   date: 2024-01-16
#   format: YANDF-0.1
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,a)
#   Q-value [MeV]:  4.248473E+00
#   E-threshold [MeV]:  0.000000E+00
#   ENDF_MF: 10
#   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
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Thank you!