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TENDL: Completeness and limitations of the ENDF-6 format

Arjan Koning, IAEA

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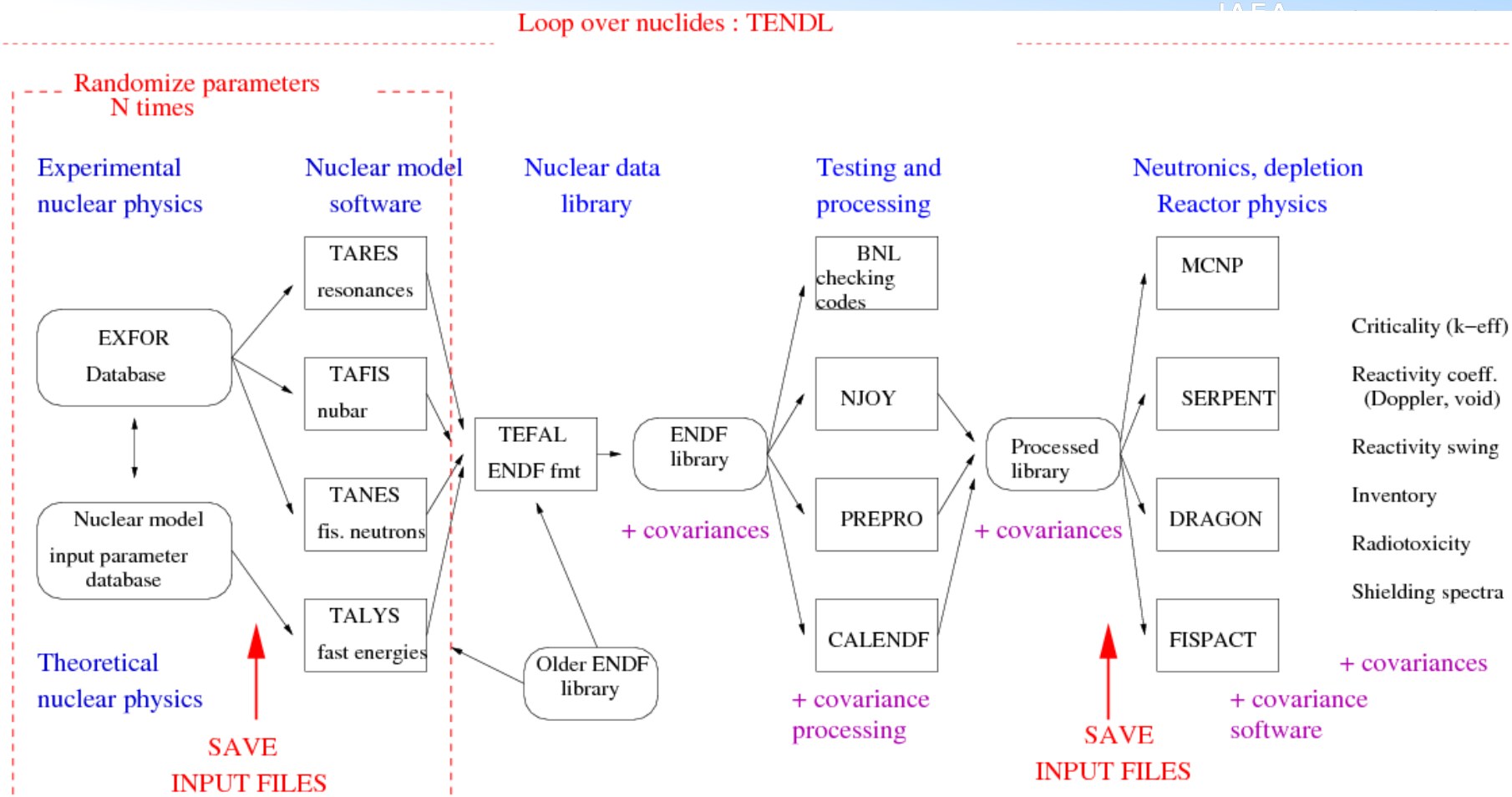
Contents

- TENDL: Prototype nuclear data pipeline
- Completeness of data file and limitations of ENDF-6 for covariance data
- A plea for efficient data retrieval
- Some new software

A nuclear data pipeline since 2009



Once the system (**T6**) works, only the input files (= "the evaluation") are important

Reproducibility

TENDL-2019

- New T6 (TALYS+TASMAN+TEFAL+TARES+TAFIS+TANES)
  - Newest code versions, (TALYS-1.95 release December 2019)
  - more verifications,
  - Linux RedHat/Mac,
  - tested with latest compilers

- TENDL-2019 available (https://tendl.web.psi.ch/tendl_2019/tendl2019.html)

- Similar structure as the previous TENDL libraries
  - 2813 isotopes, 200 MeV
  - Incident neutrons, protons, deuterons, tritons, He3, alphas, and gammas
  - Uncertainty Quantification based on Bayesian Monte Carlo
  - Complete for secondary distributions: ang. dis, DDX, recoils, discrete and continuum gamma's
  - Complete for covariance data for all that ENDF format allows
  - ACE, multi group
  - ENDF-6 files in different options (MF3 MT5 at 0, 20 or 60 MeV, EAF files)
  - MF32 and/or MF33 for resonance range
  - Automated plots versus EXFOR and other world libraries
  - Random files for use in Total Monte Carlo

TENDL-2019

- TARES-1.4: resonance formatting and analyzing tool

- Measured/compiled/evaluated resonances:
  - Based on latest JENDL-4.0, ENDF/B-VIII.0 and JEFF-3.3
  - Based on the latest Atlas, 6th edition (2018)
  - RESONANCETABLES: code to produce unifying and prioritized data library for thermal cross sections, resonance integral, MACS, D_0, Gamma_gamma, S_0 etc. based on Atlas, RIPL, EXFOR
  - **Best of all worlds, expect global superiority in RRR and URR**
- Covariances in MF32 and MF33
  - Consistency between both format
  - Consistent with the random files (using the ENDSAM from IJS)

TENDL may be overcomplete

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Same general structure for every isotopic data file

MF1: description and average fission quantities
MF2: resonance data
MF3: cross sections
MF4: angular distributions
MF5: energy spectra
MF6: double-differential spectra, particle yields and residual products
MF8-10: isomeric cross sections and ratios
MF12-15: gamma yields, spectra and angular distributions
MF31: covariances of average fission quantities
MF32: covariances of resonance parameters
MF33: covariances of cross sections
MF34: covariances of angular distributions
MF35: covariances of fission neutron spectra and particle spectra
MF40: covariances of isomeric data

All output data of TALYS (fast region) and TARES (resonance range) +
all associated covariance data including cross-channel correlations have been encrypted in ENDF-6 format. Thermal neutron capture gamma lines (EGAF) is the only missing component

“Impossible” covariance data for ENDF-6 format

- MF36 does not, and will not, exist: no covariance data for DDX, recoils, gamma-ray branching ratios.
- MF38 does not exist, hampering full covariance representation for FY and decay data
- MF40: covariance for residual production cross section theoretically possible, will lead to huge data files in unattractive format + processability not guaranteed
- MF42-45 does not exist: no covariance for gamma-ray production for discrete levels or continuum
- Uncertainty quantification/propagation for the above classes requires Total Monte Carlo and/or new format (GNDS)

TENDL paradigm for nuclear data evaluation

- All historical nuclear data of importance:
  - EXFOR
  - Other experimental data sets (EGAF, etc.)
  - Resonance compilations/evaluations (Atlas)
  - Existing nuclear data libraries (ENDF/B, etc)
- ….need to be available on the spot, with command-line access, in order to be manipulated into better nuclear data libraries, with the help of a nuclear model code

Options for data retrieval

- One extreme: GUI with click-by-click options, date retrieval per case (JANIS, ZVVIEW etc.)
- Other extreme: Complete translation of entire data libraries (EXFOR, ENDF) into direct-access logical directory structure (used by TALYS system)
- Optimal (?) solution: online command-line API, e.g.
  - getexfor -element Nb -mass 93 -reaction n,2n -quantity xs -format json
  - getendf -element U -mass 235 -reaction n,f -library jendl4.0
- Options to accomplish this (?):

"getexfor"

Special extensions of:

EXFORtables
X4toC4
IAEA retrieval scripts
Other software

"getendf"

Special extensions of:

DECE
ENDVER
ENDFTABLES
FUDGE
NJOY
PREPRO

Ni-58: Create the best TALYS input file

```
/Users/koning/talys/structure/best/Ni058> cat n-Ni058.talys
#
# General
#
ldmodel 2
m2constant 1.30
#
# (n,tot), (n,el), (n,inl)
#
#
# (n,p), (n,2n), (n,np)
#
rvadjust p 1.10
aadjust 27 57 0.95
pshift 27 57 -0.8
pshift 27 58 -0.85
#
# (n,a)
#
rvadjust a 1.02
avadjust a 1.02
cknock a 0.5
cstrip a 0.5
#
# (n,g)
#
gamgamadjust 28  59 0.33
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
#
branch 27 58 2 2 1 0.8 0 0.2
branch 27 58 12 1 1 1.0
branch 27 58 17 1 1 1.0
branch 27 58 20 1 1 1.0
/Users/koning/talys/structure/best/Ni058>
```

talys < talys.inp > talys.out

Autonorm: Normalize TALYS to data from other NDL's

```
/Users/koning/talys/structure/best/Ni058> cat n-Ni058.auto
projectile n
element Ni
mass 058
library irdff2.0
norm mt=2 width=0.05 lib=endfb8.0 emin=0. emax=10. ebeg=0. eend=8.
norm mt=16 width=0.05 emin=0. emax=50. ebeg=0. eend=48.
norm mt=51 width=0.05 lib=endfb8.0 emin=0. emax=14. ebeg=0. eend=10.
norm mt=52 width=0.05 lib=endfb8.0 emin=0. emax=14. ebeg=0. eend=10.
norm mt=53 width=0.05 lib=endfb8.0 emin=0. emax=14. ebeg=0. eend=10.
norm mt=54 width=0.05 lib=endfb8.0 emin=0. emax=14. ebeg=0. eend=10.
norm mt=103 width=0.05 emin=0. emax=30. ebeg=0. eend=28.
```

autonorm < autonorm.inp

talys < talys.inp > talys.out

(i.e. run TALYS again)

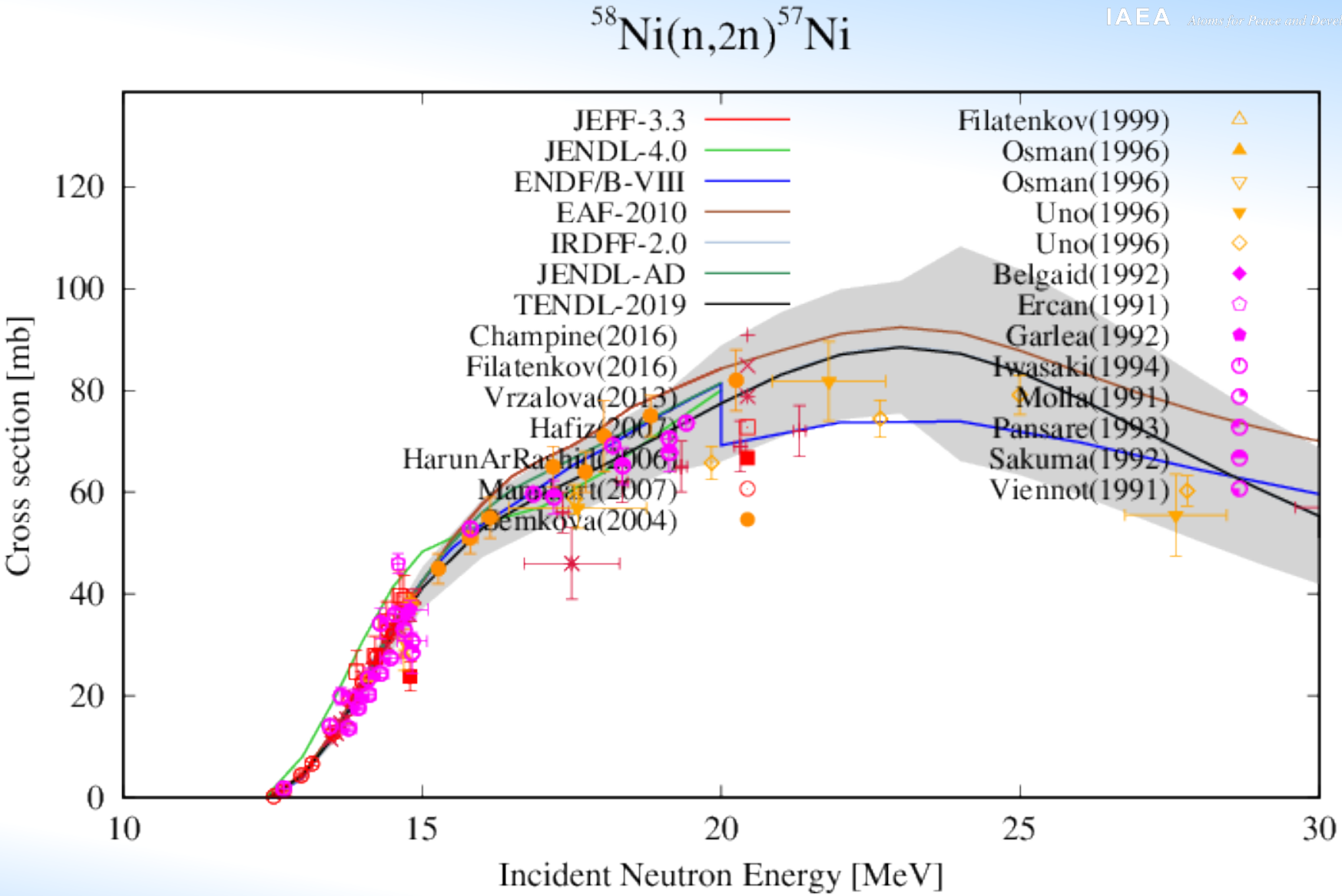
autotalys -element Ni -mass 58

```
tares < tares.inp > tares.out
   (produce the resonance paramaters + covariances)

talys < talys.inp > talys.out
   (run TALYS)

autonorm < autonorm.inp
  (optional: create ratio's between TALYS and selected NDL channels)
talys < talys.inp > talys.out
  (optional: run TALYS with ratio's)

tasman < tasman.inp > tasman.out
 (produce full covariance matrix + random ENDF files for Total Monte Carlo)
```

Ideally, we should also have, **on the spot** (as opposed to getting integral feedback months later)

```
Comparison with integral activation cross sections/reaction rates
  (FISPACT/EASY) (this is already done)

geticsbep Ni (future API?)

getsinbad Ni (future API?)

getirphe Ni (future API?)

Run all the MCNP etc codes, make automated C/E, plots etc.
```

…and then return to the input files to make improvements



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)

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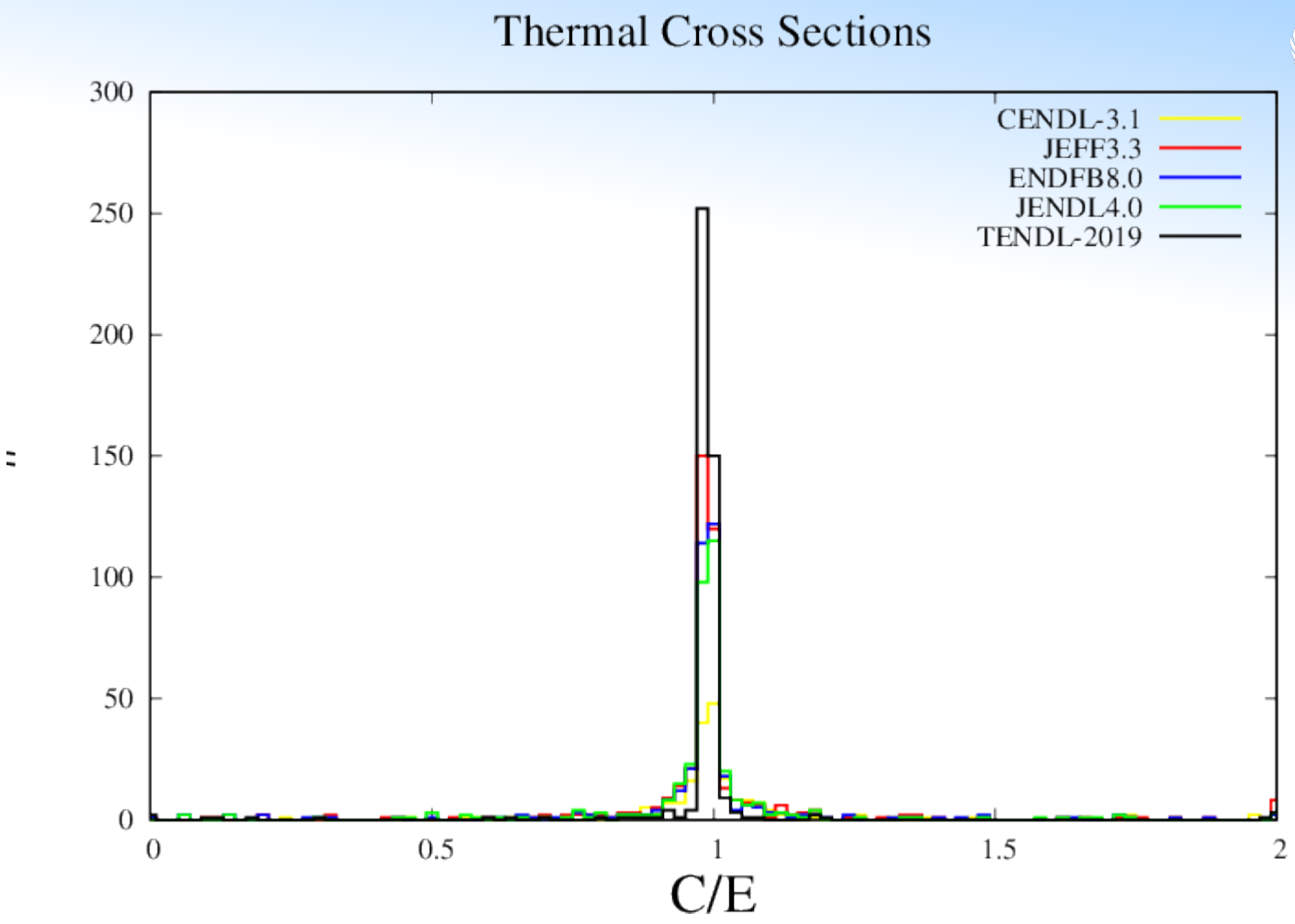
nds.iaea.org/talys

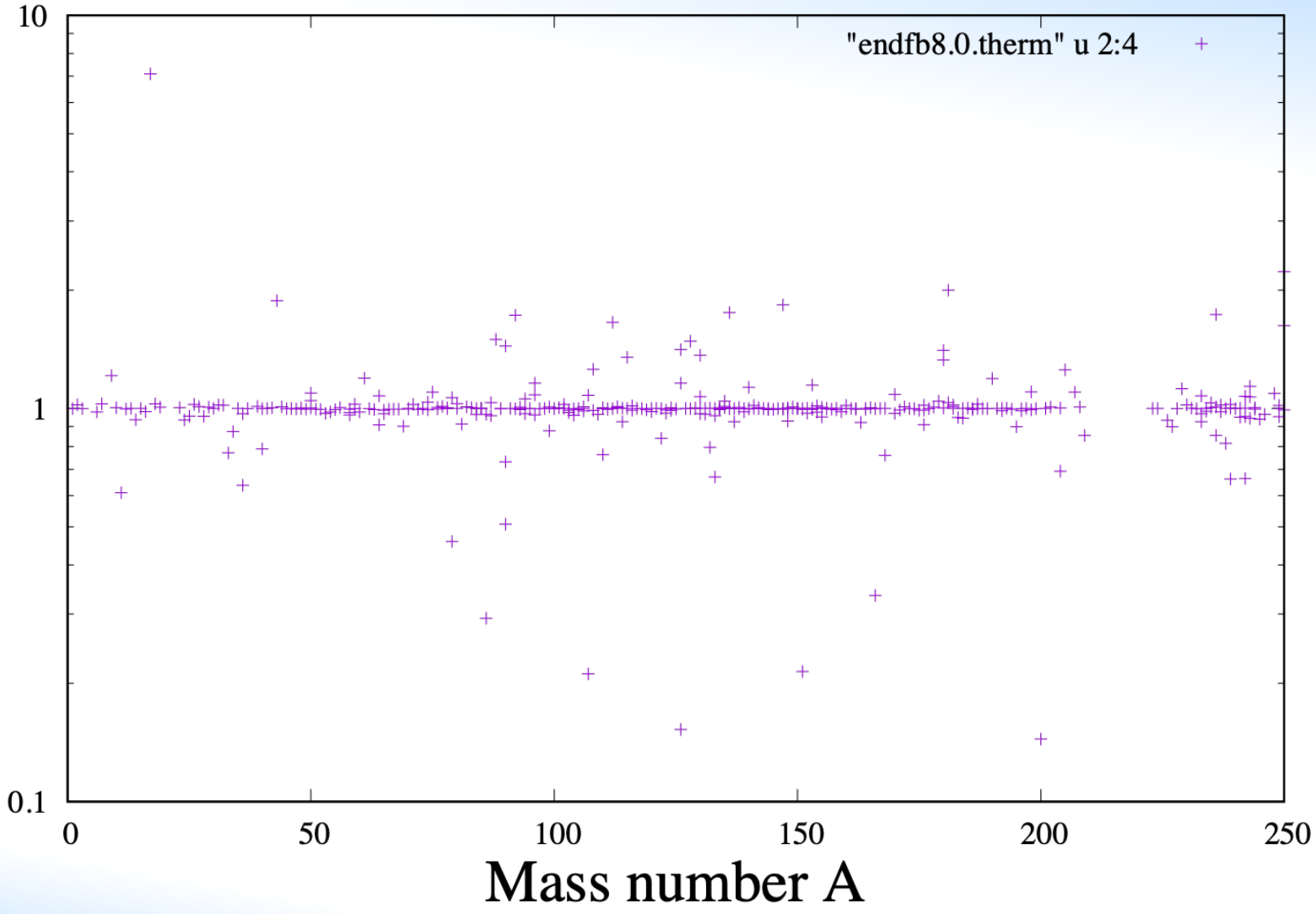
TASMAN, TEFAL, and Tools for TALYS (“T6”) soon to follow



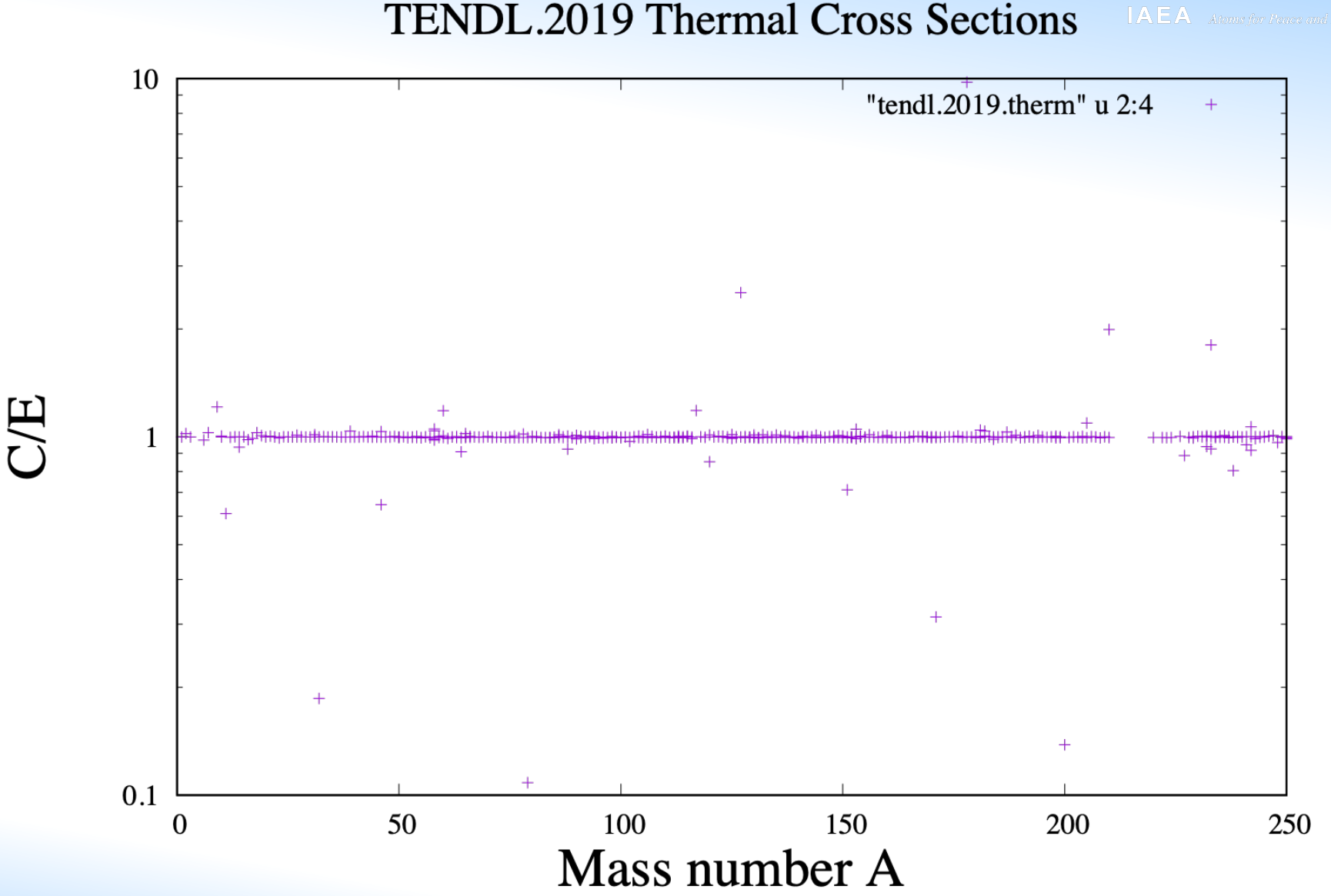
Lib	F(C/E)	N	N <5%	N < 20%	N < 50%
CENDL-3.1	1.036	201	129(0.642)	177(0.881)	187(0.930)
ENDFB-8.0	1.022	375	284(0.757)	332(0.885)	351(0.936)
JEFF-3.3	1.024	425	315(0.741)	377(0.887)	398(0.936)
JENDL-4.0	1.025	359	269(0.749)	320(0.891)	334(0.930)
TENDL-2019	1.008	446	416(0.933)	431(0.966)	434(0.973)

Ratio over final database

ENDFB8.0 Thermal Cross Sections



Ratio over final database



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Thank you!