IAEA 60 Years
Atoms for Peace and Development

Status of TENDL and its role for JEFF-4

Arjan Koning, IAEA
Dimitri Rochman, PSI

JEFF Meeting, Nov 23-27 2020, NEA, Boulogne-Billancourt (virtual)

Contents

- TENDL: Paradigm shift
- TENDL-2019: Global comparison with other libraries
  - Thermal cross sections, Res Int and MACS
  - Comparison vs. EXFOR
- Integral validation
- TENDL4JEFF
- Summary and future

“The split”: IAEA Meeting on long term nuclear data needs (2011)

An Alternative Future: An International Evaluated Nuclear Database (“ENDF/I” or “WENDF” or “WEF or …”)

M.B. Chadwick

X-CP Computational Physics Division, LANL,

What users need: nuclear data libraries of the highest possible quality for all nuclides, incident particles, energies, reaction channels, including uncertainties:

A plea for reproducibility

Arjan Koning

CIELO

All effort on 6 most important isotopes

Successful collaboration between experimentalists, nuclear modelers, evaluators and validators

No change in evaluation/validation paradigms

TENDL

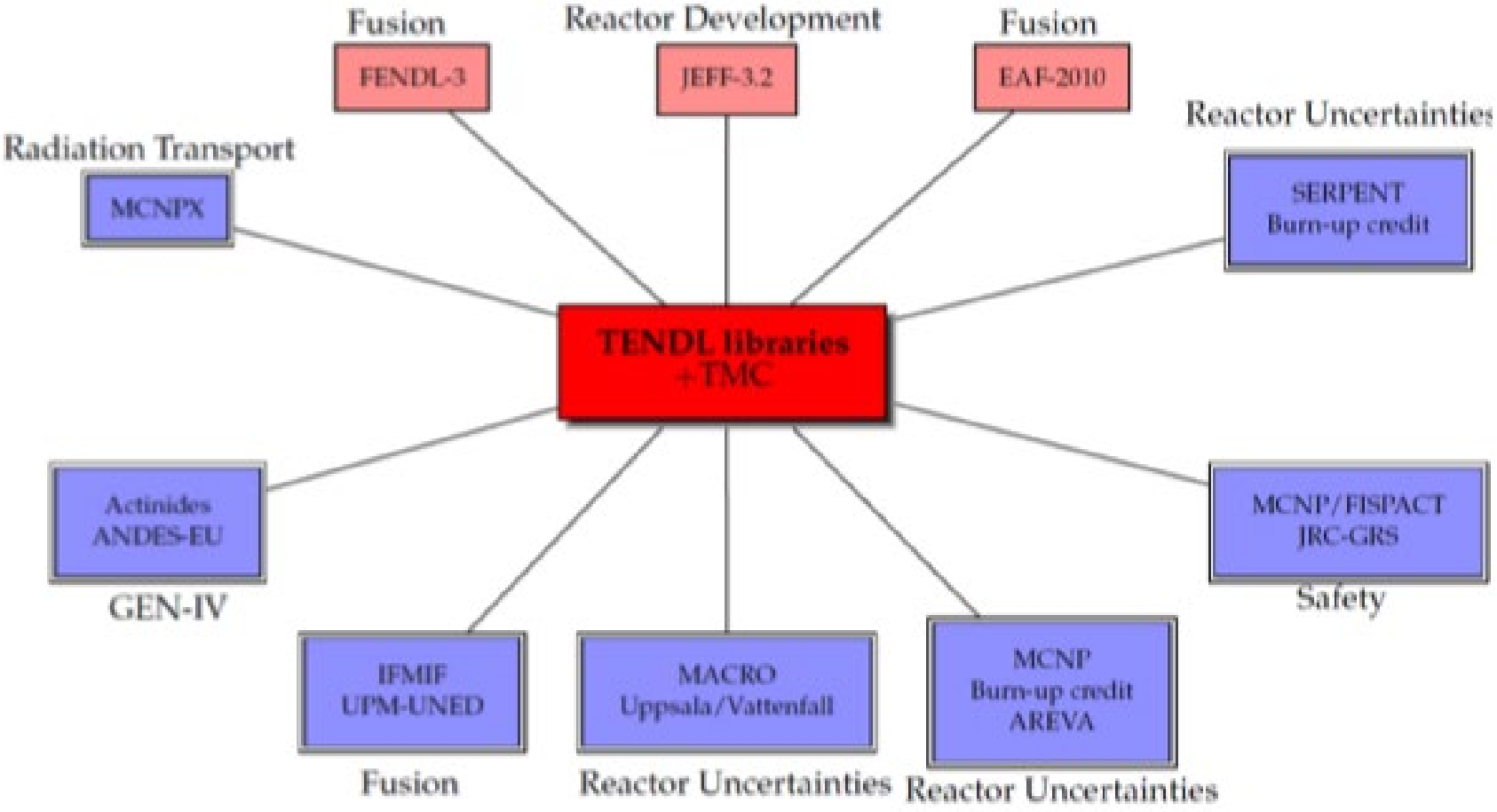
All effort distributed among everything

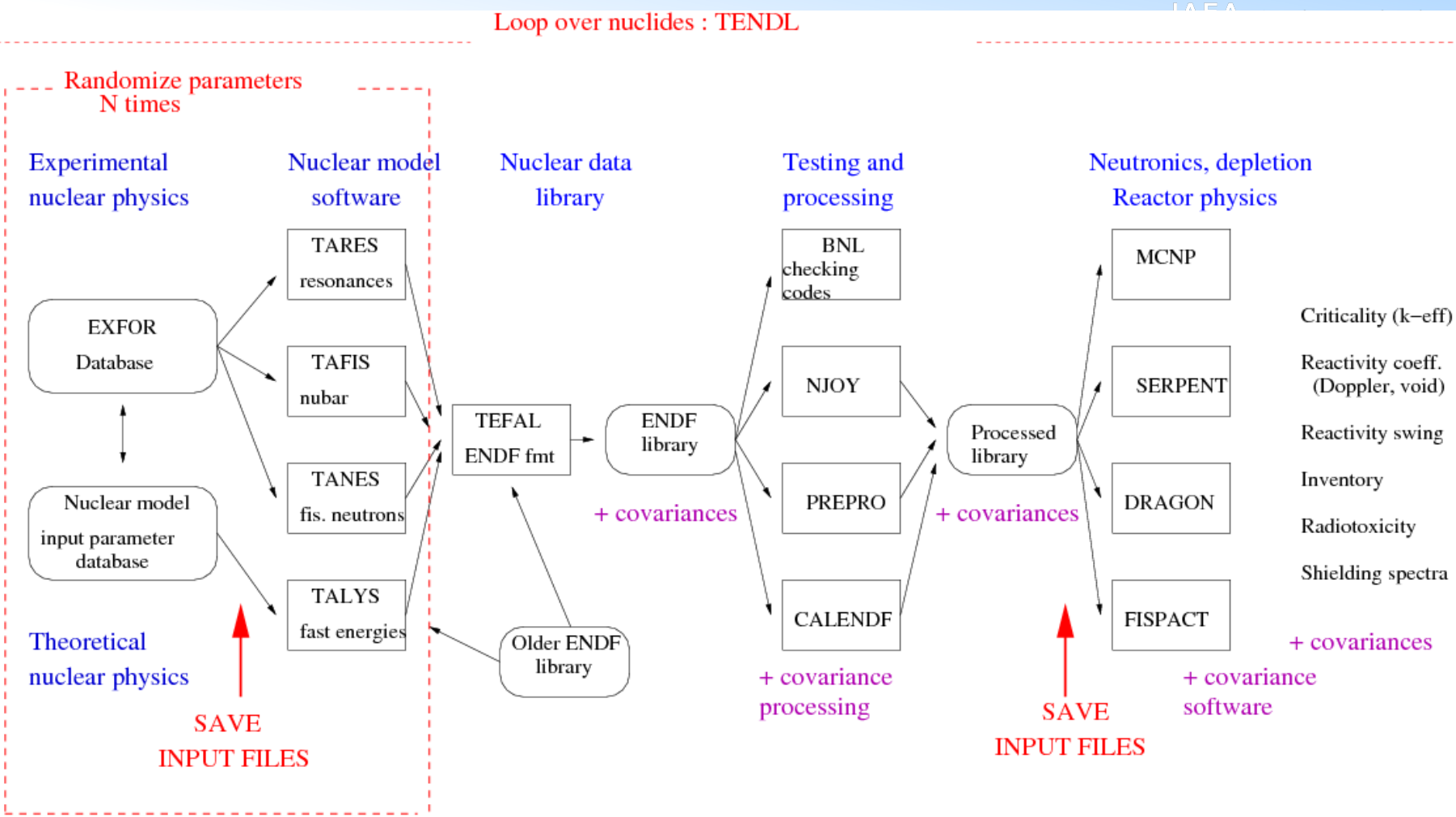
Automated use of “all knowledge up to now”: EXFOR, TALYS, existing libraries CIELO (challenging!), AK + DR

Reproducibility and completeness

What is the TENDL project ?

- Fully implemented in FISPACT-II, part of GEANT, CASMO…,
- Used in fission, fusion applications, medical isotope productions





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

Reproducibility

TENDL-2019

TALYS-based evaluated nuclear data library

Home | Reference & us | Citations | Feedback | TALYS

"We believe that our great goal can be achieved with systematism and reproducibility. We are so outside the box, that the box is a point"

How to reference

Sub-library files

1. Neutron
2. Proton
3. Deuteron
4. Triton
5. He3
6. Alpha
7. Gamma

Application libraries & tar

Random files

1. Random fission yields
2. Random thermal scattering
3. Random ENDF-6 files
4. Random ACE files

V&V

TENDL-2019: (release date: December 31, 2019)

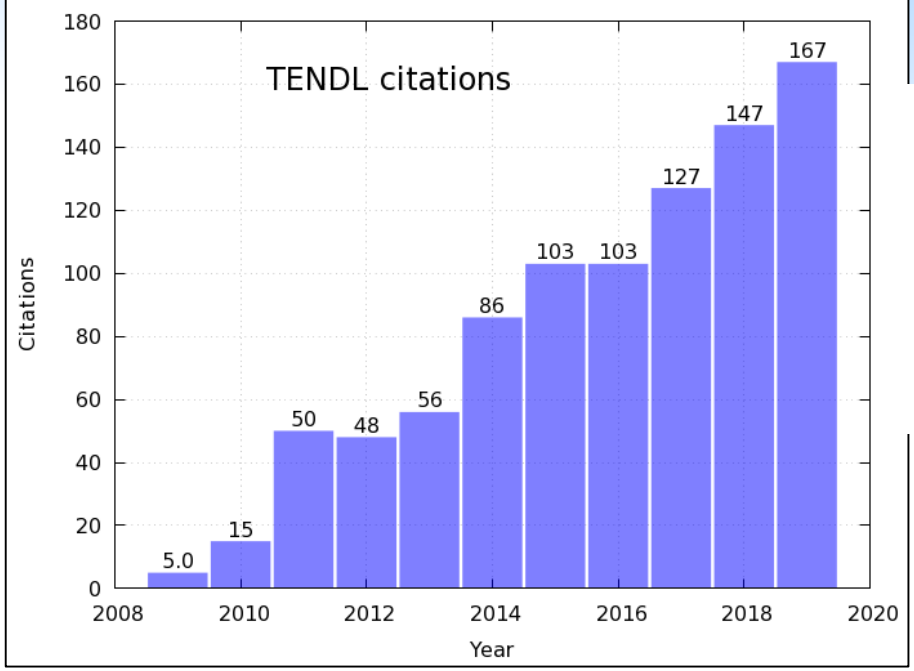
Last update: 13 December 2019

TENDL is a nuclear data library which provides the output of the **TALYS** nuclear model code system for direct use in both basic physics and applications. The 10th version is **TENDL-2019**, which is based on both default and adjusted **TALYS** calculations and data from other sources (previous releases can be found here: 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, and 2017).

Up to 2014, TENDL was produced at NRG Petten. Since 2015, TENDL is mainly developped at PSI and the IAEA (Nuclear Data Section). Still, many people contributes to TENDL with the testing and processing of the files.

TENDL contains evaluations for seven types of incident particles, for all isotopes living longer than 1 second: Z=1 ^{1}H to Z=115 ^{291}Mc (about 2800 isotopes), up to 200 MeV, with covariances.

TENDL is not a default or shadow library. Not a single neutron evaluation is based on default calculations. With the HFR approach, all resonances follow statistical hypothesis. For major isotopes, greater care was used during the evaluation process.



ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

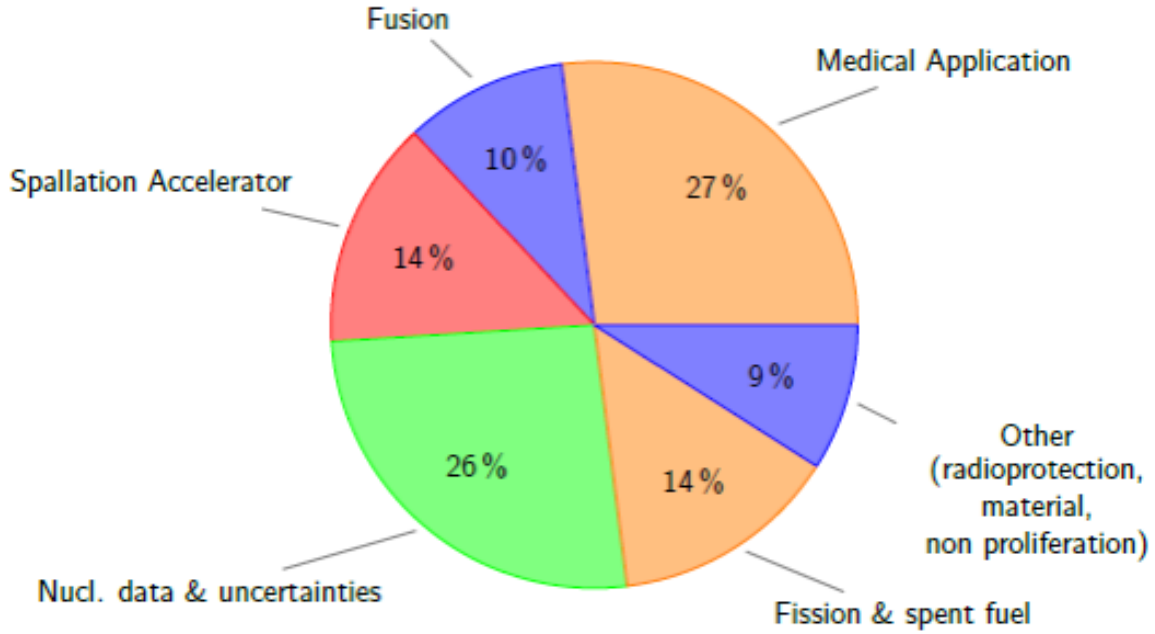
Nuclear Data Sheets

Nuclear Data Sheets 155 (2019) 1–55

www.elsevier.com/locate/nds

TENDL: Complete Nuclear Data Library for Innovative Nuclear Science and Technology

A.J. Koning,[1,2,*] D. Rochman,[3] J.-Ch. Sublet,[1] N. Dzysiuk,[4,5] M. Fleming,[6,7] and S. van der Marck[4]



TENDL-2019, what is new ?

- 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)

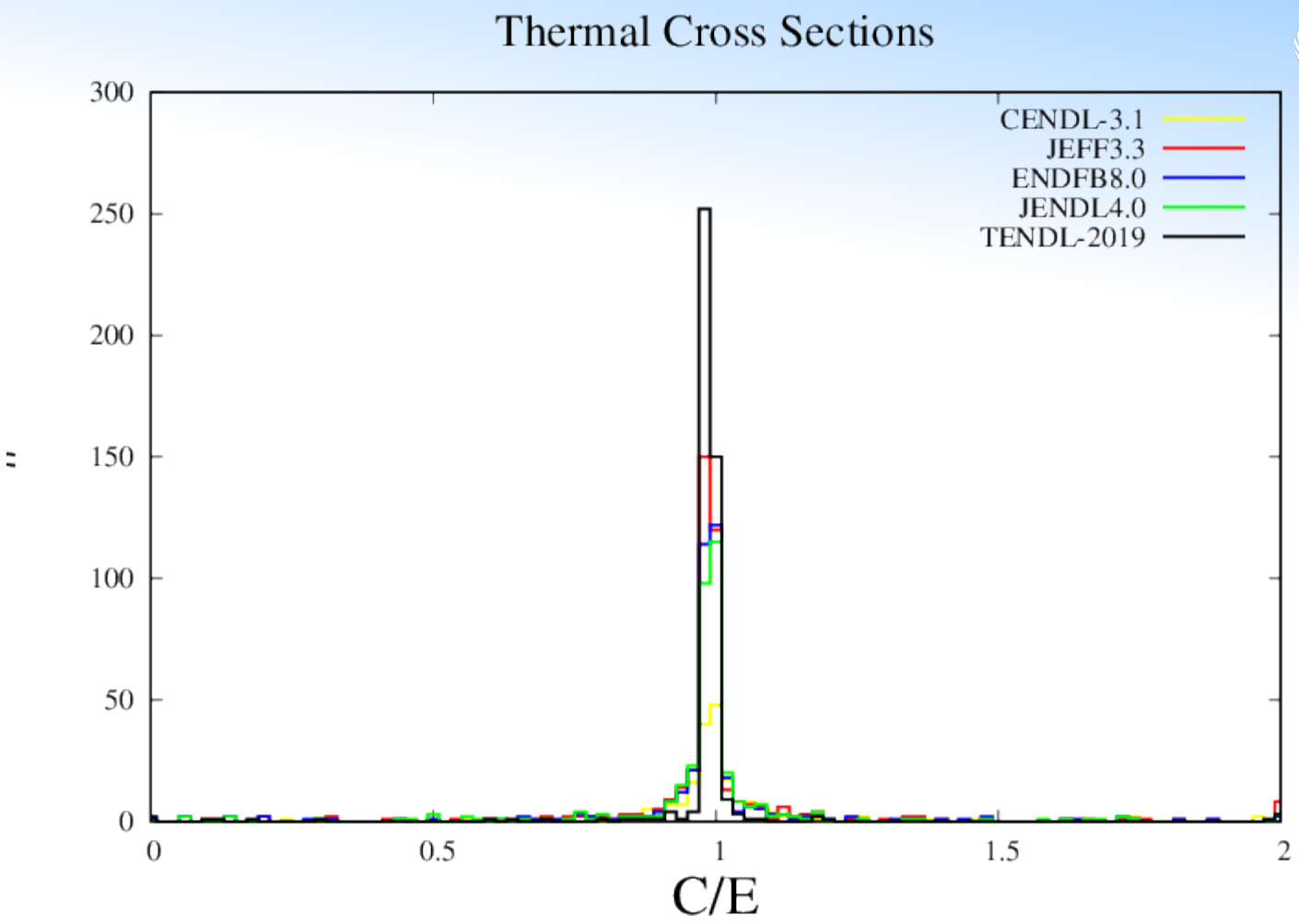
- Similar structure as the previous TENDL libraries
  - 2813 isotopes, 200 MeV
  - Incident neutrons, protons, deuterons, tritons, He3, alphas, and gammas
  - Uncertainty Quantification based on Bayesian Monte Carlo
  - Complete for secondary distributions: ang. dis, DDX, recoils, discrete and continuum 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, what is new ?

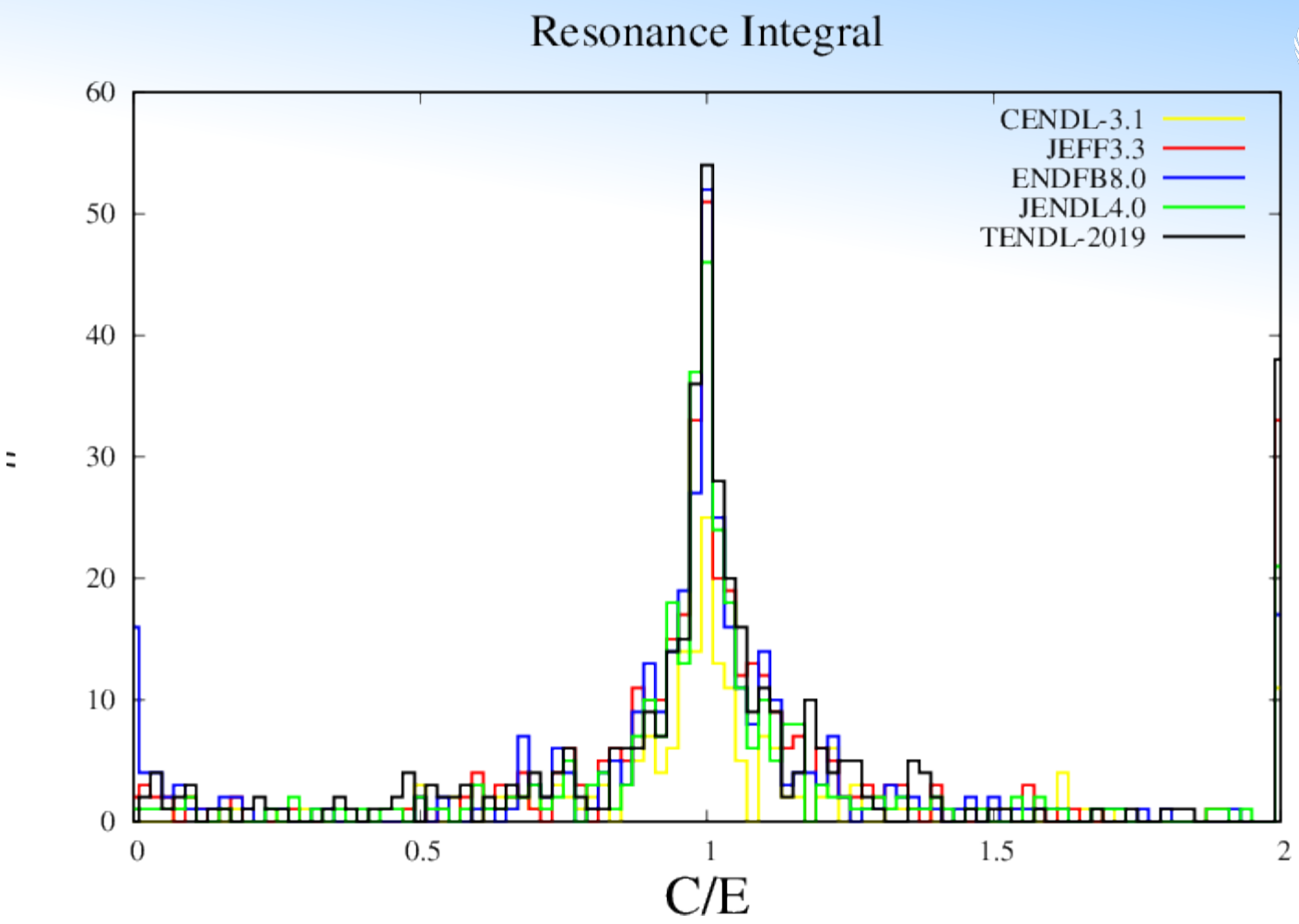
- TARES-1.4: resonance formatting and analyzing tool

- 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**
- Statistical resonances:
  - Based on CALENDF
  - Translating the unresolved range from TALYS into statistically resolved range
  - Consistency between the RRR, URR and fast range

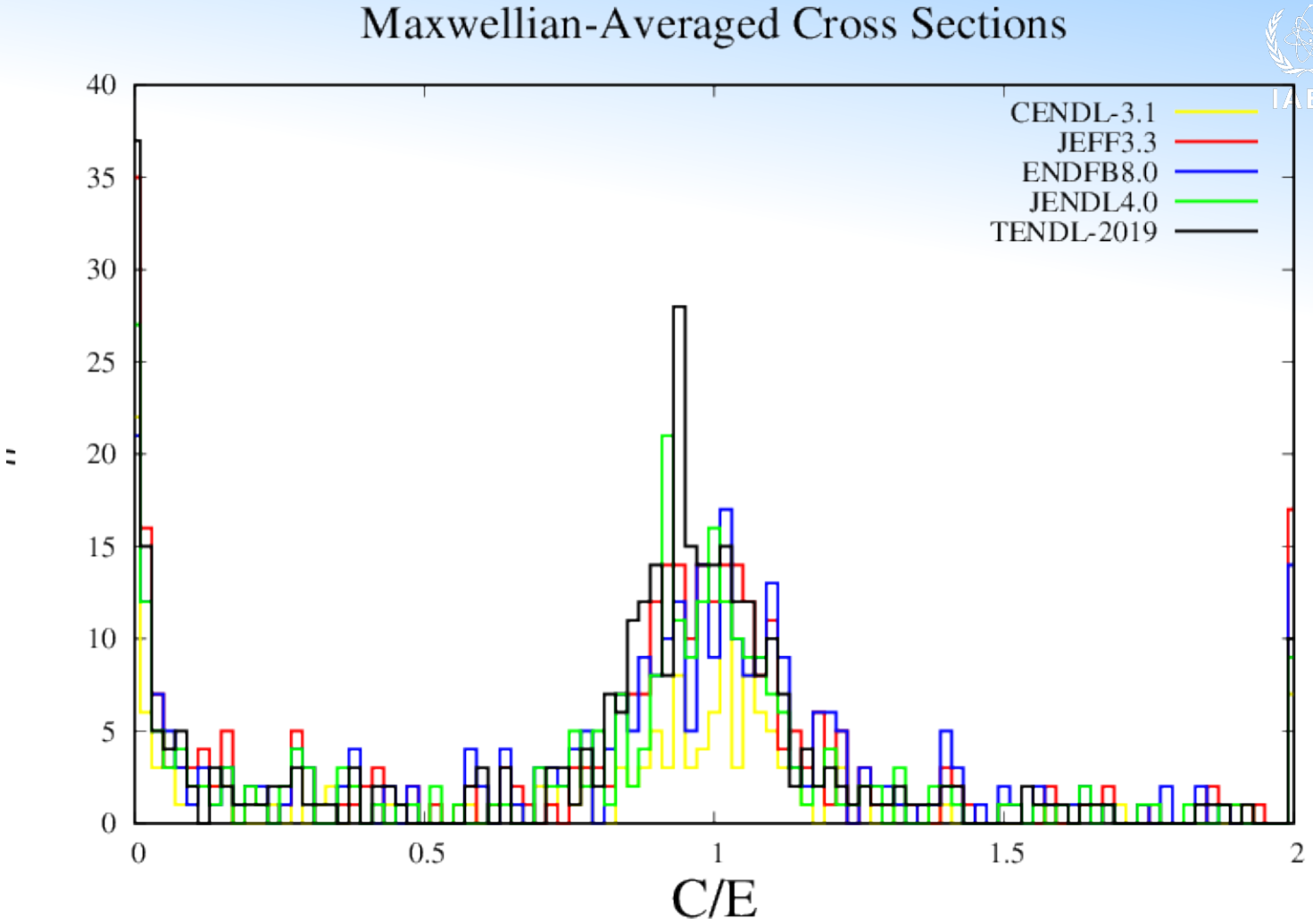
- Covariances in MF32 and MF33
  - Consistency between both format
  - Consistent with the random files (using the ENDSAM from IJS)



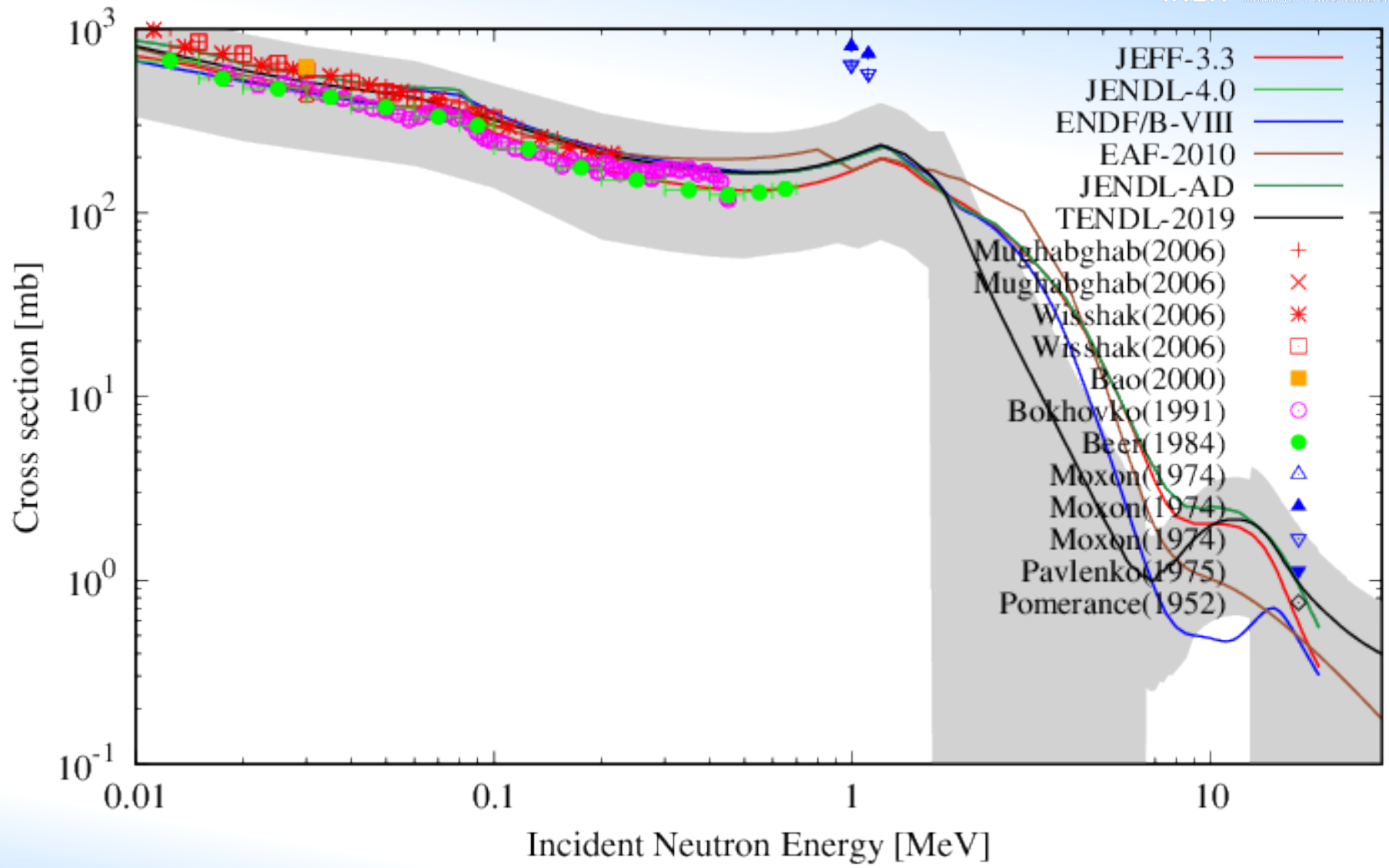
Lib	F(C/E)	N	N <5%	N < 20%	N < 50%
CENDL-3.1	1.036	201	129(0.642)	177(0.881)	187(0.930)
ENDFB-8.0	1.022	375	284(0.757)	332(0.885)	351(0.936)
JEFF-3.3	1.024	425	315(0.741)	377(0.887)	398(0.936)
JENDL-4.0	1.025	359	269(0.749)	320(0.891)	334(0.930)
TENDL-2019	1.008	446	416(0.933)	431(0.966)	434(0.973)

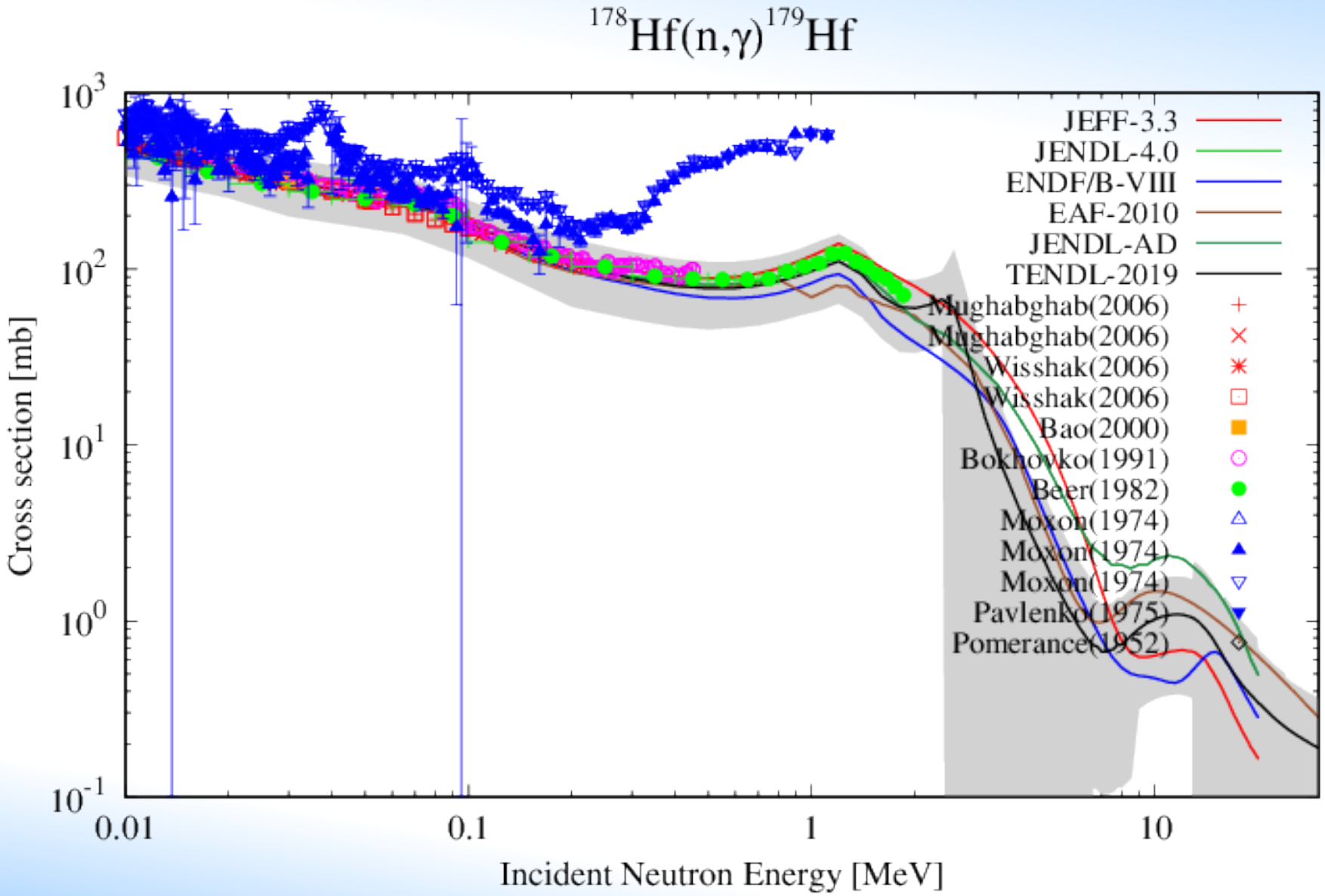


Lib	F(C/E)	N	N < 5%	N < 20%	N < 50%
CENDL-3.1	1.056	194	73(0.376)	126(0.649)	158(0.814)
ENDFB-8.0	1.060	377	138(0.366)	249(0.660)	300(0.796)
JEFF-3.3	1.059	386	133(0.345)	257(0.666)	312(0.808)
JENDL-4.0	1.054	334	133(0.398)	233(0.698)	275(0.823)
TENDL-2019	1.058	412	146(0.354)	263(0.638)	321(0.779)

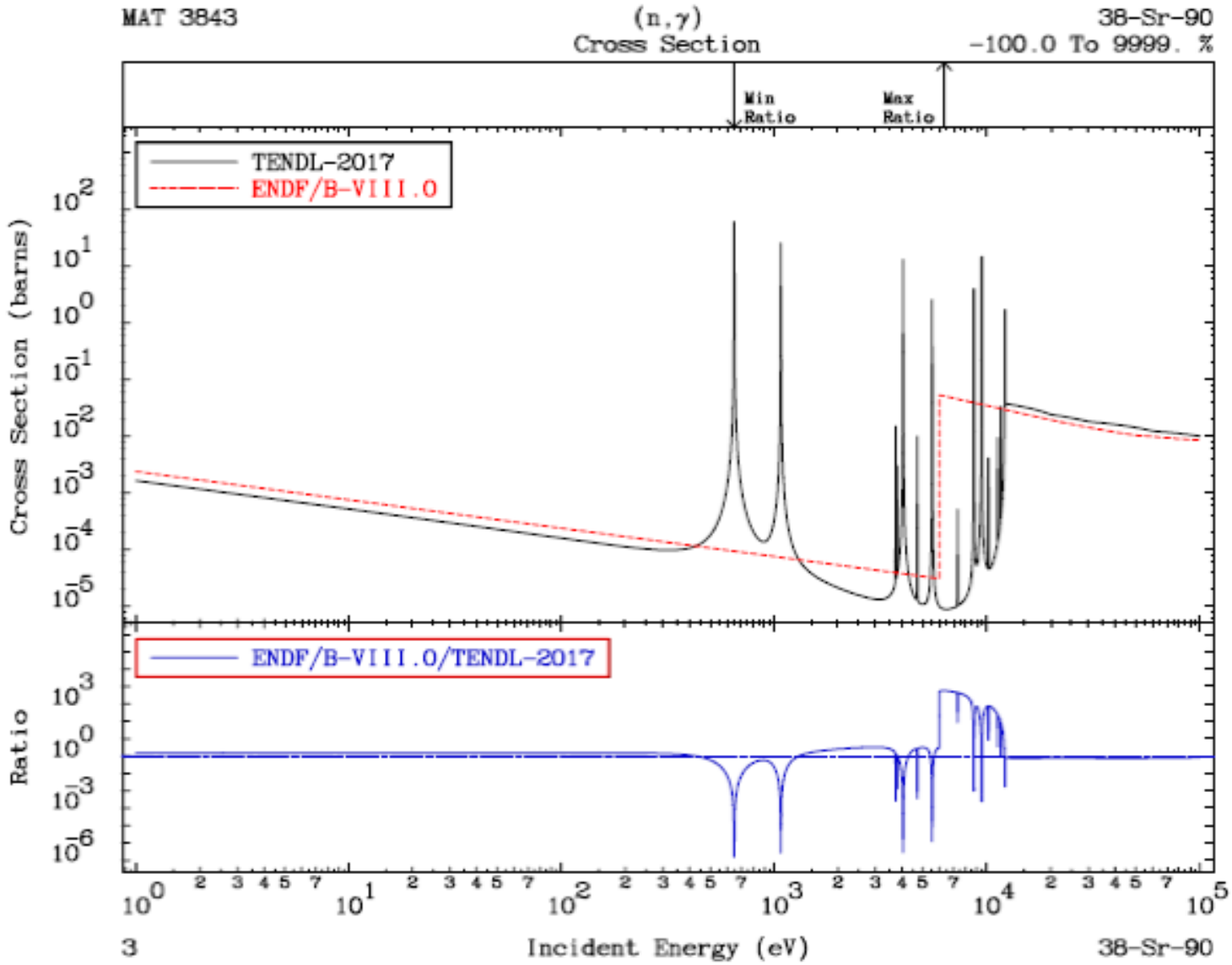


Lib	F(C/E)	N	N < 5%	N < 20%	N < 50%
CENDL-3.1	1.073	176	29(0.165)	78(0.443)	101(0.574)
ENDFB-8.0	1.082	328	56(0.171)	157(0.479)	208(0.634)
JEFF-3.3	1.078	346	67(0.194)	175(0.506)	208(0.601)
JENDL-4.0	1.070	292	59(0.202)	149(0.510)	187(0.640)
TENDL-2019	1.076	357	75(0.210)	196(0.549)	233(0.653)

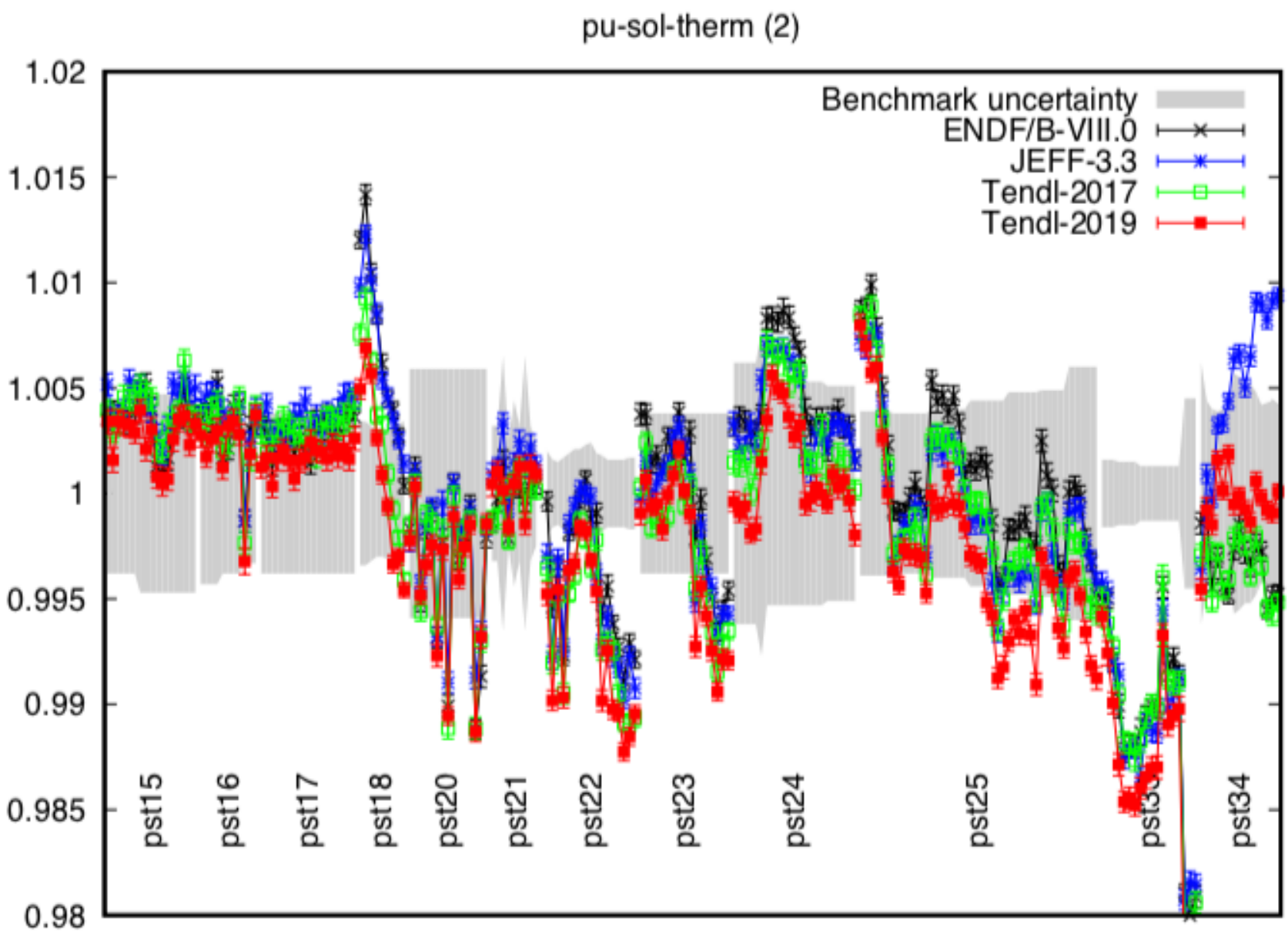



^{178}Hf(n,γ)^{179}Hf
Cross section [mb]
Incident Neutron Energy [MeV]
JEFF-3.3
JENDL-4.0
ENDF/B-VIII
EAF-2010
JENDL-AD
TENDL-2019
Mughabghab(2006)
Mughabghab(2006)
Wisshak(2006)
Wisshak(2006)
Bao(2000)
Bokhovko(1991)
Beer(1982)
Moxon(1974)
Moxon(1974)
Moxon(1974)
Pavlenko(1975)
Pomerance(1952)

Comparison with ENDF/B-VIII: Sr-90



Steven van der Marck MCNP benchmarking (2500 cases)



Challenges for TENDL…and JEFF

- TENDL production is basically a part-time 2-person project. (TENDL validation and feedback involves more persons).
- Release of portable understandable software to produce evaluations including all documentation (working on it……)
  - Danger of a future helpdesk function for the two authors
  - Will T6 be as user-friendly as TALYS?
- **Combine the TENDL production line with the quality of individual evaluations/evaluators**

Example for Ni-58: Can other evaluators do this?

- Choose the best resonance data (DR, subjective), in this case JENDL-4.0 and complement will complete covariances
- tares < tares.inp > tares.out
- MF2 for RRR+URR is now available
- MF32 for covariance data for RRR+URR **or** point wise covariance data in MF33 is now available

ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Nuclear Data Sheets 163 (2020) 163–190

Nuclear Data Sheets

www.elsevier.com/locate/nds

A Statistical Analysis of Evaluated Neutron Resonances with TARES for JEFF-3.3, JENDL-4.0, ENDF/B-VIII.0 and TENDL-2019

D. Rochman,[1,*] A.J. Koning,[2,3] and J.-Ch. Sublet[2]

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)

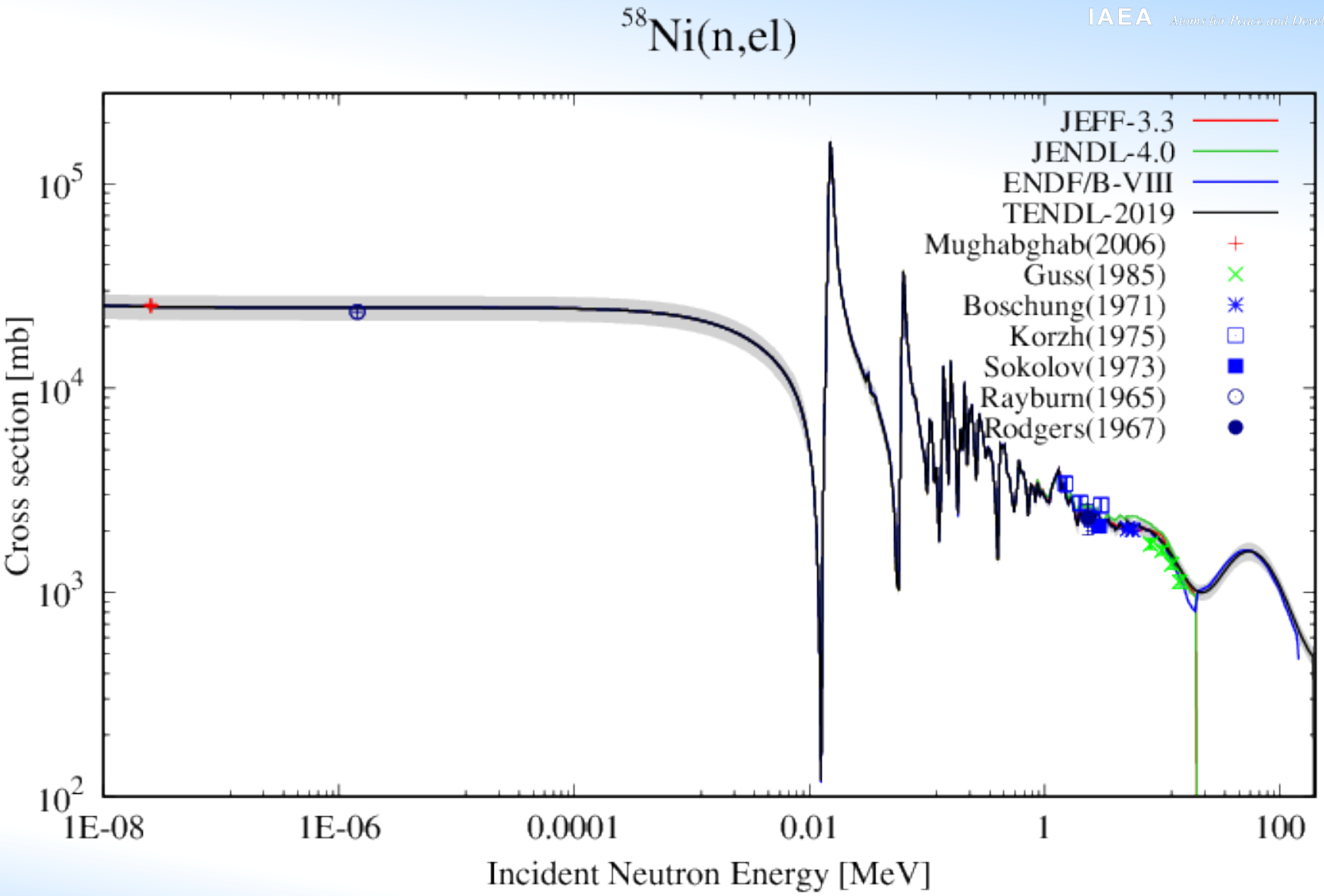
autotalys -element Ni -mass 58

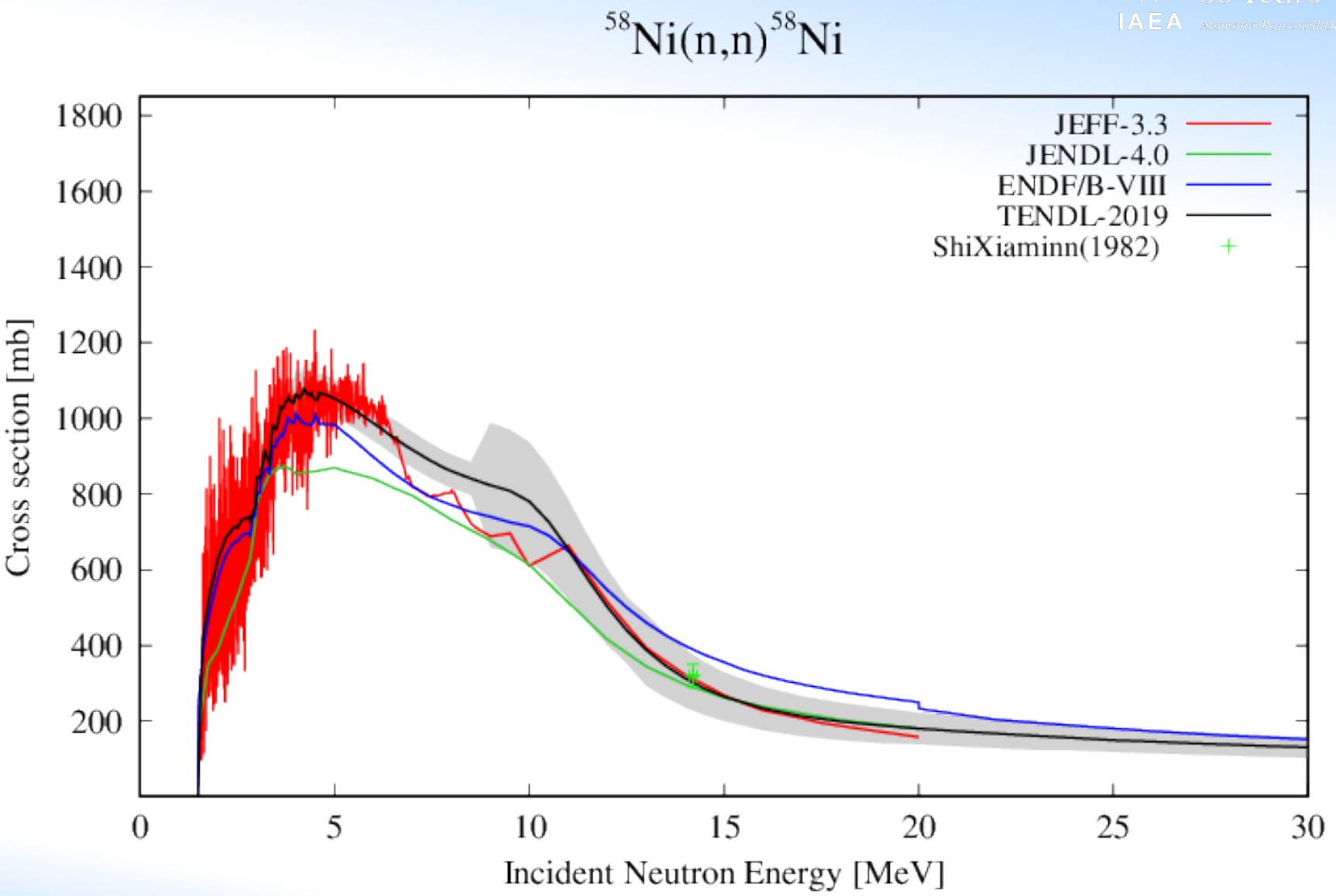
```
tares < tares.inp > tares.out
   (produce the resonance paramaters + covariances)

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)
```

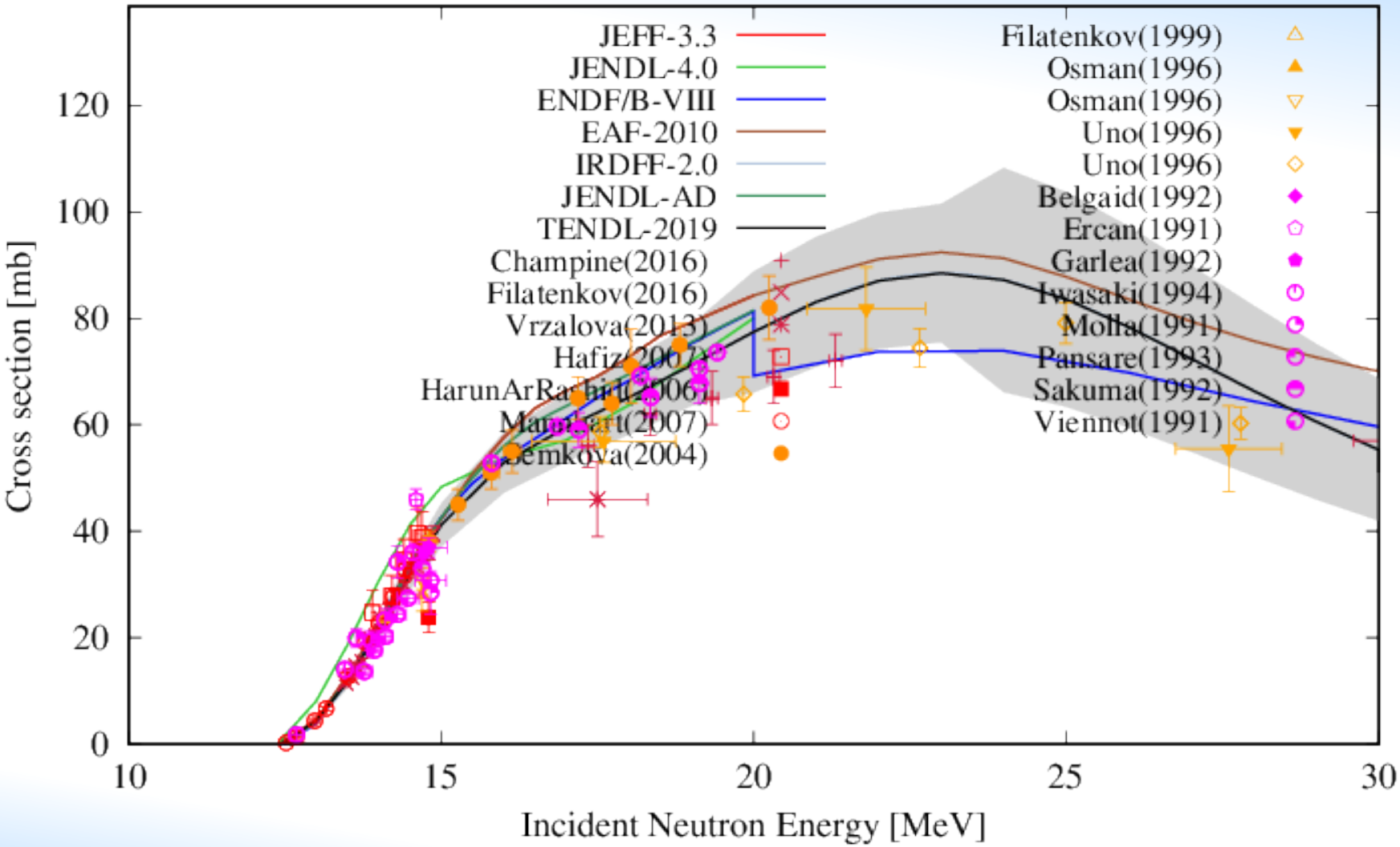
Ideally, we should also have, **on the spot** (as opposed to getting integral feedback months later)

```
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.
```

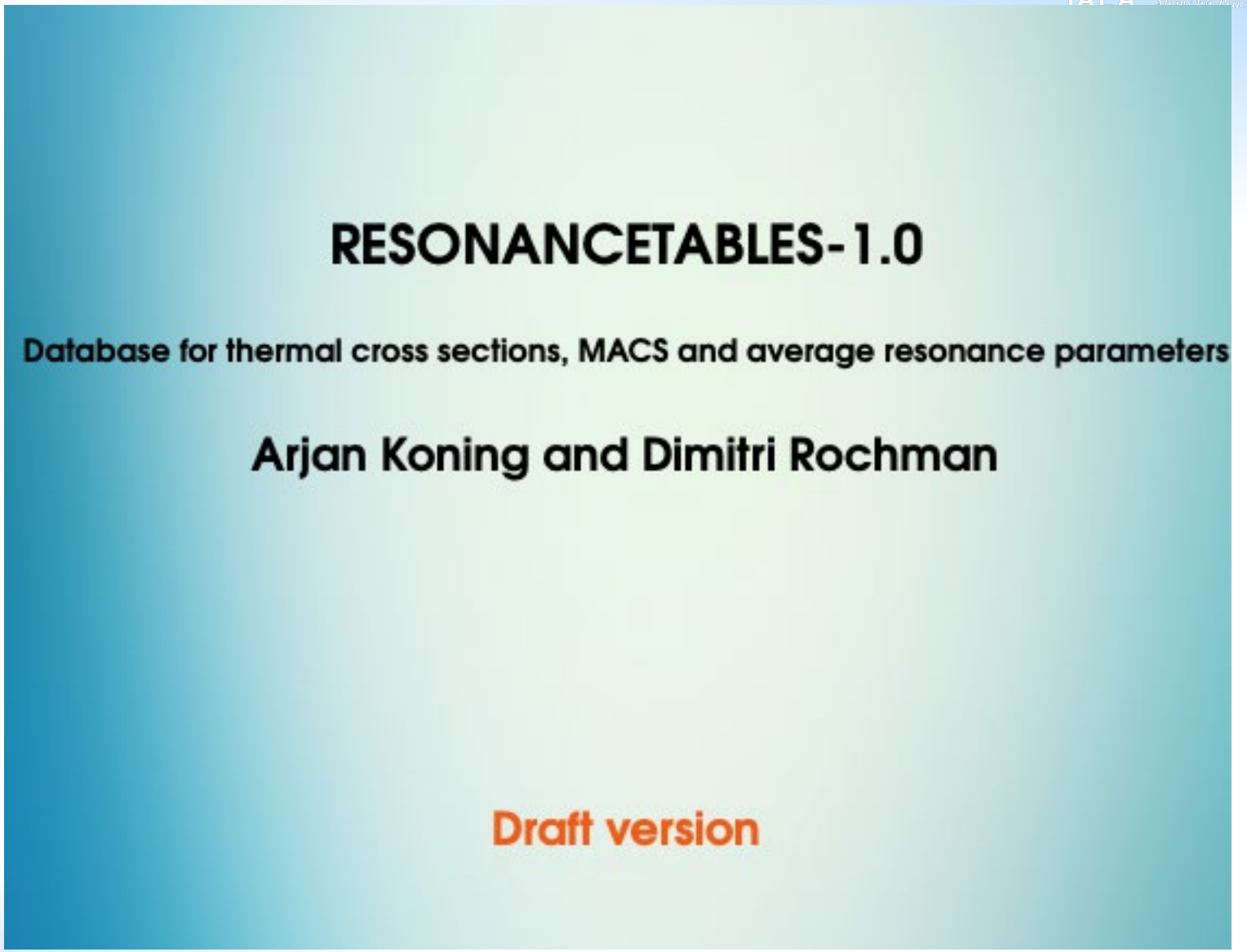
…and then return to the input files to make improvements







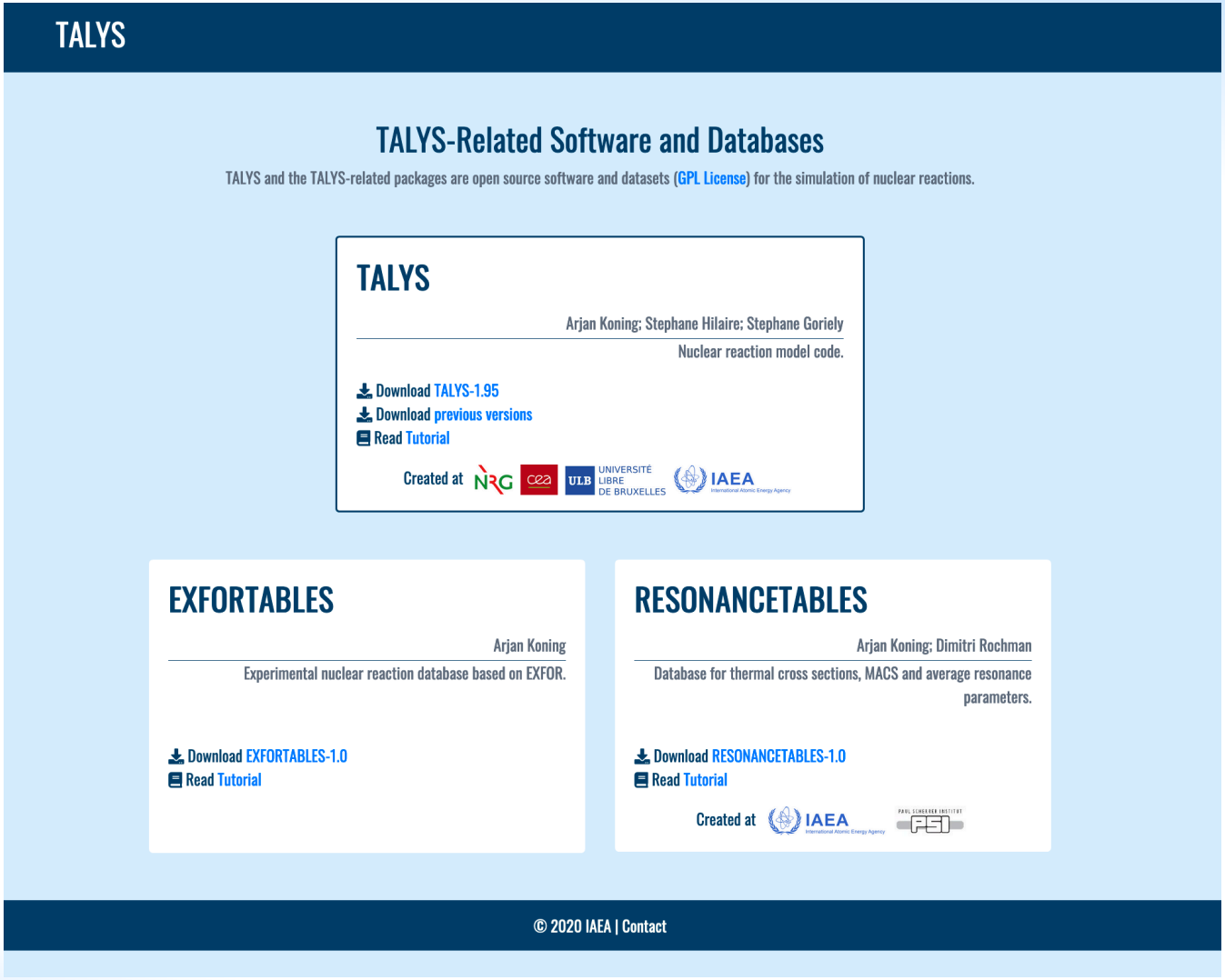
Portable software + complete documentation



Available on new website soon, together with other TALYS-related software

Contents

New webpage under construction at IAEA



TASMAN, TEFAL, Libraries, plots, ENDFTABLES, ISOTOPIA and Tools for TALYS (“T6”) soon to follow

Summary and future

- At least one more….: TENDL-2021
- Focus on more different output formats, more applications do not require/want ENDF
  - Straight from TALYS + TARES to GNDS (C. Mattoon)
  - Tables with human/machine readable covariance data
- Automate validation as much as evaluation (challenging!). Now:
  - Criticality validation by van der Marck
  - Decay heat and activation validation by UKAEA (Gilbert et al)
  - Scattered results from other places in 1-2 years after release
- Extinction of evaluators works to advantage of TENDL approach
  - Bulk of materials already better with TENDL (which is NOT a theoretical nuclear data library)
  - However, need to work on our PR for neutron applications
- Strong coupling with Machine Learning, EXFOR usability
- Release **autotalys** (“T6”), the system that produces (among others) TENDL

IAEA 60 Years
Atoms for Peace and Development

Thank you!