Reproducible nuclear data evaluation

An example: the T6 system

Arjan Koning

Nuclear Data Section, IAEA

NEA, November 27 2019

Outline

First, another paradigm shift

- "Those companies or institutions that can assure and reduce the cycle time for innovations and quality improvements in nuclear data have a distinct advantage in either research or the industrial markets." *Nuclear data for sustainable nuclear energy* (CANDIDE), EU report EUR 23977 EN - 2009

Translation for TALYS, T6 and TENDL (and soon JEFF): Quantify all information and knowledge

- All evaluated nuclear data libraries for reactions (ENDF) and structure (ENSDF), experimental reactions (EXFOR) and other compilations (resonances. integral data, etc.) should be accessible unambiguously, instantaneously and in readable form.

This will open up efficient evaluation, validation, Machine Learning etc.

Challenges for accessibility of all data

- Many important data in compilations rather than accessible input databases (Resonances, EXFOR)
- The nuclear data community never bothered to unify ENDF filenames like they agreed on the format in the files. Collecting all important historic data libraries and processing them is non-trivial
- All ENDF and EXFOR databases need to be dismantled first to get access to important data. No general command-line API's for ENDF or EXFOR retrieval exist (to my knowledge) ("getendf Nb 093 n2n xs endfb8.0")
- After the dismantling of an existing ENDF file and EXFOR, an evaluation and an improved data library can be made.

Nuclear Data Tables: 3 tools for BIG data

EXFORtables

- Aims to transform the EXFOR compilation into a computer-usable database
- Based on XC4 format
- EXFOR in directory structure (aka "newbase", WPEC-SG30)
- x-y-dy file per reaction channel
- Statistical analysis and comparison with nuclear data libraries

ENDFtables

- Transforms ENDF in directory structure
- One x-y-dy file per reaction channel
- Many libraries: ENDF/B, JEFF, JEFF, CENDL, TENDL, IRDFF, EAF, IBANDL, IAEA-MED, other special libraries.
- Makes ENDF data accessible for flexible and efficient use (**not** by GUI)

Nuclear Data Tables: 3 tools for BIG data

Resonancetables

- Thermal cross sections, MACS, average resonance parameters
- Based on previous compilations, evaluations and EXFOR
- Statistical analysis and comparison with nuclear data libraries

Are the above 3 tools good candidates for Gitlab?

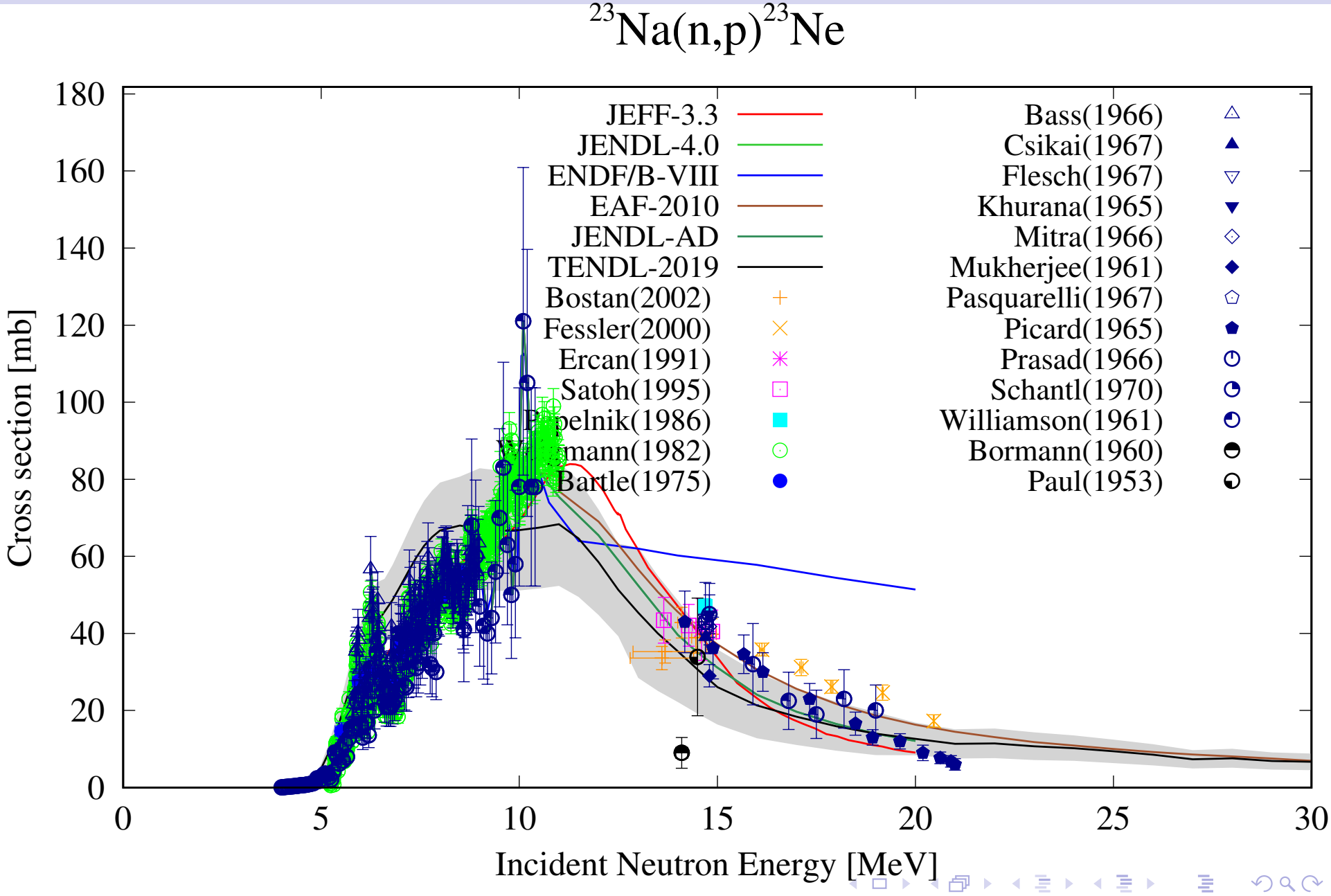
libraries: ENDF ($\sim$ 10 000 000 files)

```
/Users/koning/k/libraries/n/Y089> ls -1 */tables/xs/*MT016.*
endfb8.0/tables/xs/n-Y089-MT016.endfb8.0
irdff2.0/tables/xs/n-Y089-MT016.irdff2.0
jeff3.3/tables/xs/n-Y089-MT016.jeff3.3
jendl.ad/tables/xs/n-Y089-MT016.jendl.ad
jendl4.0/tables/xs/n-Y089-MT016.jendl4.0
tendl.2019/tables/xs/n-Y089-MT016.tendl.2019
/Users/koning/k/libraries/n/Y089>  head endfb8.0/tables/xs/n-Y089-MT016.endfb8.0
# n + Y  89 : (n,2n)
# endfb8.0   Rochman,Chadwick,Herman,Kawano+   EVAL-AUG06
# uncertainties: y
# # energies =    19
#   E(MeV)      xs(mb)      xslow(mb)     xsupp(mb)
 1.16067E+01   0.00000E+00   0.00000E+00   0.00000E+00
 1.20000E+01   7.25038E+01   6.44448E+01   8.05628E+01
 1.25000E+01   2.73305E+02   2.55084E+02   2.91526E+02
 1.30000E+01   4.87844E+02   4.66732E+02   5.08956E+02
 1.35000E+01   6.70103E+02   6.51145E+02   6.89061E+02
```

libraries: EXFOR ($\sim$ 200 000 files)

/Users/koning/k/libraries/n/Y089/exfor/xs/016> ls -1
n-Y089-MT016-Abboud-30274002.1971
n-Y089-MT016-Agrawal-23031004.2008
n-Y089-MT016-Araminowicz-30264026.1973
n-Y089-MT016-Bayhurst-10536008.1975
n-Y089-MT016-Bayhurst-10536009.1975
n-Y089-MT016-Bayhurst-10536010.1975
n-Y089-MT016-Begun-32204002.2000
n-Y089-MT016-Begun-32205012.2002
n-Y089-MT016-Berrada-30805003.1984
n-Y089-MT016-Bormann-20614011.1976
n-Y089-MT016-ChuanxinZhuu-32696004.2011
n-Y089-MT016-Chudoba-31787002.2018
n-Y089-MT016-Csikai-30033005.1967

∼ 14 000 plots


^{23}Na(n,p)^{23}Ne
Cross section [mb]
Incident Neutron Energy [MeV]
0
20
40
60
80
100
120
140
160
180
0
5
10
15
20
25
30
JEFF-3.3
JENDL-4.0
ENDF/B-VIII
EAF-2010
JENDL-AD
TENDL-2019
Bostan(2002)
Fessler(2000)
Ercan(1991)
Satoh(1995)
Bartle(1975)
Bass(1966)
Csikai(1967)
Flesch(1967)
Khurana(1965)
Mitra(1966)
Mukherjee(1961)
Pasquarelli(1967)
Picard(1965)
Prasad(1966)
Schantl(1970)
Williamson(1961)
Bormann(1960)
Paul(1953)

EXFOR I

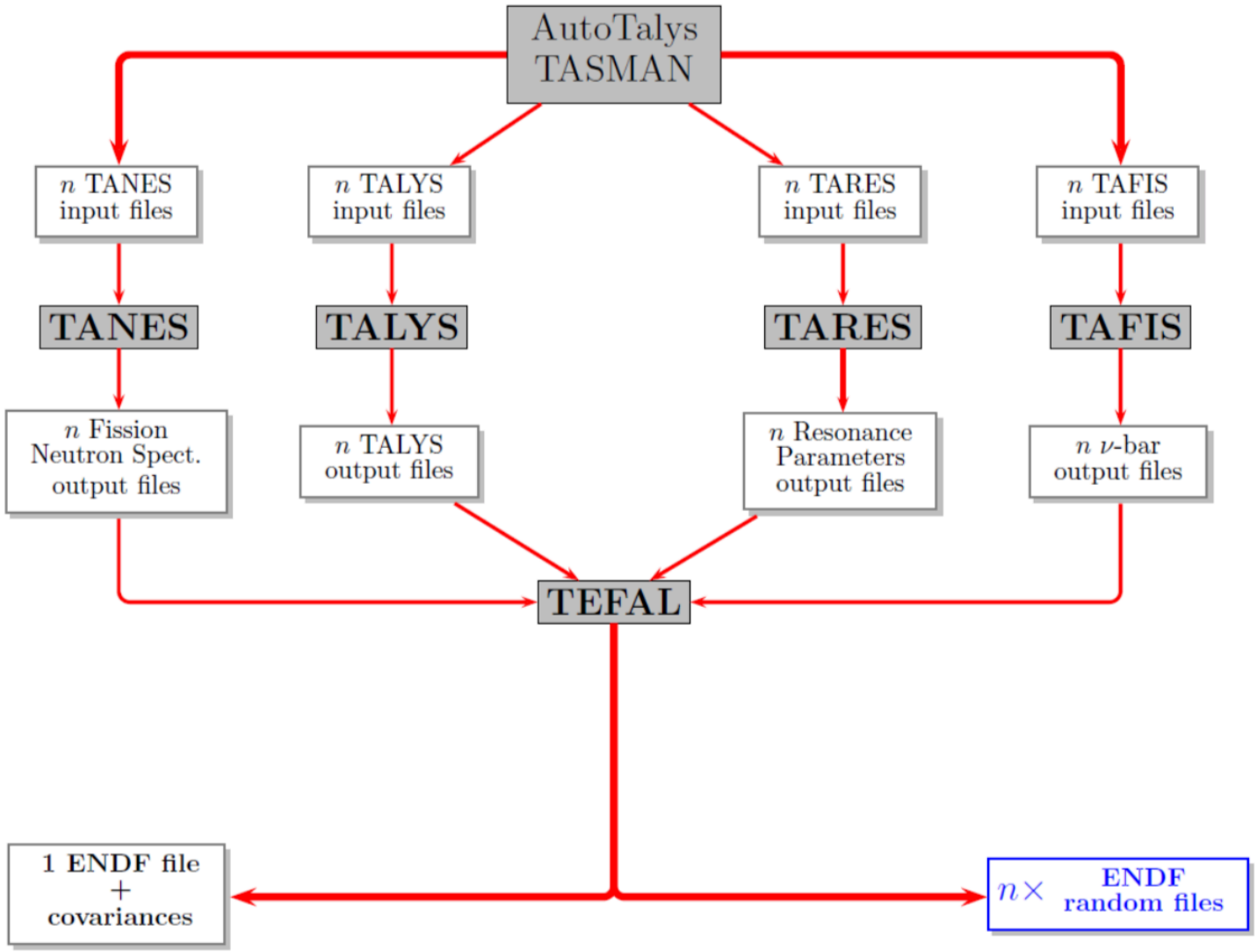
- Make ready for machine learning
- Unification of metadata
- Quantification of opinions (i.e. the original meaning of the word **evaluation**) and **store** this
  - Reject or accept entries, per evaluator
  - Different quality classes (Koning, SG30, NEA/DB/DOC(2017) 1)
  - Apply normalizations, per evaluator
- Natural language processing: software analyzes pdf's and quantifies opinions of EXFOR entries

EXFOR II

- Continuous availability of **all** data
  - Future goes way beyond click-by-click retrievals with a GUI
  - XC4, JSON, GNDS, ...
- Quantify the quality of data
  - Outlier detection, statistical comparisons among exp data sets and with nuclear data libraries (NEA/DB/DOC(2017) 1.)
  - (Unsupervised) Machine Learning directly on the raw data (Catch 22: "Bad data is the largest enemy for Machine Learning")
- Format for renormalization (including rejection flags etc.) exists but not used
- Will (at least) release combined quality database from Koning (NEA DOC), Dzysiuk, Alhassan, Gaughan, Sjöstrand in unofficial format (i.e. subentry : yes/no)

What is T6

- Method: Quality evaluation, production automation, open source



Evaluation

- Knowledgable people have stored essential evaluations (opinions, choices) **directly** into nuclear data libraries,
  - ENDF files
  - "private compilations/evaluations", RIPL, Atlas of Resonances etc.
  - and in most cases we no longer know how and why
- Ideally: all such evaluations/compilations should be produced from EXFOR using scripts which include, exclude, renormalize or average data to obtain the final database. Reproducibility: these scripts + nuclear model input file are "the evaluation"
- All such basic nuclear data evaluations should be available in complete form, and *not* in ENDF format

The urge to do this is far less than doing a new measurement or making a better theoretical model.

Evaluation: Another paradigm shift

- Quantify knowledge:
  - Quantify facts
  - Quantify opinions
- Store evaluations **before** they are encrypted in ENSDF or ENDF, unless you have infinite money and (young) people who are not demotivated to re-invent the wheel everytime.
- For T6/TENDL, quantifying the opinion (i.e. evaluation) of EXFOR data is the only step which is (still) not complete. We have,
  - A "best" TALYS input file per projectile-target combination (neutrons only)
  - For many nuclides, an "autonorm" file which normalizes TALYS or TEFAL to a good evaluation (per reaction channel)
- An evaluation and a nuclear data library is not the same.

Best TALYS file for n + Y89

```
#
# General: n + Y089
#
ldmodel 2
m2constant 1.2
#
# (n,tot), (n,el), (n,inl)
#
avadjust n 1.0 5. 11. 8. 1.04
#
# (n,p), (n,2n), (n,np)
#
gnadjust 39 90 1.04 0.05
gpadjust 39 90 1.04 0.05
#
# (n,a)
#
rvadjust a 1.03
avadjust a 1.03
s2adjust 37 86 0.30
#
# (n,g)
#
gamgamadjust 39 90 1.30 0.20
Rgamma 3.
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
#
Cstrip d 2.
Cstrip t 2.4
Cknock t 2.4
branch 39 89 8 2 1 0.8 0 0.2
branch 37 86 11 1 0 1.
branch 37 86 12 1 0 1.
```

autonorm file for n + Y89

```
projectile n
element Y
mass 089
library irdff2.0
norm mt=16 width=0.05 emin=0. emax=30. ebeg=0. eend=28.
```

TASMAN-1.95

Statistical software for TALYS: Uncertainties, sensitivities and optimization

Arjan Koning

Software releases

- TALYS-1.95: Nuclear reactions (manual: 621 pages)
- TASMAN-1.95: Statistical software for TALYS: Uncertainties, sensitivities and optimization (manual: 186 pages)
- TEFAL-1.95: Making ENDF-6 nuclear data libraries from TALYS (manual: 112 pages)
- EXFORTABLES-1.0: An experimental nuclear reaction database based on EXFOR (manual: 82 pages)
- ENDFTABLES-1.0: Translate ENDF-6 files into x-y-dy tables (Part of "Tools for TALYS" manual)
- RESONANCETABLES-1.0: A database for thermal cross sections, MACS and average resonance parameters (manual: 27 pages)

Release via website (static) or Gitlab (dynamic) or both?

Running checking and processing codes

Bash scripts for CHECKR, FIZCON, PSYCHE, INTER, PREPRO, NJOY and FUDGE,

- **run.bnl** -file n-Fe056.endfb8.0 (or e.g. **run.bnl** -file n-Fe056.endfb8.0.pendf -inter -nocheckr -nofizcon -nopsyche)
- **run.prepro** -file n-Fe056.endfb8.0 (or e.g. **run.prepro** -file n-Fe056.endfb8.0 -nomerger -noevalplot -groupie)
- **run.njoy** -file n-Fe056.endfb8.0 (or e.g. **run.njoy** -file n-Fe056.endfb8.0 -noacer -nogaspr)
- **run.fudge** -file n-Fe056.endfb8.0

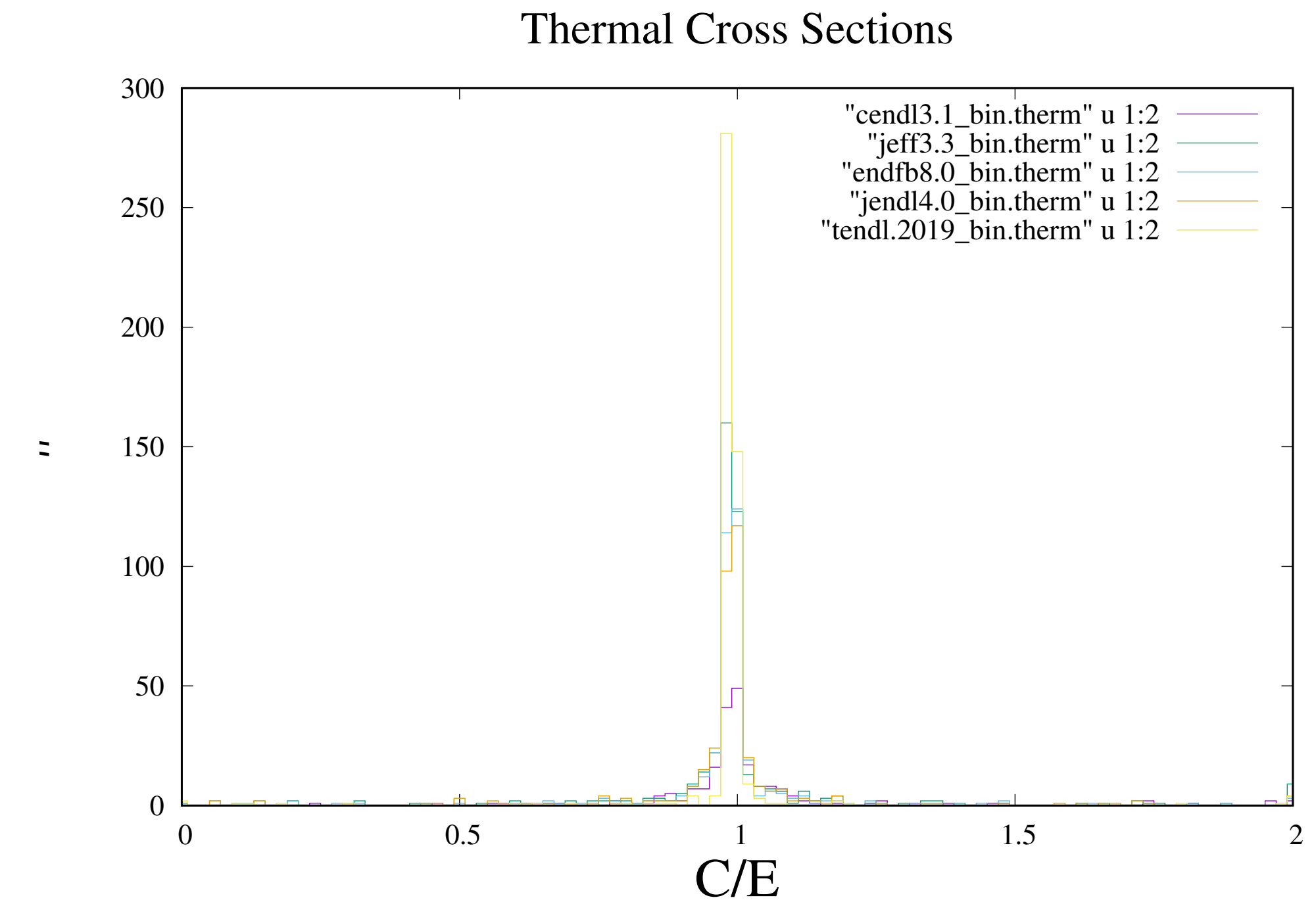
Diagnosis of checking and processing codes

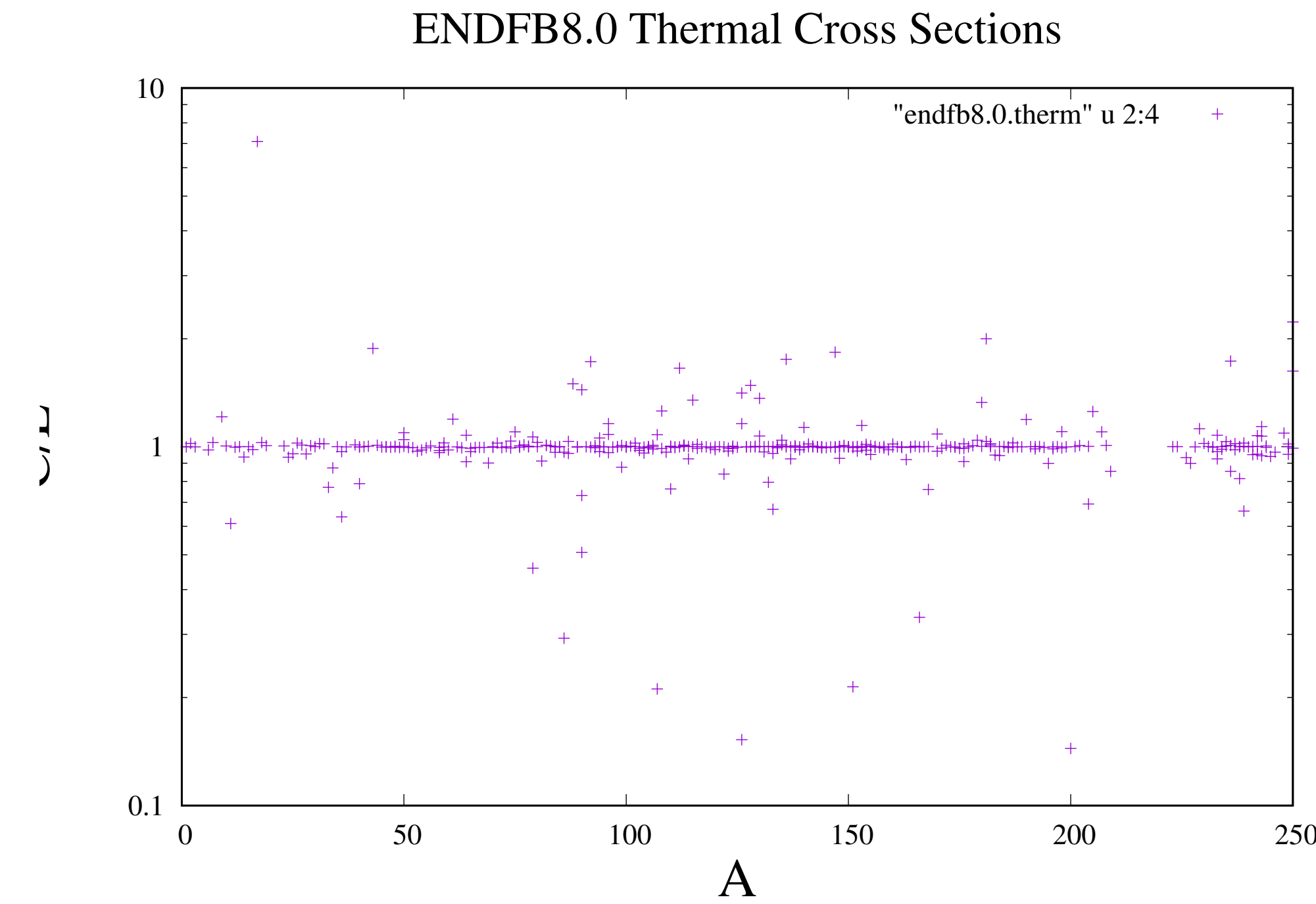
Bash scripts which filter warning and error messages, (of thousands of output files)

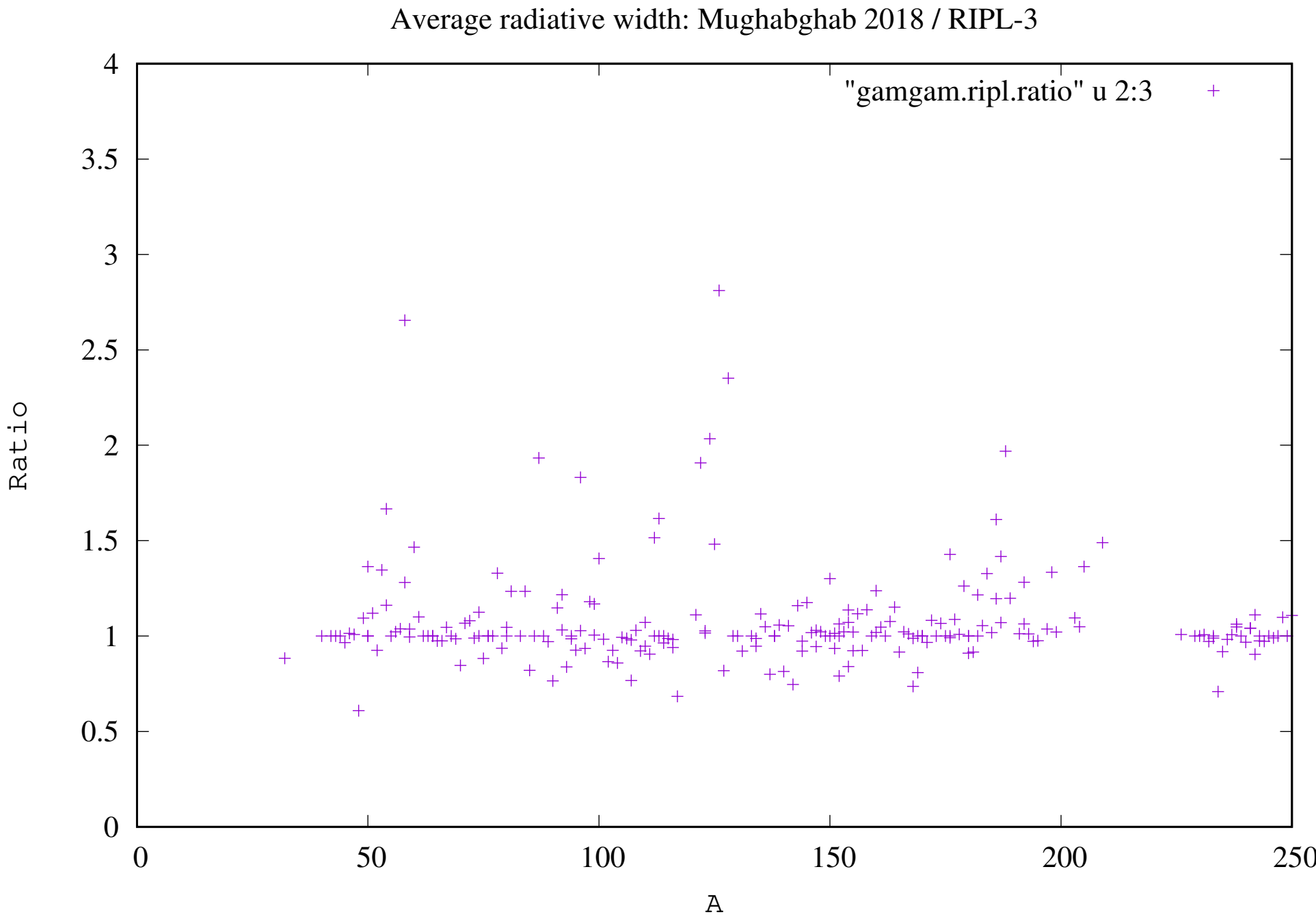
- **diag.checkr**, **diag.fizcon**, **diag.psyche**
- **diag.prepro**
- **diag.njoy** (filters on 83 warning and error messages which have been grepped from NJOY source code, like 'not ready', 'not allowed', 'not complete', 'is unreasonable', etc.
- **diag.fudge**

RESONANCETABLES Information flow

- "Mother" database for thermal cross sections, MACS, Res. Int., D_0, Γ_γ,
  - RIPL-3 databases
  - Mughghabghab 2006 Atlas of Neutron Resonances
  - Mughghabghab 2018 Atlas of Neutron Resonances
  - EXFOR
- Priorities for final database are set by Resonancetables code
- Final databases, C/E versus EXFOR, lists of all choices per nuclide, comparisons among databases and nuclear data libraries etc.


Thermal Cross Sections
"cendl3.1_bin.therm" u 1:2
"jeff3.3_bin.therm" u 1:2
"endfb8.0_bin.therm" u 1:2
"jendl4.0_bin.therm" u 1:2
"tendl.2019_bin.therm" u 1:2
300
250
200
150
100
50
0
0
0.5
1
1.5
2
C/E


ENDFB8.0 Thermal Cross Sections
"endfb8.0.therm" u 2:4
10
1
0.1
0
50
100
150
200
250
A


Average radiative width: Mughabghab 2018 / RIPL-3
"gamgam.ripl.ratio" u 2:3
Ratio
A
0
0.5
1
1.5
2
2.5
3
3.5
4
0
50
100
150
200
250

Conclusions

- Knowledge can never be quantified enough
- Nuclear data library production can never be automated enough
- In-depth knowledge does not (yet) make use of reproducible, QA methods and vice versa
- Many tools ready for release via Gitlab, assuming that others than the author will work on/with it