IAEA 60 Years
Atoms for Peace and Development

RESONANCETABLES-1.0 :

Database for thermal cross sections, MACS and average resonance parameters

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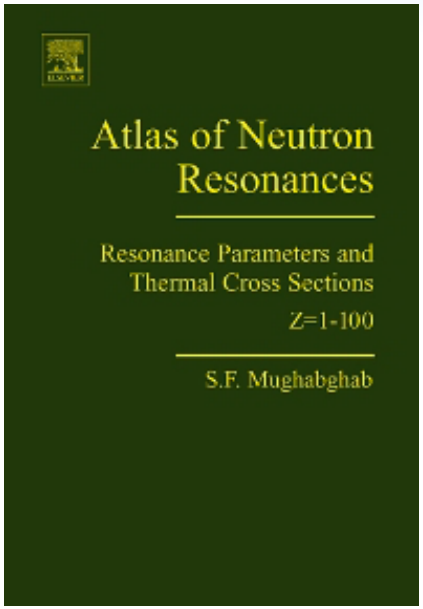
WPEC SG49 Meeting, November 16 2020, NEA, Boulogne-Billancourt
(Video meeting)

Rule number 1 for reproducibility, automation and efficiency of nuclear data evaluation

IAEA Atoms for Peace and Development

- All historical nuclear data of importance needs to be available all at once, on the spot, NOW, and machine-readable in easy format.
- This holds for all existing ENDF libraries, Atlas of resonances, EXFOR, RIPL, etc, which feed into new libraries
- Two options:
  - (Very) Large complete databases: used for the “3 T’s”: TALYS, TENDL, TMC
  - command-line API’s (not available yet)

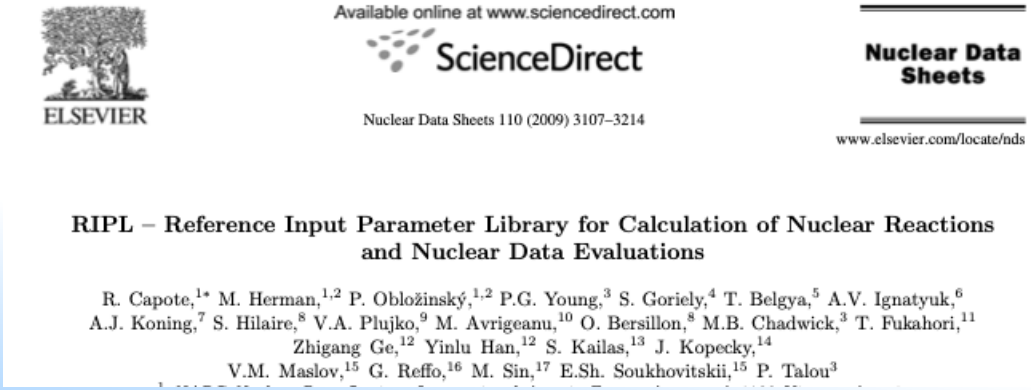
Thermal cross sections and resonance integrals: 6 sources of digital information



Mughabghab Atlas 2018
Mughabghab Atlas 2006

Sukhoruchkin 2015

Neutron Activation Analysis: http://www.kayzero.com/k0naa



RIPL: Kopecky compilation
(Includes Holden tables)

EXFOR

The “mother” databases

At the moment, the following files in the mother database are processed:

- *thermal.mugh06*: Mughabghab 2006 Atlas of neutron resonances [2], including many corrections by Dimitri Rochman
  - Thermal (n,el), (n,γ), (n,f), (n,α) cross sections, total, prompt, and delayed nubar
- *thermal.mugh18*: Mughabghab 2018 Atlas of neutron resonances [1], including many corrections by Dimitri Rochman
  - Thermal (n,tot), (n,el), (n,γ), (n,f), (n,p), (n,α) cross sections, total, prompt, and delayed nubar
  - MACS
  - Thermal (n,γ), (n,f) resonance integrals
  - D_0, S_0, Γ_γ
- *sukhoruchkin.txt*: Sukhoruchkin 2015 Neutron resonance parameters [3], digitized by Dimitri Rochman
  - Thermal (n,γ), (n,f), (n,p), (n,α) cross sections
  - Thermal (n,γ), (n,f) resonance integrals
  - MACS
- Reference Input Parameter Library (RIPL) [4]
  - *thermal.ripl*: Thermal cross section database compiled by Jura Kopecky,
  - *resonance.ripl*: Average resonance parameters D_0, S_0, Γ_γ, compiled and evaluated by Anatoli Ignatyuk.

The “mother” database

- Other compilations and evaluations
  - *kayzero.txt*: Kay-zero database for thermal (n,γ) cross sections, obtained from Andrej Trkov [5]
  - *resint.juko*: Resonance Integral database by Jura Kopecky [6]
  - *macs_kadonis.ng*: KADONIS database for MACS [7]
- EXFOR database [8]
  - *thermal_exfor.tot*: thermal (n,tot) cross sections
  - *thermal_exfor.el*: thermal (n,el) cross sections
  - *thermal_exfor.nf*: thermal (n,f) cross sections
  - *thermal_exfor.ng*: thermal (n,γ) cross sections
  - *thermal_exfor.np*: thermal (n,p) cross sections
  - *thermal_exfor.na*: thermal (n,α) cross sections
  - *thermal_exfor.nu*: thermal total nubar cross sections
  - *thermal_exfor.nup*: thermal prompt nubar cross sections
  - *thermal_exfor.nud*: thermal delayed nubar cross sections
  - *macs_exfor.ng*: MACS
  - *RI_exfor.ng*: (n,γ) resonance integral

Output of EXFORTABLES

+For comparison/validation, all corresponding values of CENDL

Processing the mother databases

- All input is returned in a unified output format
- Comparisons (ratios) between mother databases are made
- Final databases are made according to priority rules
- Comparisons (ratios) with evaluated NDL's are made.
- All output in logically named separate files.

Order of adoption for thermal cross sections, resonance integrals and MACS

1. Kayzero database
2. Mughabghab 2018 Atlas
3. Sukhoruchkin 2015 Atlas
4. Mughabghab 2006 Atlas
5. RIPL or Kopecky database
6. EXFOR (the most recent value)

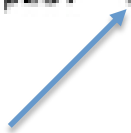
For MACS, the order of adoption is

1. Mughabghab 2018 Atlas
2. Sukhoruchkin 2015 Atlas
3. KADONIS database
4. EXFOR (the most recent value)

Final database: if 1 doesn't exist, we take 2, if it doesn't exist, we take 3, etc.

Example: the final database for thermal capture cross sections

	89	227	0	8.90000E+02	3.00000E+01	Mugh18	Ac227	6
	90	228	0	1.23000E+02	1.50000E+01	Mugh18	Th228	1
	90	229	0	6.28000E+01	6.00000E+00	Mugh18	Th229	0
	90	230	0	2.29000E+01	3.00000E-01	Mugh18	Th230	5
	90	232	0	7.34100E+00	3.90000E-02	Kayzero	Th232	27
	90	233	0	1.33000E+03	5.00000E+01	Mugh18	Th233	3
	90	234	0	1.80000E+00	5.00000E-01	Mugh18	Th234	1
	91	231	0	2.00200E+02	2.30000E+00	Mugh18	Pa231	6
	91	232	0	5.90000E+02	6.90000E+01	Mugh18	Pa232	3
	91	233	0	3.95000E+01	1.10000E+00	Mugh18	Pa233	6
#	92	0	0	7.83000E+00	4.20000E-01	Stefanescu_1961_30073009	U000	2
	92	229	0	9.88000E+01	8.00000E-01	Mugh06	U229	0
	92	232	0	7.49000E+01	1.60000E+00	Mugh18	U232	3
	92	233	0	4.57000E+01	7.00000E-01	Mugh18	U233	5
	92	234	0	1.02500E+02	1.30000E+00	Mugh18	U234	6
	92	235	0	9.88000E+01	8.00000E-01	Mugh18	U235	6
	92	236	0	5.09000E+00	1.00000E-01	Mugh18	U236	15
	92	237	0	4.43000E+02	1.67000E+02	Mugh18	U237	1
	92	238	0	2.67000E+00	1.00000E-02	Kayzero	U238	15
	92	239	0	2.20000E+01	5.00000E+00	Mugh18	U239	1
	93	235	0	1.50000E+02	2.00000E+00	Mugh18	Np235	2
	93	236	0	1.21000E+02	7.00000E+00	Sukhoruchkin	Np236	0
	93	237	0	1.78800E+02	2.90000E+00	Mugh18	Np237	13



Number of measurements
In EXFOR

Example: Table with all possible options for thermal capture cross sections

```
62 151    0     1.51400E+04     3.00000E+02    Mugh18                                  Sm151
  ripl              1.52000E+04     3.00000E+02    JUKO
  mugh06            1.51700E+04     3.00000E+02    Mugh06
  mugh18            1.51400E+04     3.00000E+02    Mugh18
  sukhoruchkin      1.51700E+04     2.99000E+02    Sukhoruchkin
  exfor             1.20000E+04     0.00000E+00    Melaika_1955_12086003
  exfor             1.51700E+04     3.00000E+02    Mughabghab_2006_V10022001
  exfor             1.50200E+04     5.25000E+02    Marrone_2006_22893007
  cendl3.1          1.51239E+04            CE=     9.98937E-01
  endfb8.0          1.51379E+04            CE=     9.99861E-01
  jeff3.3           1.51294E+04            CE=     9.99300E-01
  jendl4.0          1.51598E+04            CE=     1.00131E+00
  tendl.2019        1.51334E+04            CE=     9.99564E-01
62 152    0     2.06000E+02     3.00000E+00    Mugh18                                  Sm152
  ripl              2.06000E+02     1.50000E+01    JUKO
  mugh06            2.06000E+02     6.00000E+00    Mugh06
  mugh18            2.06000E+02     3.00000E+00    Mugh18
  sukhoruchkin      2.06000E+02     6.00000E+00    Sukhoruchkin
  exfor             1.38000E+02     2.76000E+01    Seren_1947_11447096
  exfor             2.00000E+02     6.00000E+00    Pattenden_1958_21325012
  exfor             2.24000E+02     7.00000E+00    Tattersall_1960_20638048
  exfor             2.15000E+02     1.00000E+01    Fehr_1960_12023006
  exfor             2.09000E+02     9.00000E+00    Cabell_1962_20627002
  exfor             2.09100E+02     2.07000E+01    Bernabei_1962_12099002
  exfor             2.06000E+02     6.00000E+00    Mughabghab_2006_V10022041
  exfor             2.04800E+02     6.32832E+00    Karadag_2007_22964002
  exfor             2.38930E+02     1.91100E+01    Nyarko_2010_31698006
  exfor             2.07300E+02     9.40000E+00    Agbemava_2011_31717003
  exfor             2.07000E+02     1.00000E+00    FarinaArbocco_2013_23266134
  exfor             2.12000E+02     8.00000E+00    Nguyen_2017_30843002
  cendl3.1          2.06640E+02            CE=     1.00311E+00
  endfb8.0          2.05946E+02            CE=     9.99738E-01
  jeff3.3           2.05974E+02            CE=     9.99874E-01
  jendl4.0          2.05842E+02            CE=     9.99233E-01
  tendl.2019        2.05971E+02            CE=     9.99859E-01
```

Library values obtained from point wise files (PREPRO's RECENT module)

Example: MACS as a function of time

```
/Users/koning/resonancetables/macs/nuc> cat Zr094.ng
#year          xs                dxs          Ref
1957     2.40000E-02     4.00000E-03    Macklin_1957_11399020
1963     1.90000E-02     4.00000E-03    Macklin_1963_11845005
1967     2.10000E-02     4.00000E-03    Macklin_1967_14322020
1976     3.40000E-02     5.00000E-03    Boldeman_1976_30358012
1982     2.52000E-02     3.60000E-03    Wyrick_1982_12831006
2000     2.60000E-02     1.00000E-03    Bao_2000_V0102164
2006     2.70000E-02     3.00000E-03    Mughabghab_2006_V1001379
2015     2.80000E-02     6.00000E-04    Tessler_2015_31765004
```

Example: Ratio of EXFOR MACS vs final database

#	Z	A	Tiso	Ratio	xs(this)	xs(final)	Ref	Nuc
	1	1	0	1.00000E+00	2.54000E-04	2.54000E-04	Bao_2000_V0102002	H001
	1	2	0	1.00000E+00	3.00000E-06	3.00000E-06	Bao_2000_V0102003	H002
	2	3	0	4.38095E-01	9.20000E-06	2.10000E-05	Wervelman_1989_22139002	He003
	2	3	0	4.33333E-01	9.10000E-06	2.10000E-05	Wervelman_1991_22230003	He003
	2	3	0	3.61905E-01	7.60000E-06	2.10000E-05	Bao_2000_V0102004	He003
	2	3	0	3.66667E-01	7.70000E-06	2.10000E-05	Mughabghab_2006_V1001008	He003
	3	7	0	4.52099E-01	2.10000E-05	4.64500E-05	Wiescher_1989_22171004	Li007
	3	7	0	4.32723E-01	2.01000E-05	4.64500E-05	Wiescher_1989_22171003	Li007
	3	7	0	9.04198E-01	4.20000E-05	4.64500E-05	Bao_2000_V0102005	Li007
	3	7	0	8.46071E-01	3.93000E-05	4.64500E-05	Mughabghab_2006_V1001015	Li007
	4	9	0	1.11828E+00	1.04000E-05	9.30000E-06	Bao_2000_V0102006	Be009
	4	9	0	1.03226E+00	9.60000E-06	9.30000E-06	Wallner_2008_22994002	Be009
#	6	0	0	1.00000E+00	2.00000E-04	2.00000E-04	Macklin_1963_11331002	C000
	6	12	0	1.00000E+00	1.54000E-05	1.54000E-05	Ohsaki_1994_23002004	C012
	6	12	0	1.00000E+00	1.54000E-05	1.54000E-05	Bao_2000_V0102007	C012
	6	12	0	1.00000E+00	1.54000E-05	1.54000E-05	Mughabghab_2006_V1001027	C012
	6	13	0	7.31707E-01	2.10000E-05	2.87000E-05	Bao_2000_V0102008	C013
	6	13	0	5.03484E-01	1.44500E-05	2.87000E-05	Wallner_2008_22994003	C013
	6	13	0	2.33449E-01	6.70000E-06	2.87000E-05	Wallner_2016_23295004	C013
	6	14	0	1.13067E+00	8.48000E-06	7.50000E-06	Bao_2000_V0102010	C014

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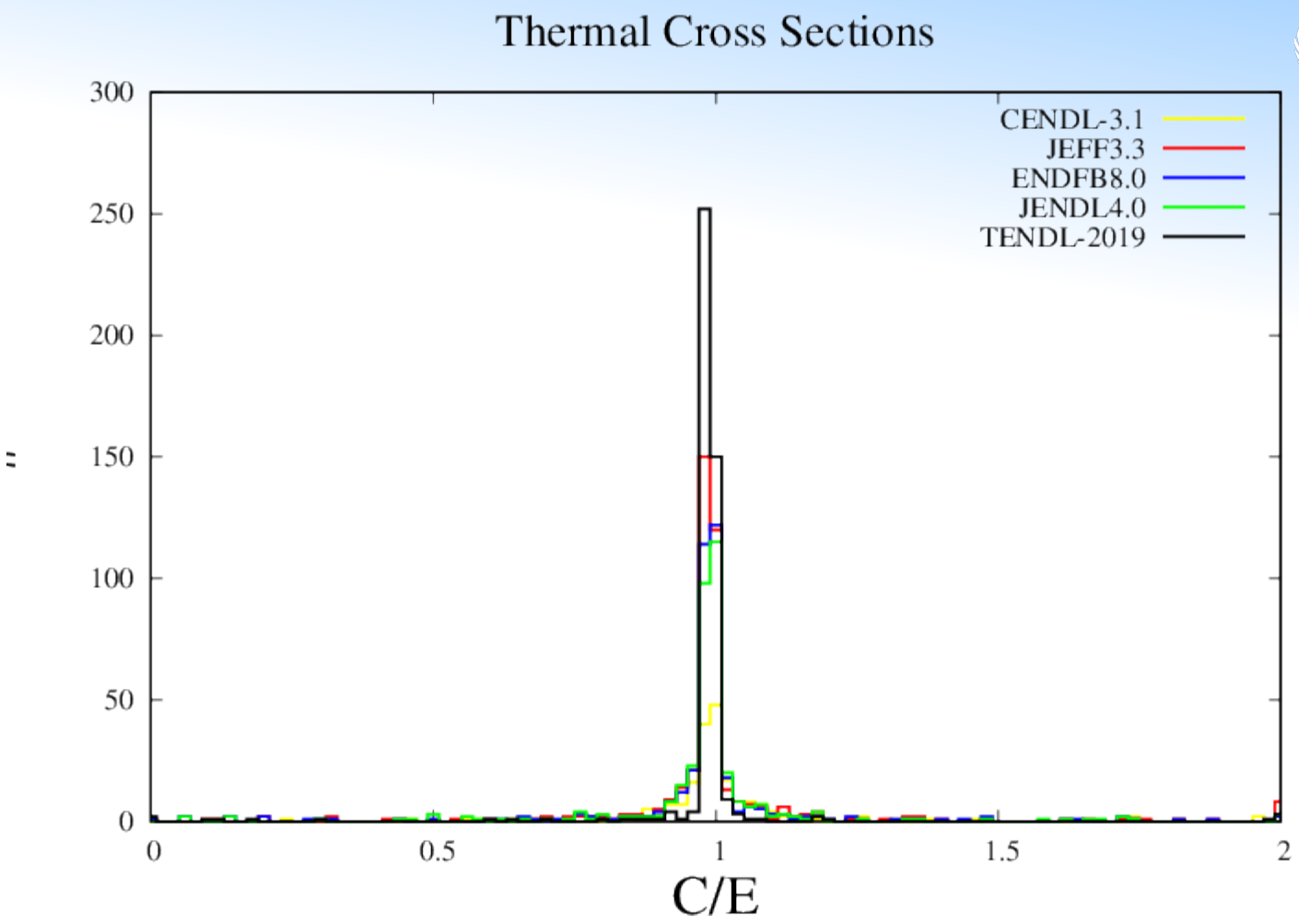
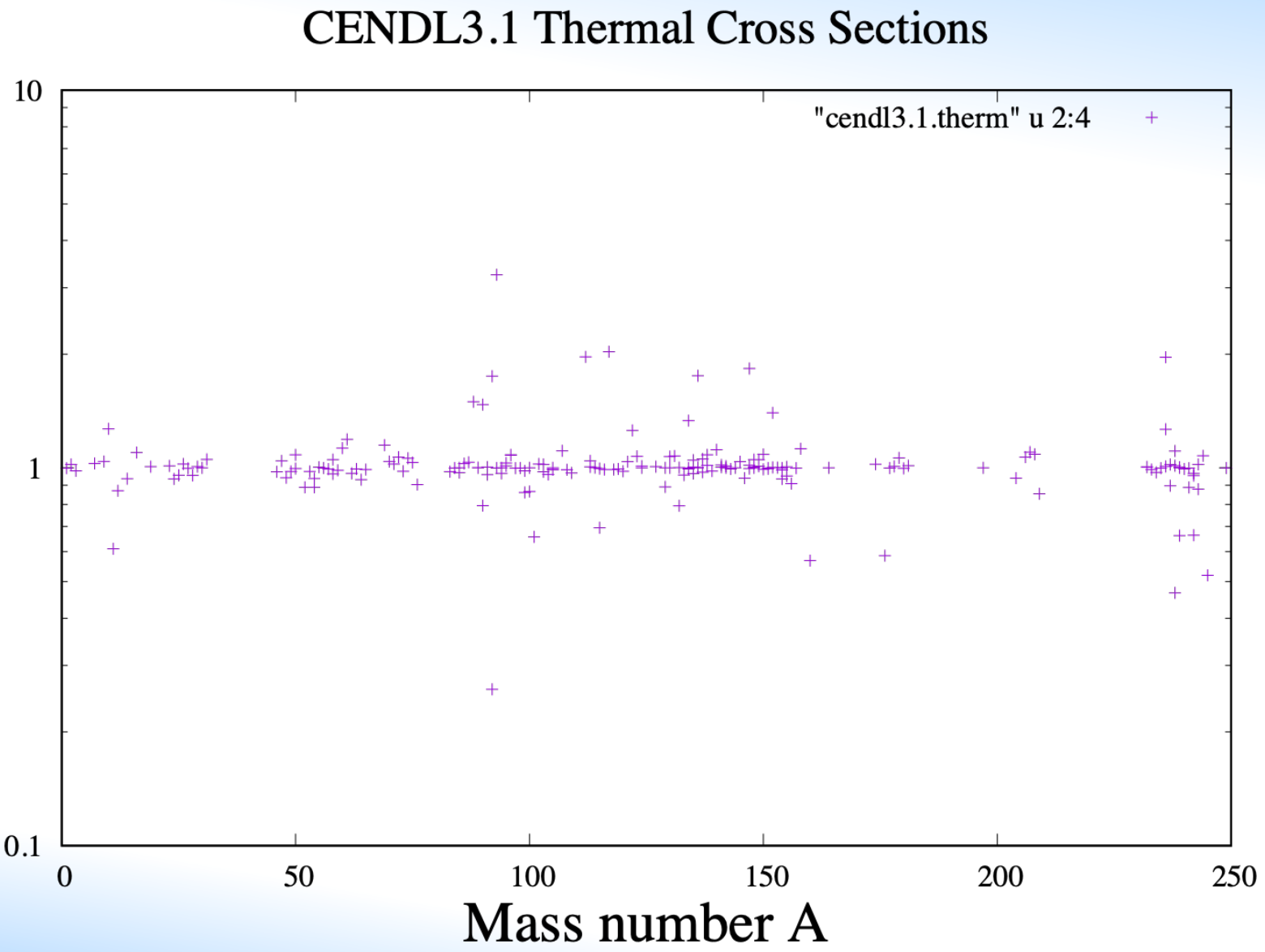


Lib	F(C/E)	N	N <5%	N < 20%	N < 50%
CENDL-3.1	1.036	201	129(0.642)	177(0.881)	187(0.930)
ENDFB-8.0	1.022	375	284(0.757)	332(0.885)	351(0.936)
JEFF-3.1	1.024	425	315(0.741)	377(0.887)	398(0.936)
JENDL-4.0	1.025	359	269(0.749)	320(0.891)	334(0.930)
TENDL-2019	1.008	446	416(0.933)	431(0.966)	434(0.973)

Ratio over final database



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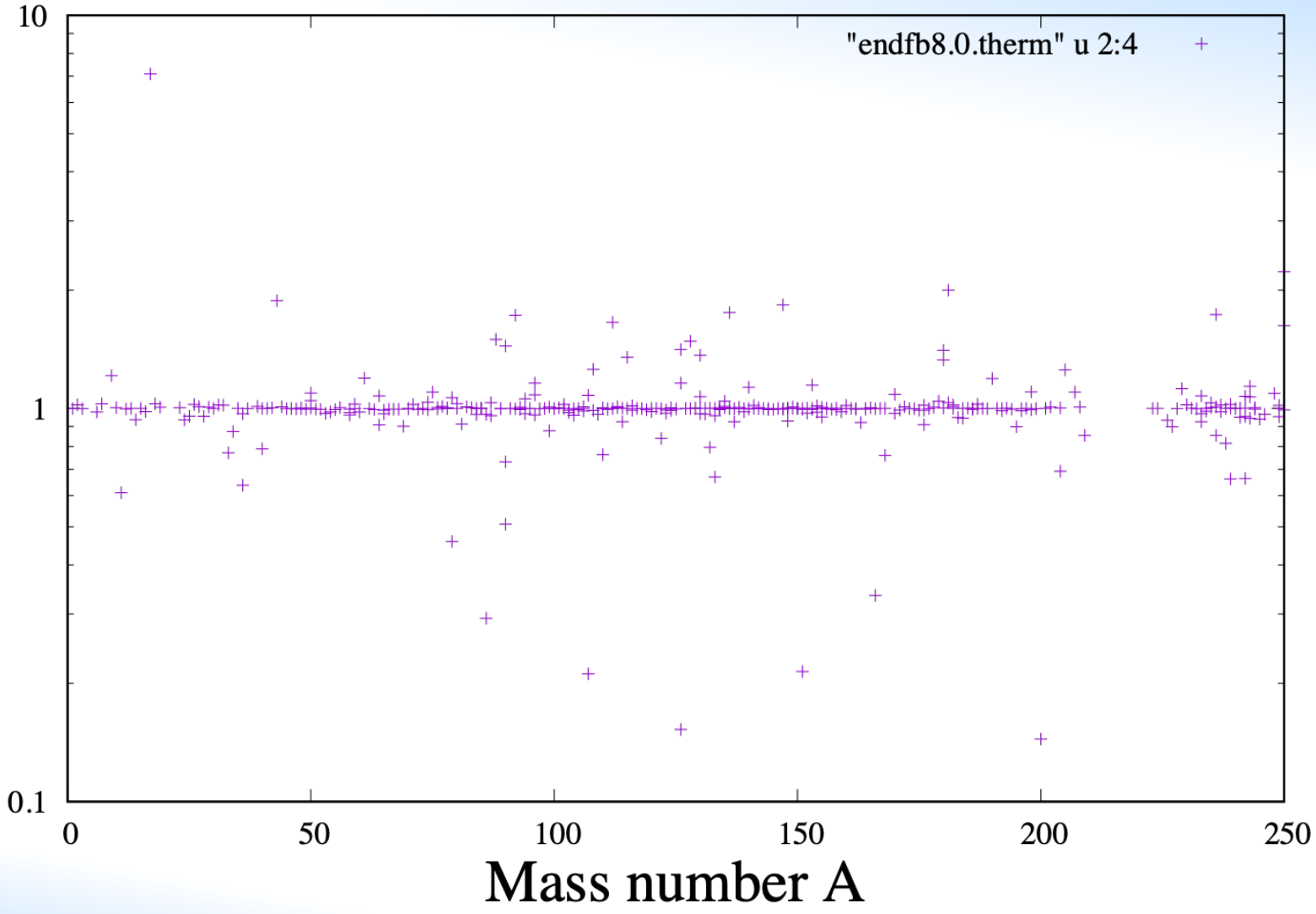
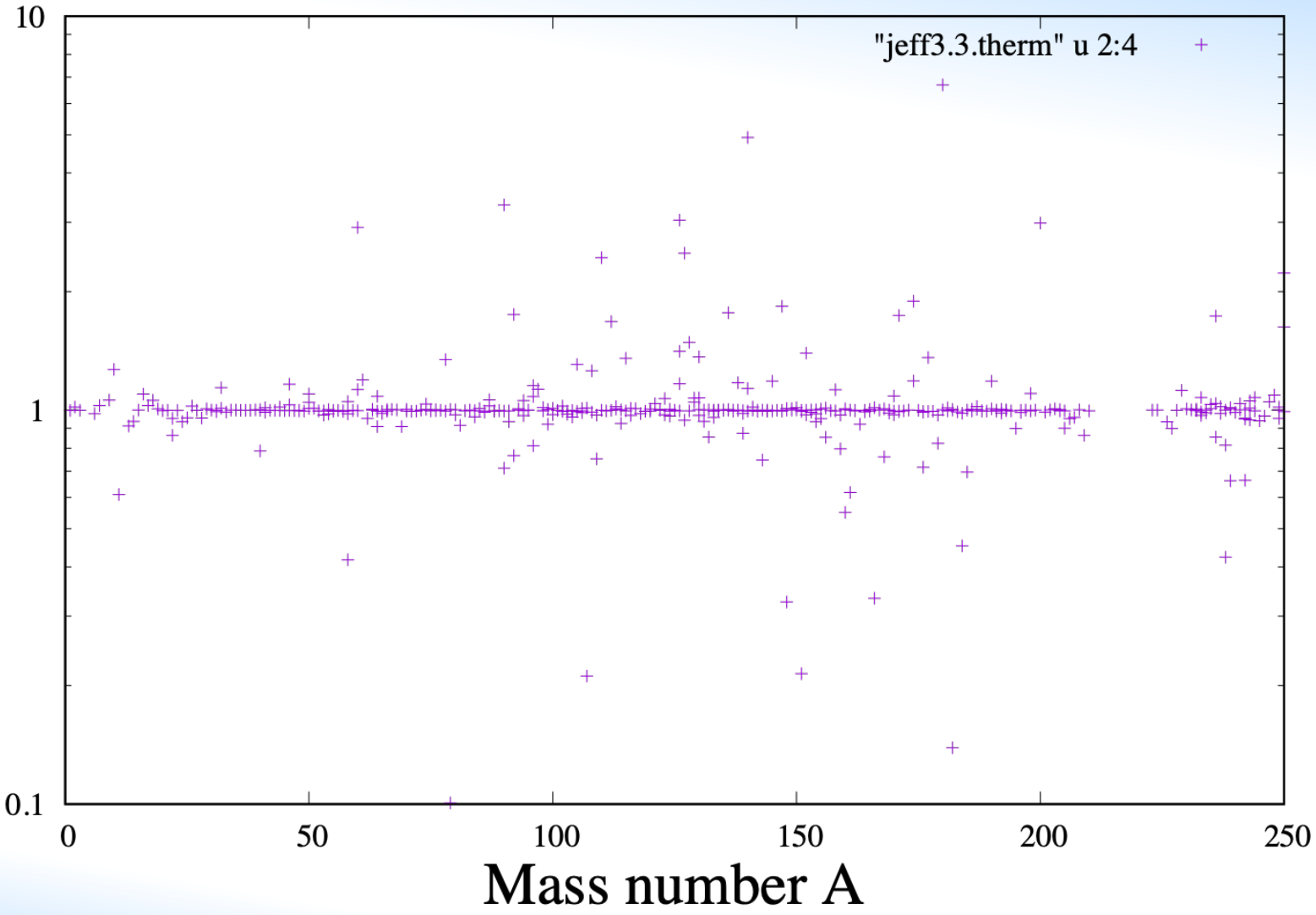


Ratio over final database

JEFF3.3 Thermal Cross Sections



Ratio over final database

JENDL4.0 Thermal Cross Sections

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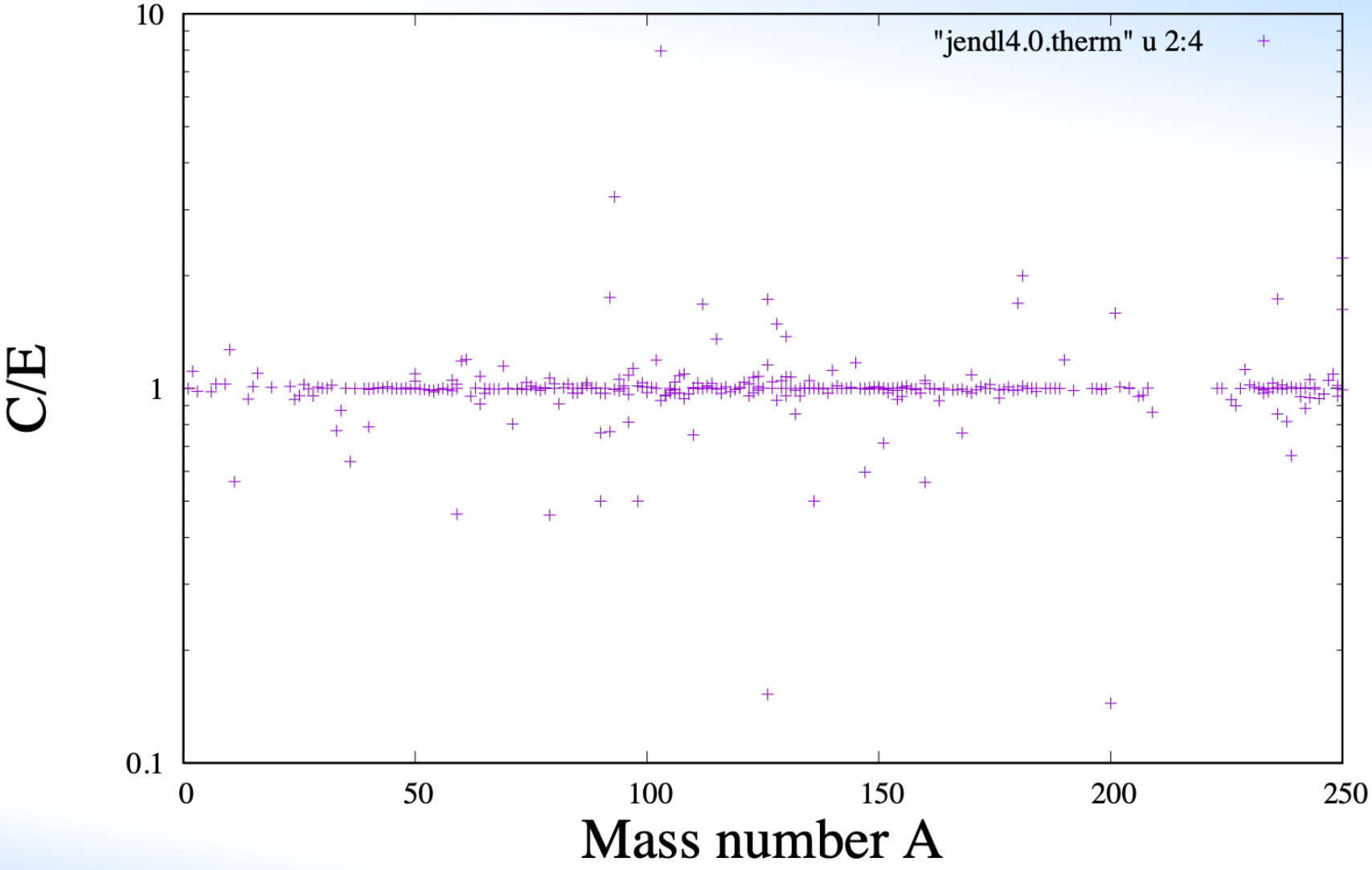
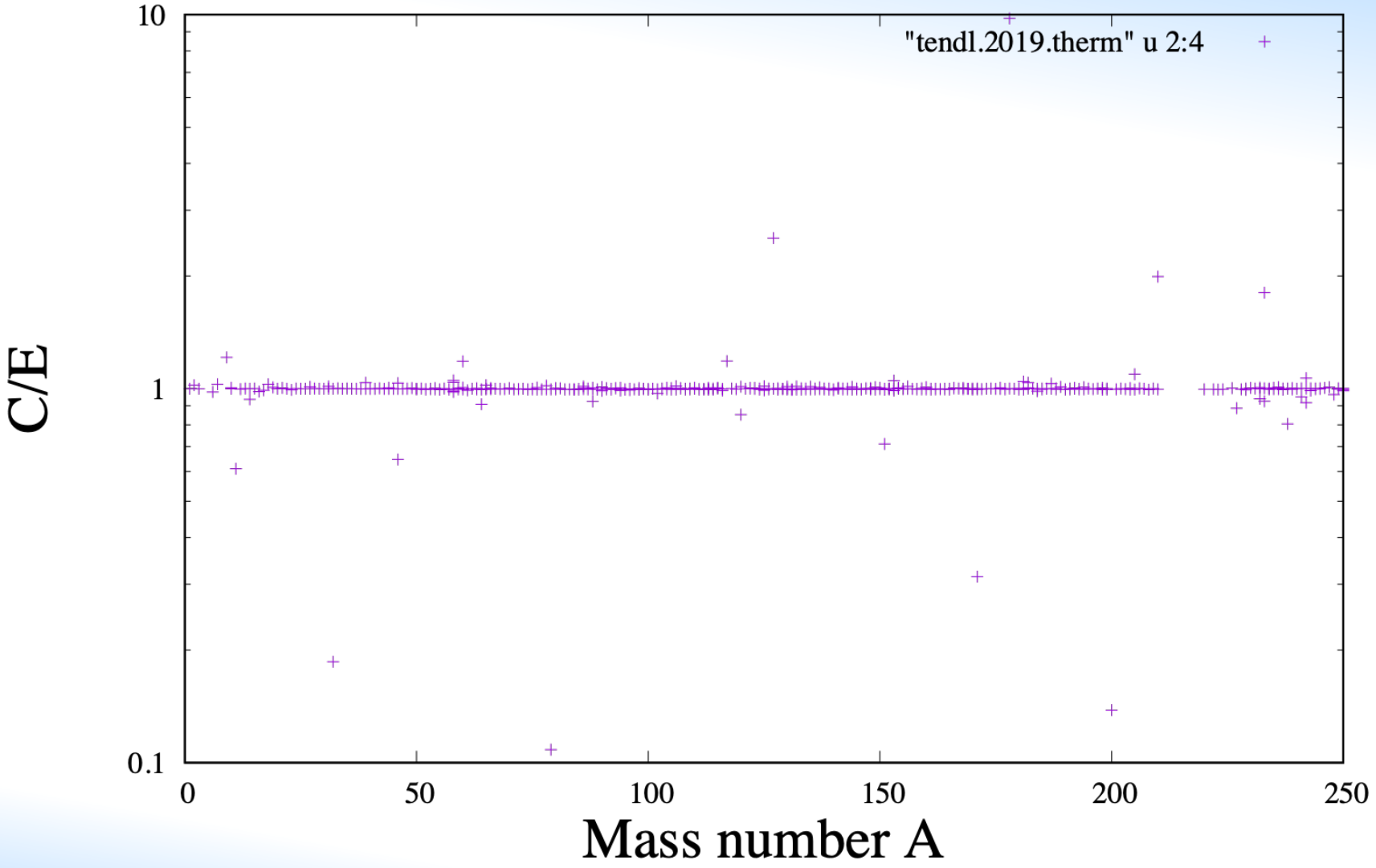
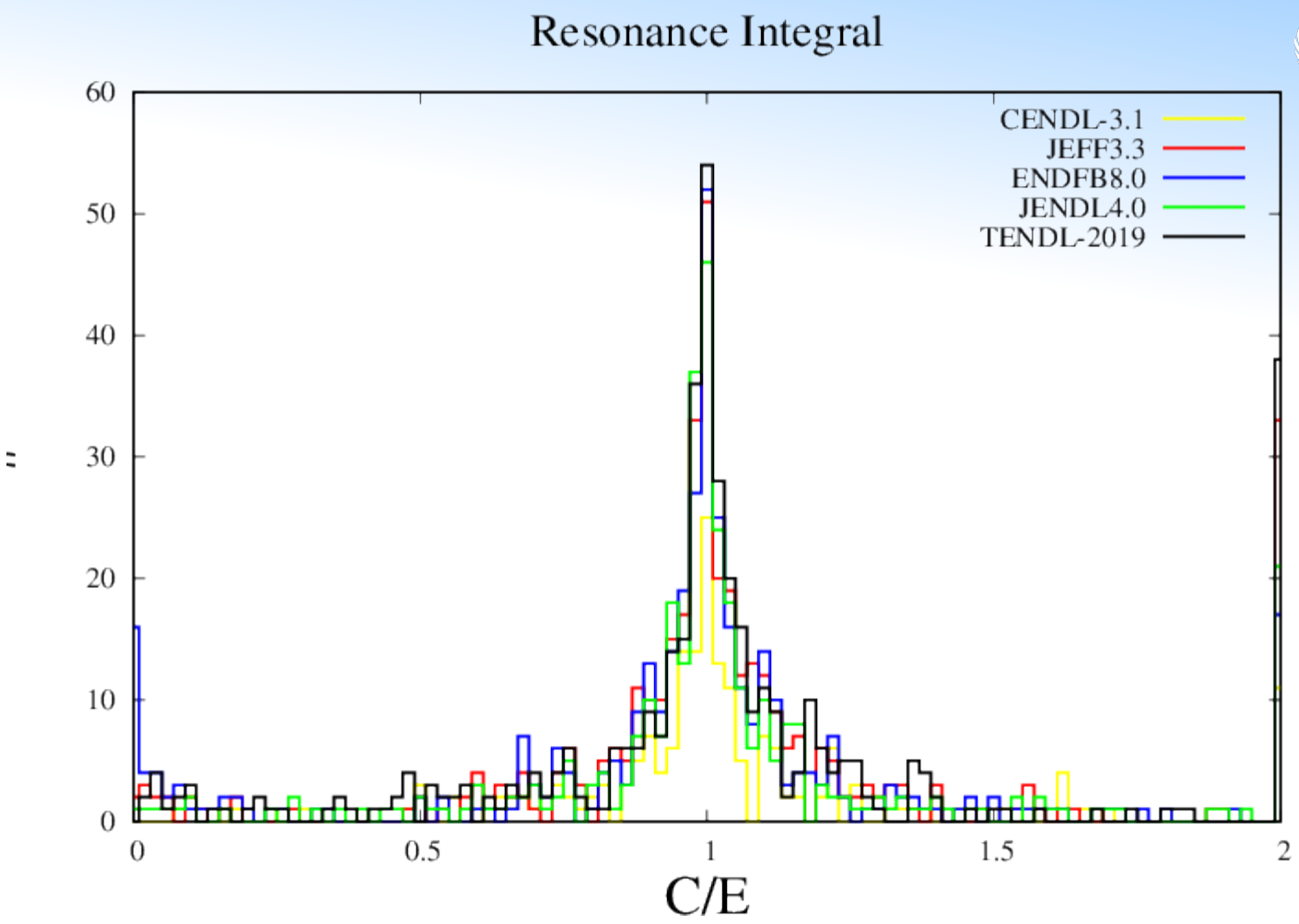


Ratio over final database

TENDL.2019 Thermal Cross Sections





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-3.1	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)

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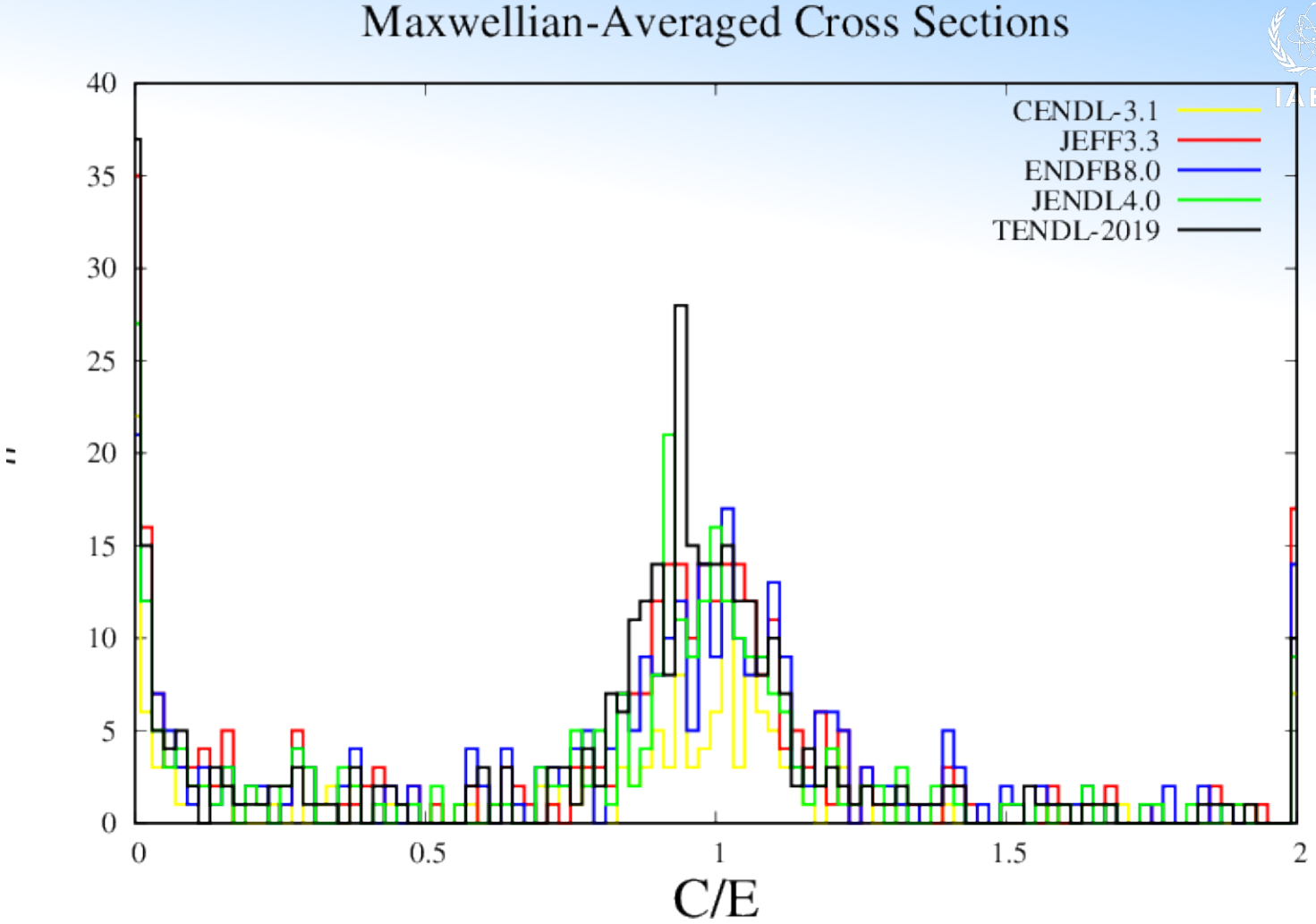


Lib	F(C/E)	N	N < 5%	N < 20%	N < 50%
CENDL-3.1	1.073	176	29(0.165)	78(0.443)	101(0.574)
ENDFB-8.0	1.082	328	56(0.171)	157(0.479)	208(0.634)
JEFF-3.1	1.078	346	67(0.194)	175(0.506)	208(0.601)
JENDL-4.0	1.070	292	59(0.202)	149(0.510)	187(0.640)
TENDL-2019	1.076	357	75(0.210)	196(0.549)	233(0.653)

RESONANCETABLES-1.0

Database for thermal cross sections, MACS and average resonance parameters

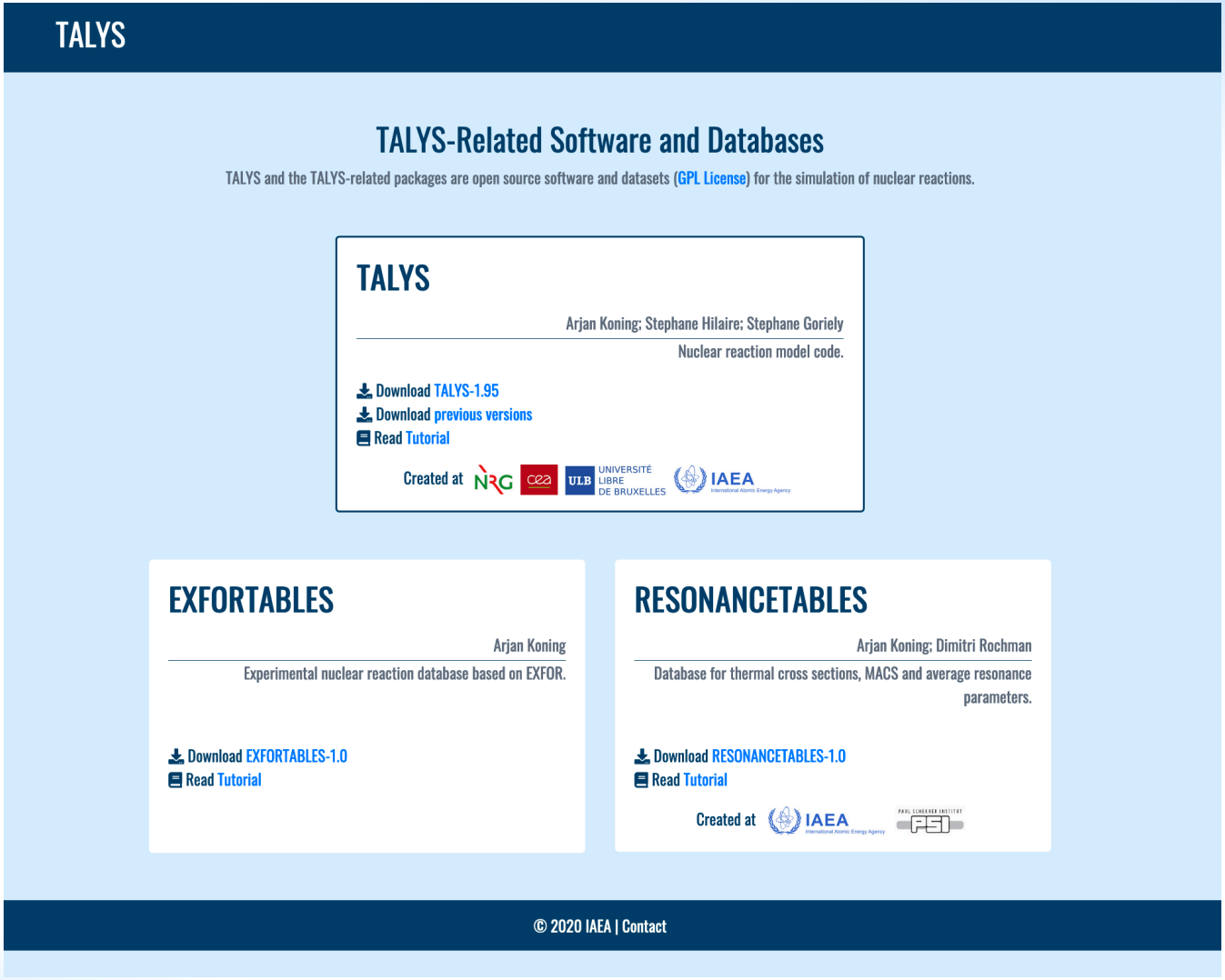
Arjan Koning and Dimitri Rochman

Draft version

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

Contents

New webpage under construction at IAEA



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

SUMMARY

- Systematic nuclear data evaluation requires all underlying data to be readily available. Preferably by API's, until that time by complete databases.
- RESONANCETABLES reads several existing compilations and evaluations for thermal cross sections, MACS and resonance integrals, and returns that in a unified tabular format
- RESONANCETABLES uses priority rules which are subjective. Evaluation of the quality of each entry is essential but also time-consuming
- The so-called final databases are used for validation of TENDL-2019 and for the production of TENDL-2021.

What next?

- Towards an evaluated, machine-readable resonance database:
  - Average or single-energy quantities, like in this work, were “easy” to digitise and maintain
  - What about the resonance parameters?
  - Copyright issues?
  - Quantify quality of a particular set of resonance parameters:
    - Differential
    - Integral
  - Be complete, i.e. include resonance parameters from all Atlases, EXFOR and major NDL’s
  - Finally use an adequate format (YAML, JSON,…)
  - Perhaps start with the average and single-energy quantities using expert knowledge: individual nuclide priorities instead of global ones
- If enough interest, IAEA could start an initiative on this

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Thank you!