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PSI

60 Years
IAEA Atoms for Peace and Development

D. Rochman, A.J. Koning and J.Ch. Sublet

Automatized nuclear data evaluation

ARIEL-H2020 International on-line school on nuclear data: the path from the detector to the reactor calculation -- NuDataPath, March 2, 2022, online

Zertifiziertes Managementsystem STARS ISO 9001

Summary

- Me, and why nuclear data evaluation
- TENDL: Main goal

- Subjects discussed in this presentation
    - What is an automatized evaluation: the TENDL library
    - Differences between the computer driven and human approach.
    - Nuclear models, tools and codes used in an automatized evaluation
    - Evaluation of the resolved resonance region (RRR) and the continuum.
    - Quality assessment of an evaluation.
    - Comparison with the differential and integral data.
    - Uncertainties for application, user's aspect

- All slides are available here: https://tendl.web.psi.ch/bib_rochman/presentation2.html

Me, at the Laboratory for Reactor Physics and Thermal-Hydraulics, PSI

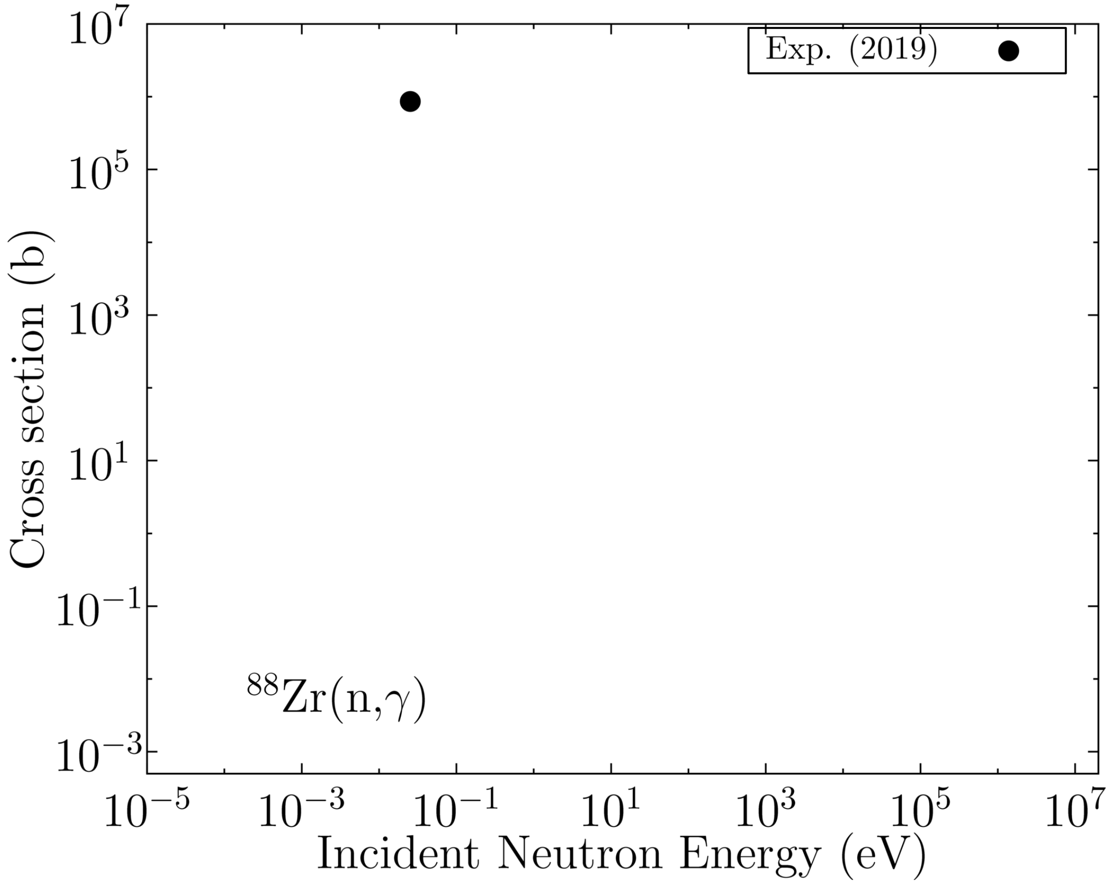
- 48 years old, married, two kids, one dog

- Our partners:
  - Regulator ENSI
  - Power plant consortium: SwissNuclear
  - Radioactive Waste Management Agency: NAGRA
  - EU projects, Swiss National Foundation
  - EUROfusion
  - And international partners

- My involvement:
  - Core licensing analyses for PWRs for new cycles
  - Spent Nuclear Fuel assessment (source term, radiations…)
  - Nuclear data (evaluation)
  - Uncertainty assessment

Why evaluation: the recent case of $^{88}Zr(n,\gamma)$

- The thermal $^{88}Zr(n,\gamma)$ cross section was recently measured at Livermore, see Nature (2019).
- Its value is 861 000 barns ± 8 %
- The last time such a large cross section was “discovered” was in the 1940s.



Why evaluation : the recent case of $^{88}Zr(n,\gamma)$

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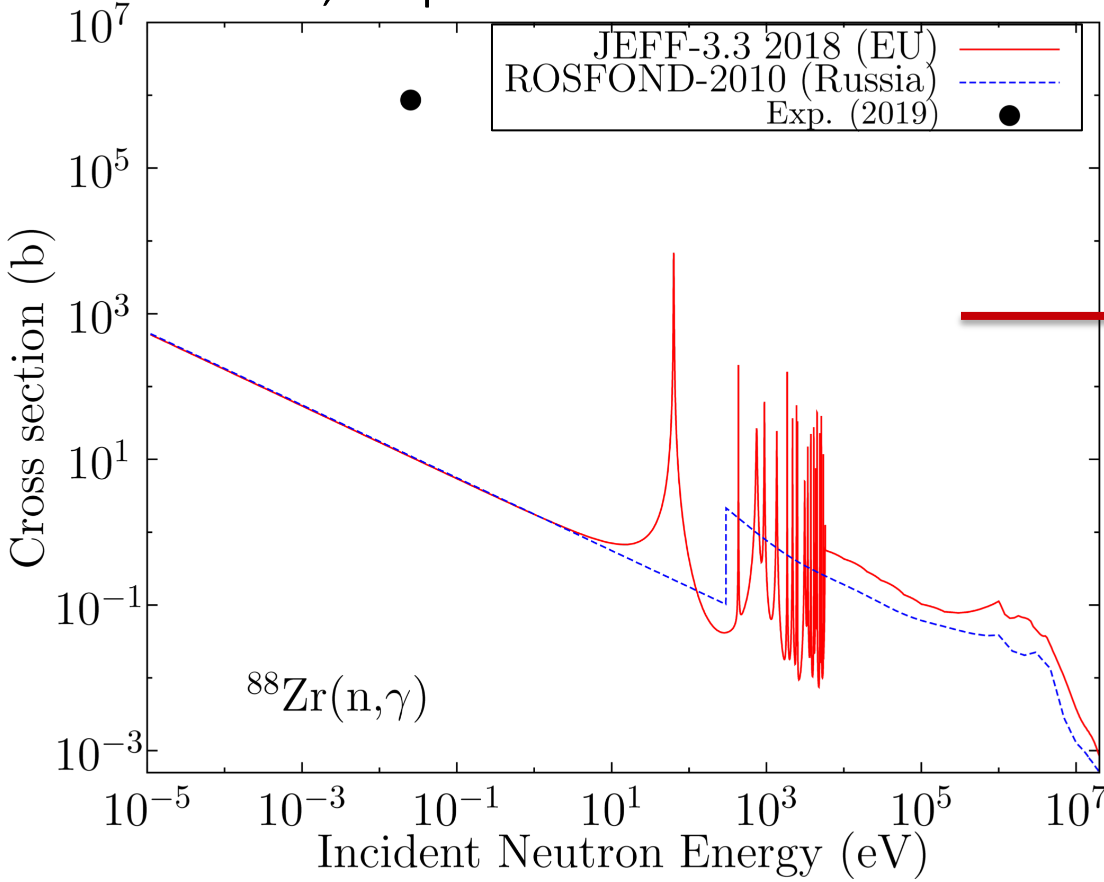
- Its value is 861 000 barns ± 8 %
- The last time such a large cross section was "discovered" was in the 1940s.
- Before the measurement, the prediction from the "nuclear data libraries" was



Current Modelling = No predictive power

Main goal: the TENDL project

- TENDL: TALYS evaluated nuclear data library,

- Goal: improve simulations for TENDL and/or other libraries, or solving

$$0 \leq \chi^2 \leq 1$$

$$\chi^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{C_i - E_i}{\Delta E_i}\right)^2$$

- Available at https://tendl.web.psi.ch/home.html

- Comes from T6 (software package)

- T6 leads to TENDL, TMC, BMC, HFR…

- See for instance NDS 155 (2019) 1

ELSEVIER
Available online at www.sciencedirect.com
ScienceDirect
Nuclear Data Sheets 155 (2019) 1–55
Nuclear Data Sheets
www.elsevier.com/locate/nds

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

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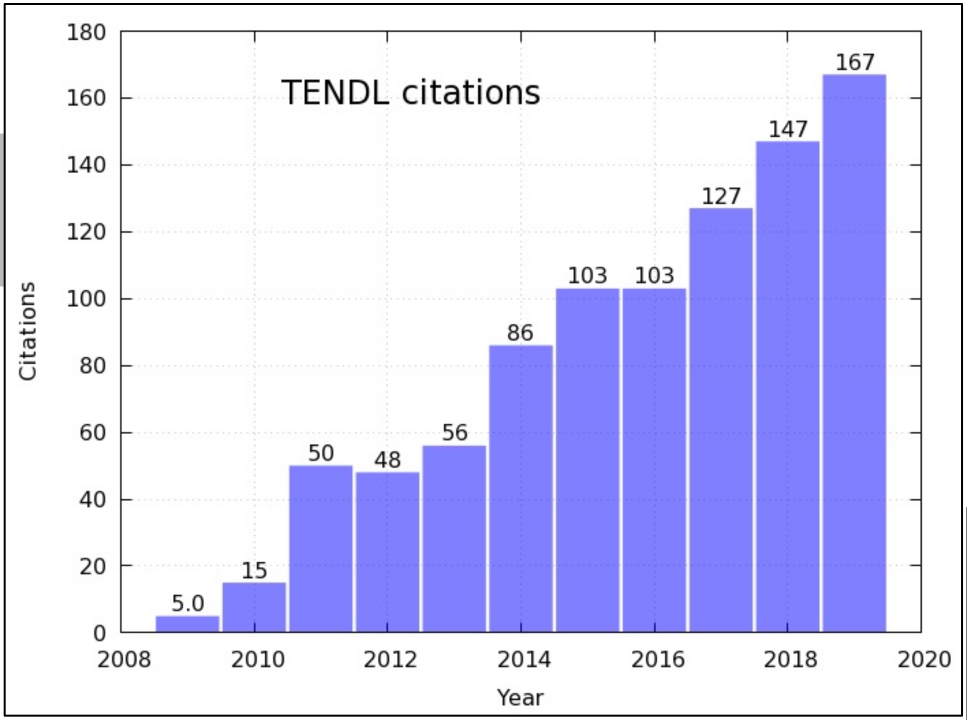
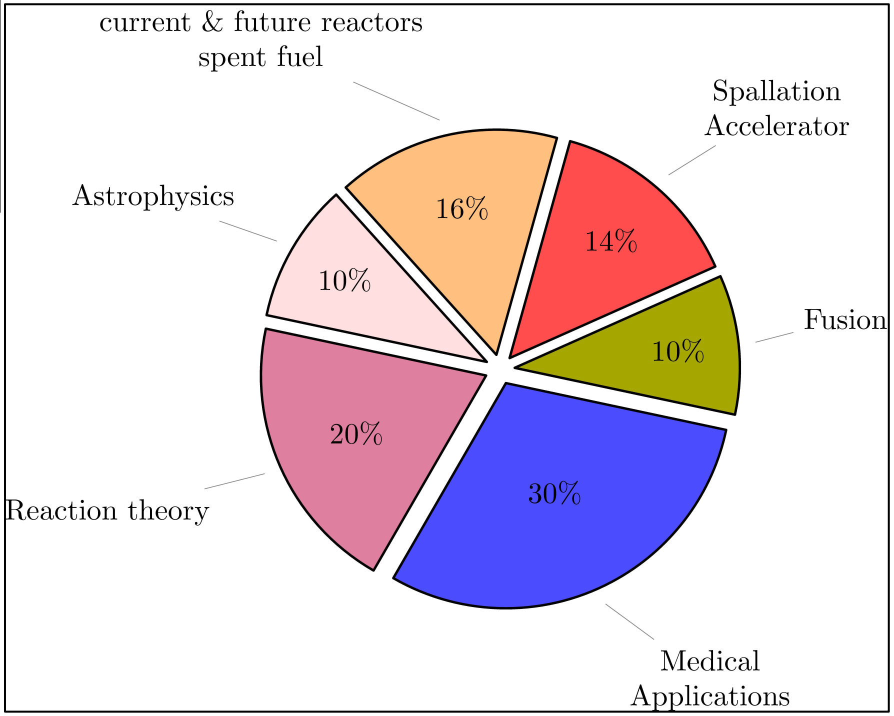
(Received 3 August 2018; revised received 7 November 2018; accepted 29 November 2018)

Automatized evaluation: TENDL

- TENDL is in fact a by-product of a series of codes,
- This is one fundamental difference with other libraries (no manual work),
- It allows to perform „TMC“ for Total Monte Carlo (uncertainty propagation)
- Methods: reproductibility & completeness, development of a portable system, and making use of the knowledge included in other libraries (JEFF, ENDF/B, JENDL),
- Background: theoretical calculations (TALYS) with experimental inputs, with original resonance evaluations,
- Impact:
  - TENDL-2008 to 2021 (2800 isotopes),
  - Neutrons, protons, deuterons, tritons, He3, alpha and gamma induced,
  - all isotopes, all cross sections with covariances, 0-200 MeV,
  - more than 300 isotopes in the NEA JEFF-3.3 library,
  - more than 50 isotopes in the US ENDF/B-VIII.0 library,
  - more than 500 publications using TENDL

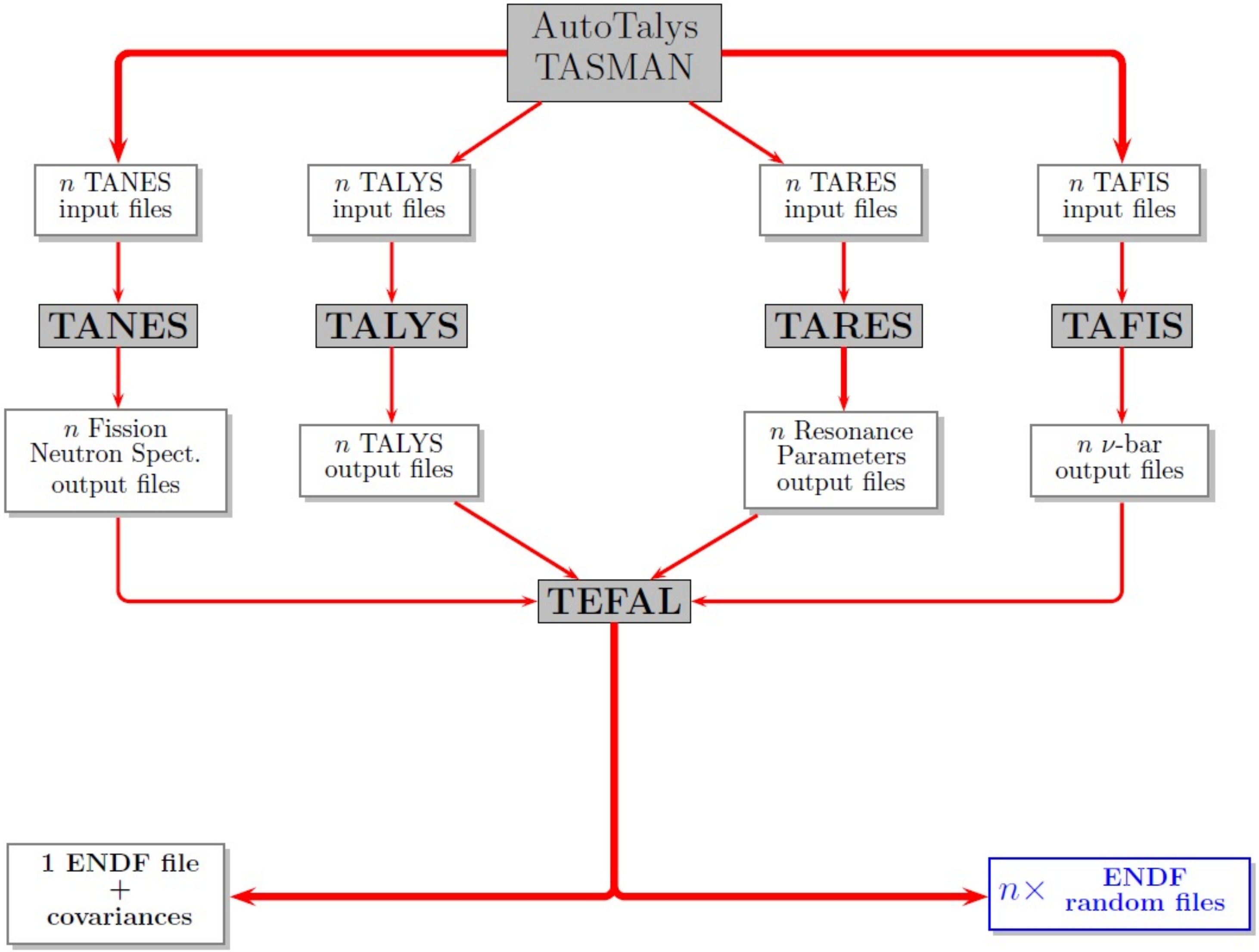
What is the TENDL project ?





What is T6

- Method: Quality evaluation, production automation, open source



What is T6

- t6.tar: 2.3 Gb
- t6 extended: 19 Gb, 880 000 files
- Necessary additional libraries: 20 Gb, 410 000 files (only for neutrons)

- Production of TENDL-2021 on 300 cpu: 1.5 months

- Tested with different compilers, Linux versions

- Developed now between IAEA (80 %) and PSI (20%)

How to produce TENDL:

```
> autotalys -Zbeg 3 -Zend 124 -lifetime 1.e-12
```

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TENDL, T6 and more

TALYS

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.

TALYS

Arjan Koning, Stephane Hilaire, Stephane Goriely

Nuclear reaction model code.

- Download TALYS-1.96
- 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)
- View Data Explorer

https://nds.iaea.org/talys/

EXFORTABLES: formatted experimental data for automatic use (plots, fit)

RESONANCETABLES: ready to use resonance tables

ENDFTABLES: ready to use x-y cross sections

Libraries-2020: systematically processed data libraries

TENDL

- Latest release: 2021 (every 2 years)
- Mainly developed between IAEA and PSI (+ CEA, ULB)

- New T6:
  – Newest code versions,
  – more verifications,
  – Linux RedHat/Mac,
  – tested with latest compilers

- New and simplified T6 available “on demand”

- TALYS-1.96 (above resonances)
- TARES-1.4 (resonances)
- NJOY-2016
- PREPRO-2018
- Other codes/tools

- New “library” database (comparisons, import…)

TENDL: Resolved Resonance Range

- 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)
  - Based on the Sukhoruchkin 2009 and 2015

- 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)

- Publications: *NDS 163 (2020) 163*, *NDS155 (2019) 1*, *ANE 51 (2013) 60*, *NDS113 (2012) 2841*

- Acknowledgments: A. Koning, J.Ch. Sublet and J. Kopecky

TARES developments

- Started in 2008
  - Translate tabulated resonance parameters into ENDF-6 format: MF2, MF32 and MF32c
  - Based on the ATLAS-2006
  - Used in combination with TALYS for TENDL production

- 2012:
  - Addition of the “HFR”: generation of statistical resonances using CALENDF
  - Read the ATLAS and other libraries (JEFF, ENDF/B, JENDL)
  - Add missing information (uncertainties)

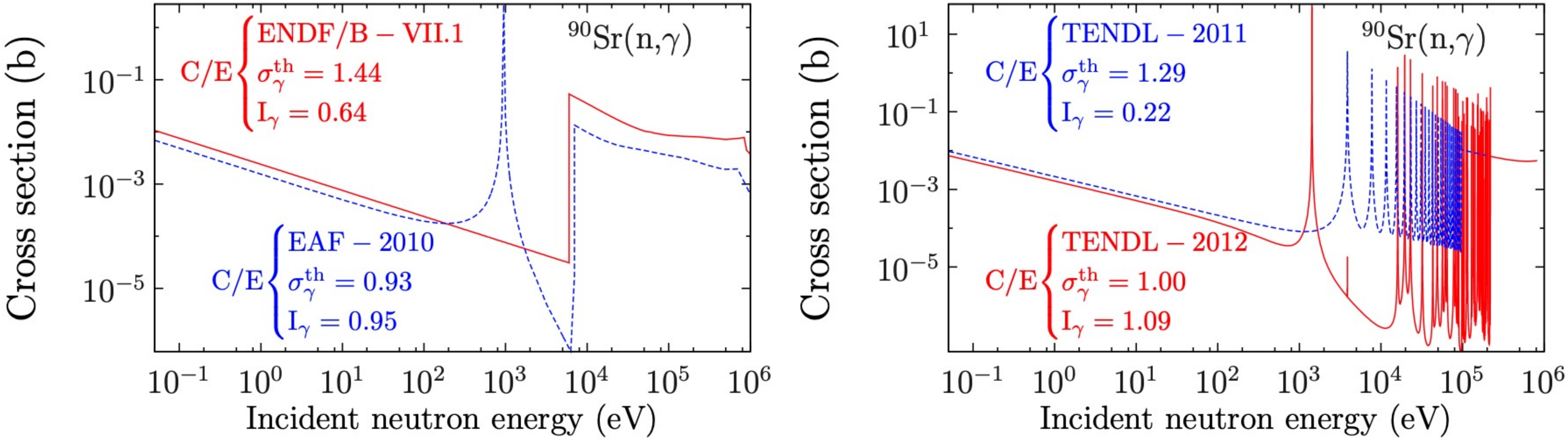
- 2015:
  - Automatic match of the thermal (n,g) points
  - Generation of MF33

- 2018:
  - Read many ATLAS versions, k0 database, some Sukhoruchtin data

TARES focus on the "HFR"

- Started with the Single Resonance Approximation from the EAF library

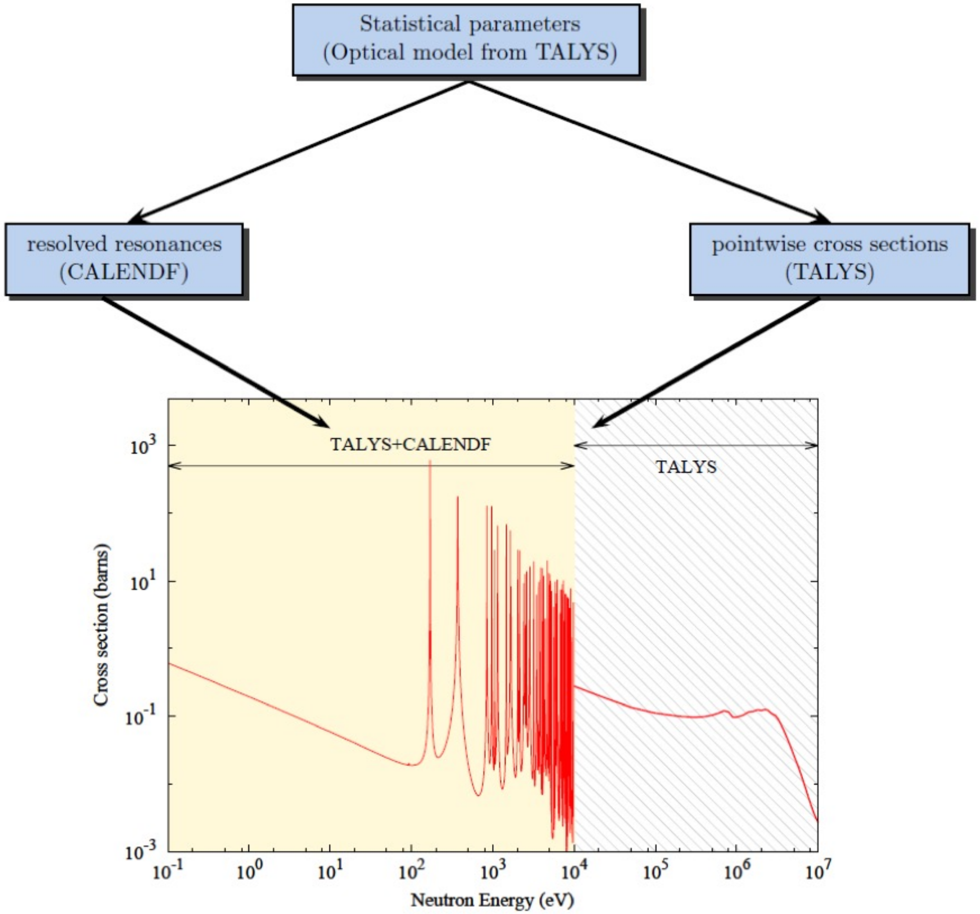
Examples of different approaches for ^{90}Sr ($h_{1/2} = 28$ sec) in the low energy region.



Left: basic optical model calculation for ENDF/B-VII.1 and Single Resonance Approximation (SRA) for EAF-2010. Right: multi-SRA for TENDL-2011 and the present methodology from TENDL-2012 to TENDL-2014.

TARES focus on the "HFR"

- In TENDL, all 2800 isotopes have unique resonances
  - Only about 10 % of the resonances are measured,
  - The rest comes from the HFR method (statistical resonances),
- Presented in ANE 50 (2013) 60
  - Combine the 3 previous models (ld, omp and γ-str) to produce statistical resonances
- Uses the following scheme:
  - TALYS (input: ld + omp + γ-str)
  - CALENDF (input: TALYS output)
  - Output: statistical resonances

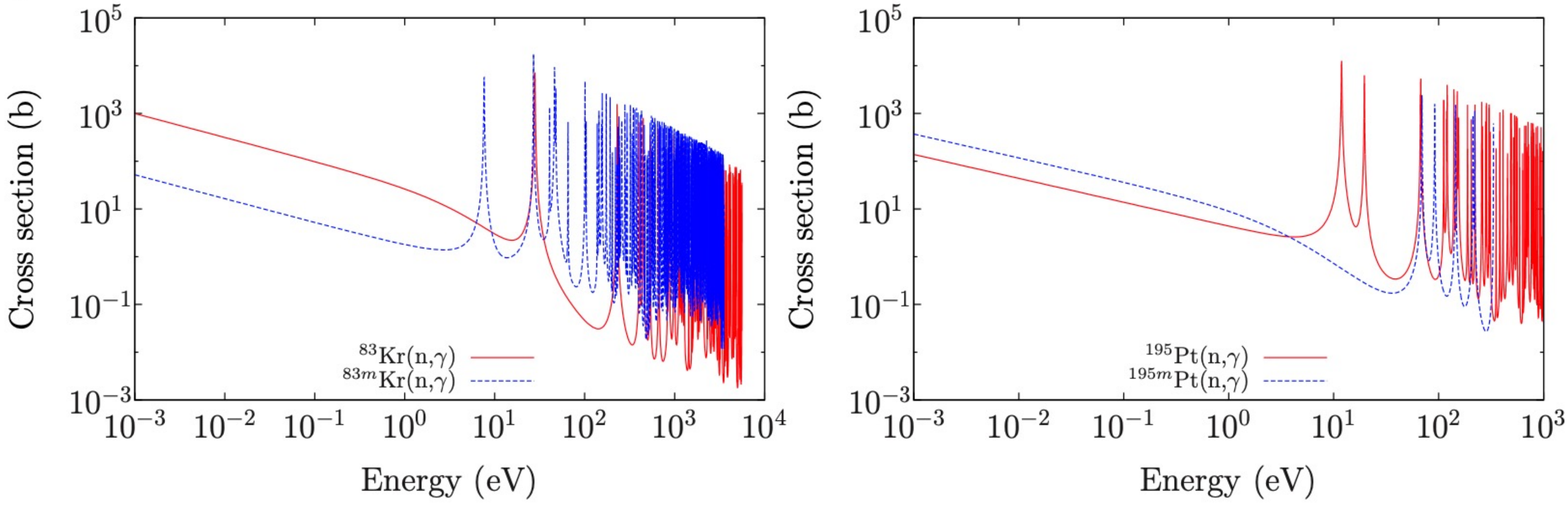


TARES focus on the "HFR"

- HFR applied for ground state and isomeric states

$$\sigma_\gamma^{\text{isomer}} = \sigma_\gamma^{\text{ground}} \frac{\sum_j \frac{g\Gamma^0_{nj}\Gamma_{\gamma j}}{E^2_{0j}}}{\sum_i \frac{g\Gamma^0_{ni}\Gamma_{\gamma i}}{E^2_{0i}}}$$

$\sigma_\gamma^{\text{ground}} \Longrightarrow$ known from measurements (or systematics)
$\sum_j$ and $\sum_i \Longrightarrow$ taken (as before) from the global OMP of TALYS.



TARES: physical checks

- Spacing distribution, Wigner distribution
- Cumulative level distribution
- Average total capture width

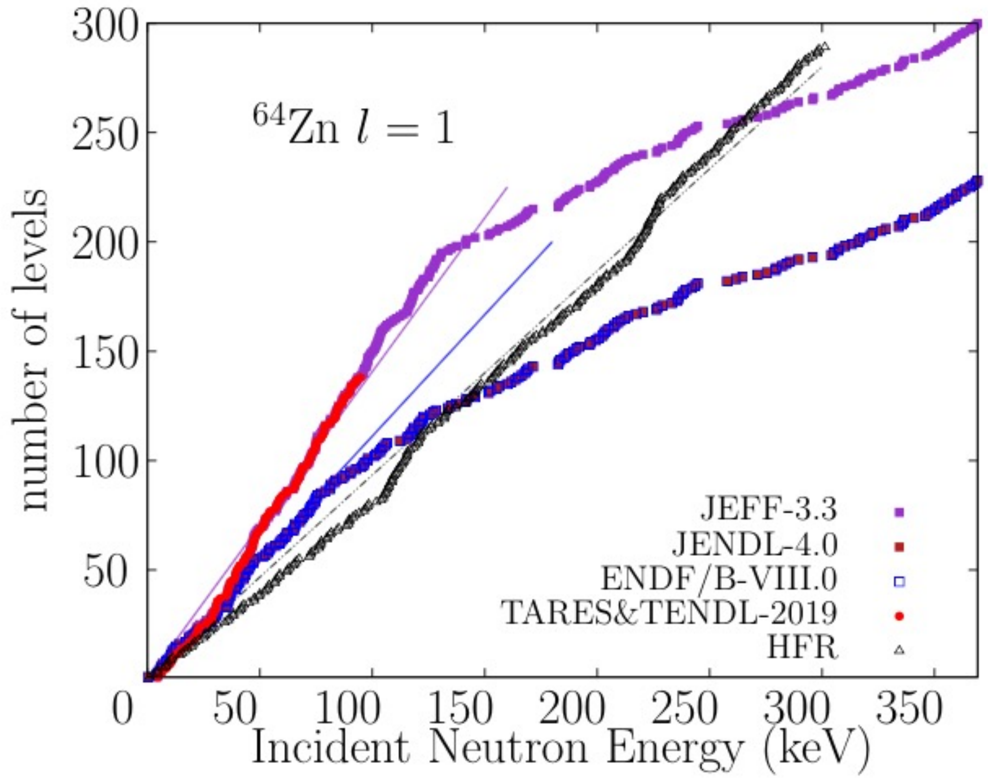
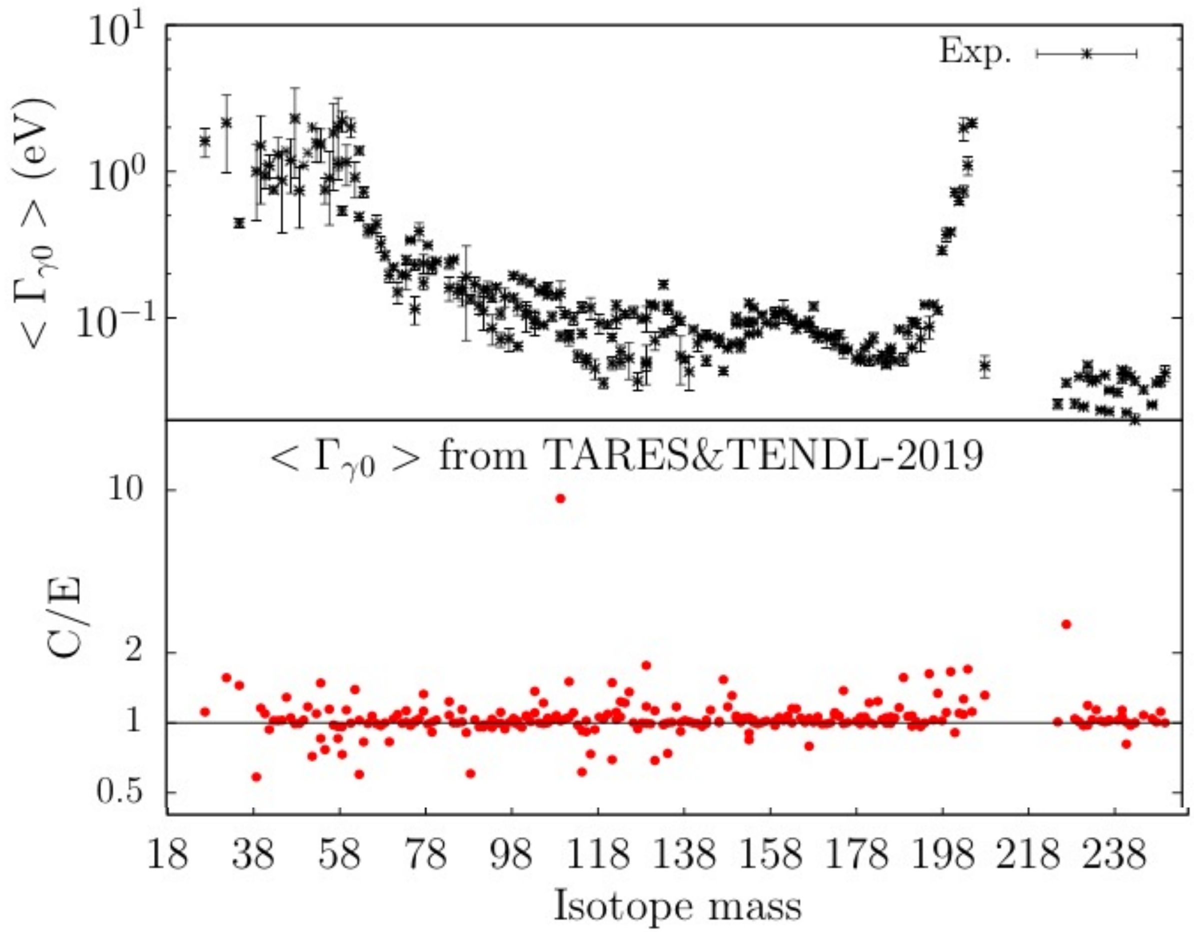


FIG. 16. (Color online) Top: cumulative level distribution for ^{120}Sn and $l = 0$; Bottom: same for ^{64}Zn and $l = 1$.

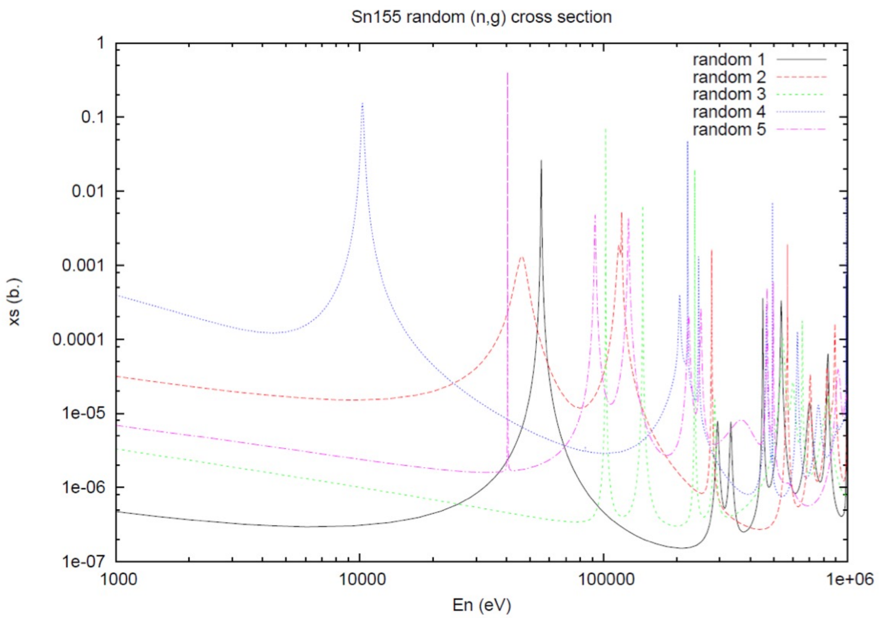
TARES: physical checks

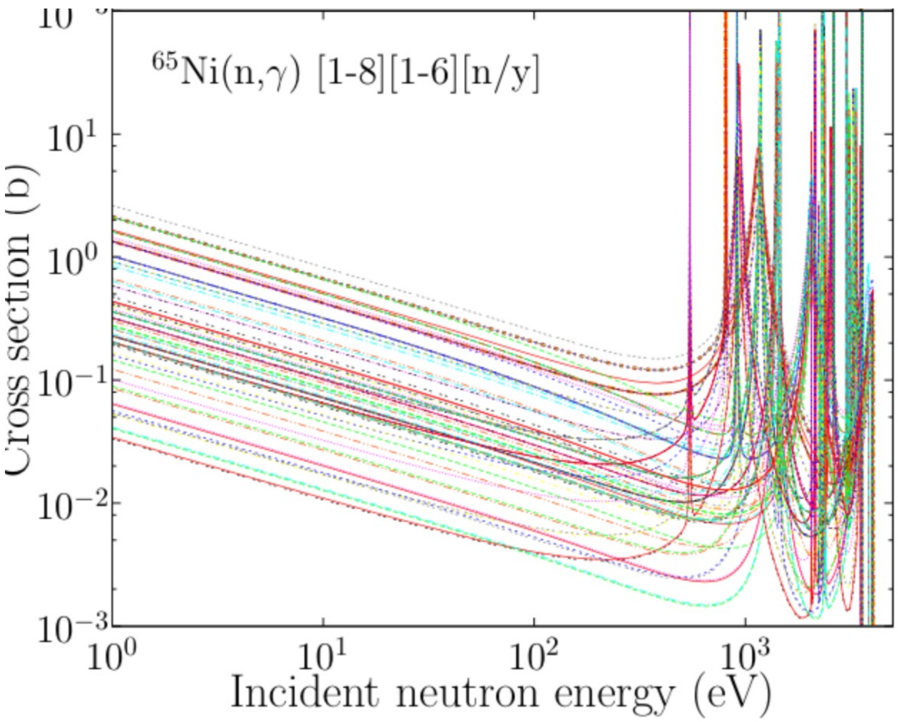
- Spacing distribution, Wigner distribution
- Cumulative level distribution
- Average total capture width



TARES: generation of MF32 and MF33

- For all resonance parameters:
  - Uncertainties are assigned to match thermal (n,g) and RI uncertainties
  - Otherwise, default uncertainties are assigned
  - Sampling of parameters are performed to produce group average cross sections



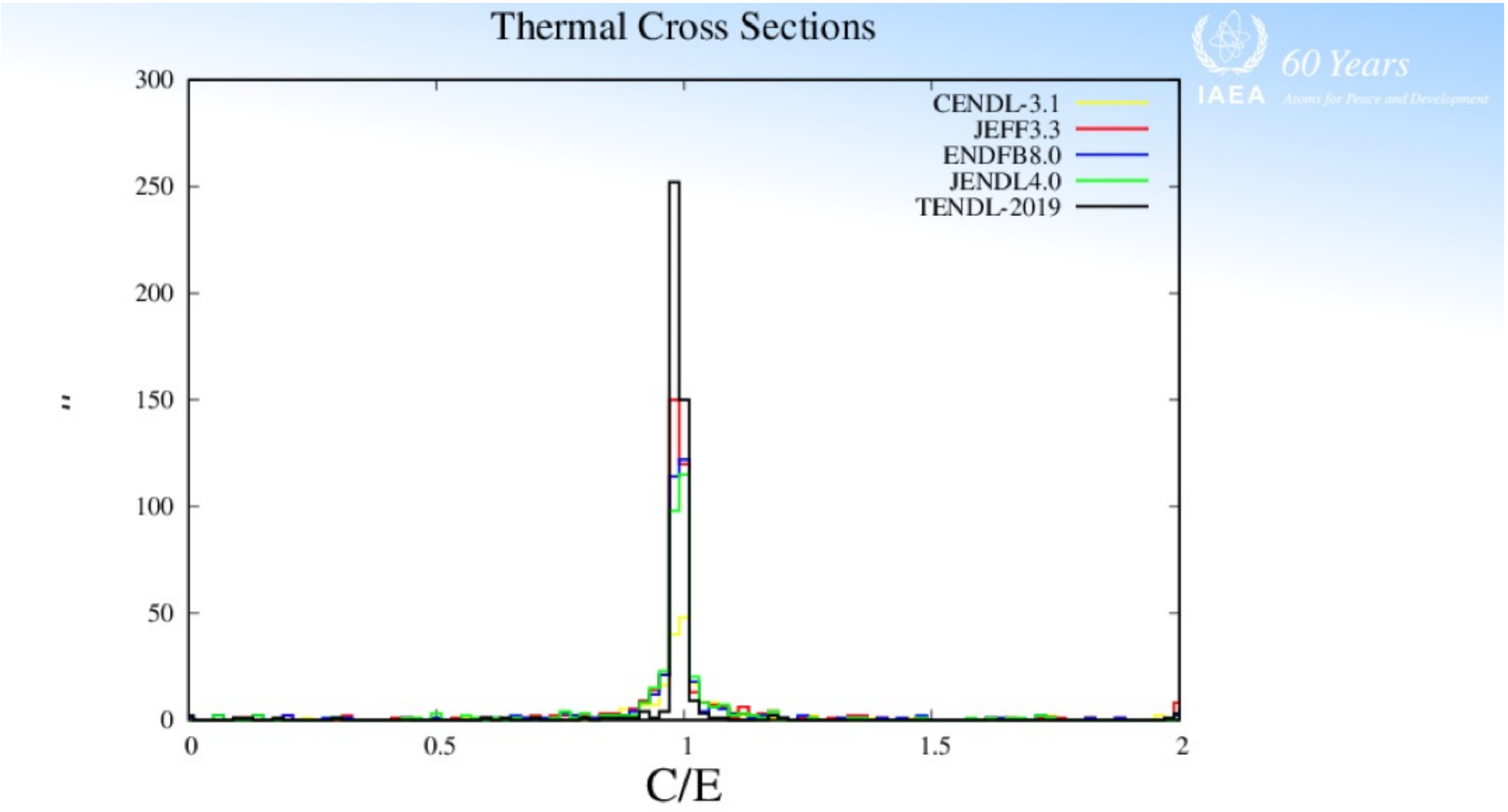


TARES outputs

- For all TENDL isotopes (2800), different outputs are produced together
  - MF1, MF2, MF32c, MF33,
  - .tex, .txt, inter & psyche ouputs
  - Reconstructed pointwise and groupwise cross sections, processed covariances

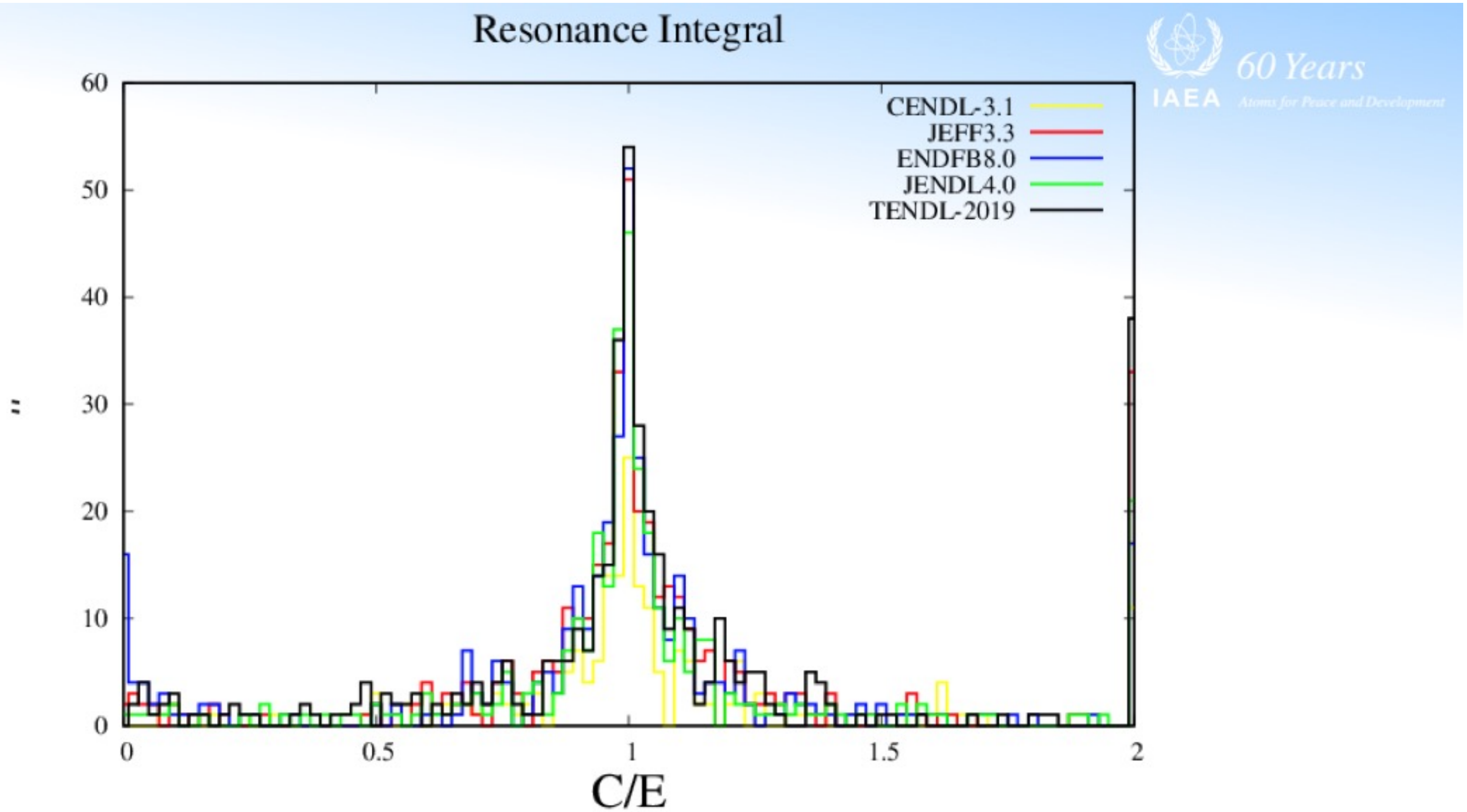
```
# D. Rochman  TARES version 1.43, Villigen   , Switzerland
# Time: Wed Mar 10 06:06:06 2021
#
# Element           : Sm
# Z                 : 62
# A                 : 151
# I                 : 0
# Data origin       : TENDL
# Formalism         : Multi-level Breit-Wigner
# Emin (RRR)        : 1e-5 eV
# Emax (RRR)        : 1.002000E+03 eV
# Emax2 (background): 1.002000E+03 eV
# Nbr. res. (<Emax) : 524
# Nbr. res. (<Emax2): 525
# Thermal  (n,g) xs : 1.514970E+04 b. (Calc.)
# Thermal  (n,g) xs : 15140 +/- 300 b. (Exp.)
# Res. Int (n,g) xs : 3.423830E+03 b. (Syst.)
# MACS 30 keV       : 4.863000E+01 b.
#
# Thermal (n,el) xs : 1.307810E+02 b. (Calc.)
# Thermal (n,el) xs : 61 +/- 3.05 b. (Exp.)
# Res. Int (n,el) xs: 1.525730E+02 b. (Calc.)
#
# Scattering radius : 5.82 fm +/- 10.00 %
#
# Ave. Gtotal   l=0 : 1.295430E-01 eV
# Ave. redu. Gn l=0 : 1.257650E-03 (Gn^0)
# Ave. Gg       l=0 : 1.019440E-01 eV
# Ave. D        l=0 : 1.919540E+00 eV (level spacing)
# Ave. S        l=0 : 3.829210E-04 eV (gamma strength function)
#
#
#
#
#
#   Energy (eV)     +/- DE (eV)      l         J         Gn (eV)       +/- DGn (eV)      Gg (eV)      +/- DGg (eV)
#<--------------><--------------><-----><----------><--------------><--------------><--------------><-------------->
  -2.200000E-01     1.000000E-03     0       +3.00     2.357140E-03    4.285710E-05    7.530000E-02    5.000000E-04
  +4.560000E-01     1.000000E-02     0       +3.00     2.199430E-05    8.571430E-07    1.000000E-01    2.000000E-03
  +1.093000E+00     2.000000E-03     0       +3.00     6.857140E-04    2.571430E-05    1.195000E-01    3.000000E-03
  +1.704000E+00     2.000000E-03     0       +3.00     3.000000E-04    5.142860E-05    9.840000E-02    1.700000E-03
  +2.036000E+00     3.000000E-03     0       +3.00     5.228570E-04    2.571430E-05    9.990000E-02    2.000000E-03
  +4.132000E+00     3.000000E-03     0       +3.00     9.171430E-04    8.571430E-05    9.590000E-02    1.000000E-03
  +6.395000E+00     4.000000E-03     0       +3.00     4.722860E-03    1.714290E-04    1.077000E-01    2.000000E-03
  +1.044800E+01     2.000000E-02     0       +3.00     1.054290E-02    4.285710E-04    1.153000E-01    5.000000E-03
```

Global verification



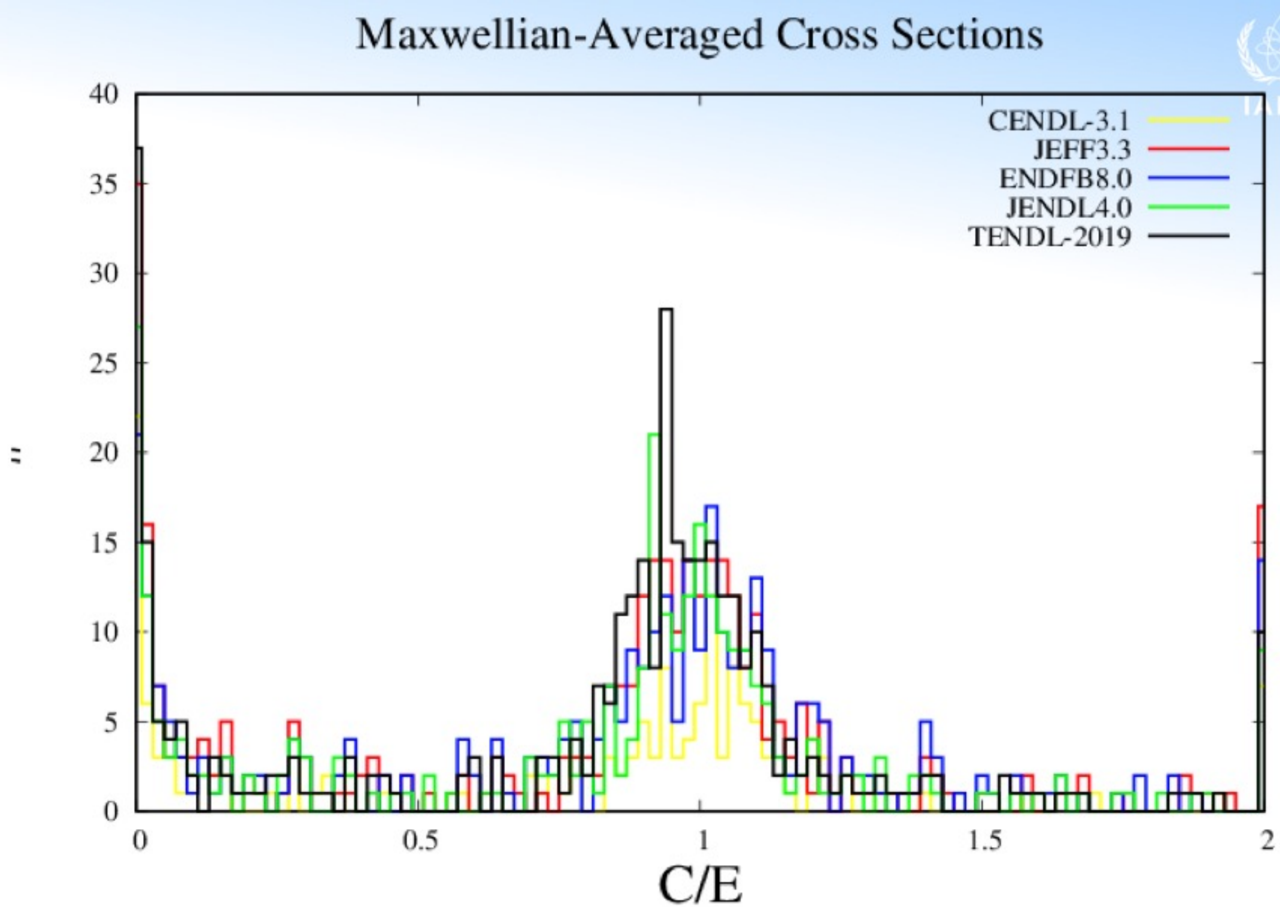
Lib	F(C/E)	N	N <5%	N < 20%	N < 50%
CENDL-3.1	1.036	201	129(0.642)	177(0.881)	187(0.930)
ENDFB-8.0	1.022	375	284(0.757)	332(0.885)	351(0.936)
JEFF-3.1	1.024	425	315(0.741)	377(0.887)	398(0.936)
JENDL-4.0	1.025	359	269(0.749)	320(0.891)	334(0.930)
TENDL-2019	1.008	446	416(0.933)	431(0.966)	434(0.973)

Global verification



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)

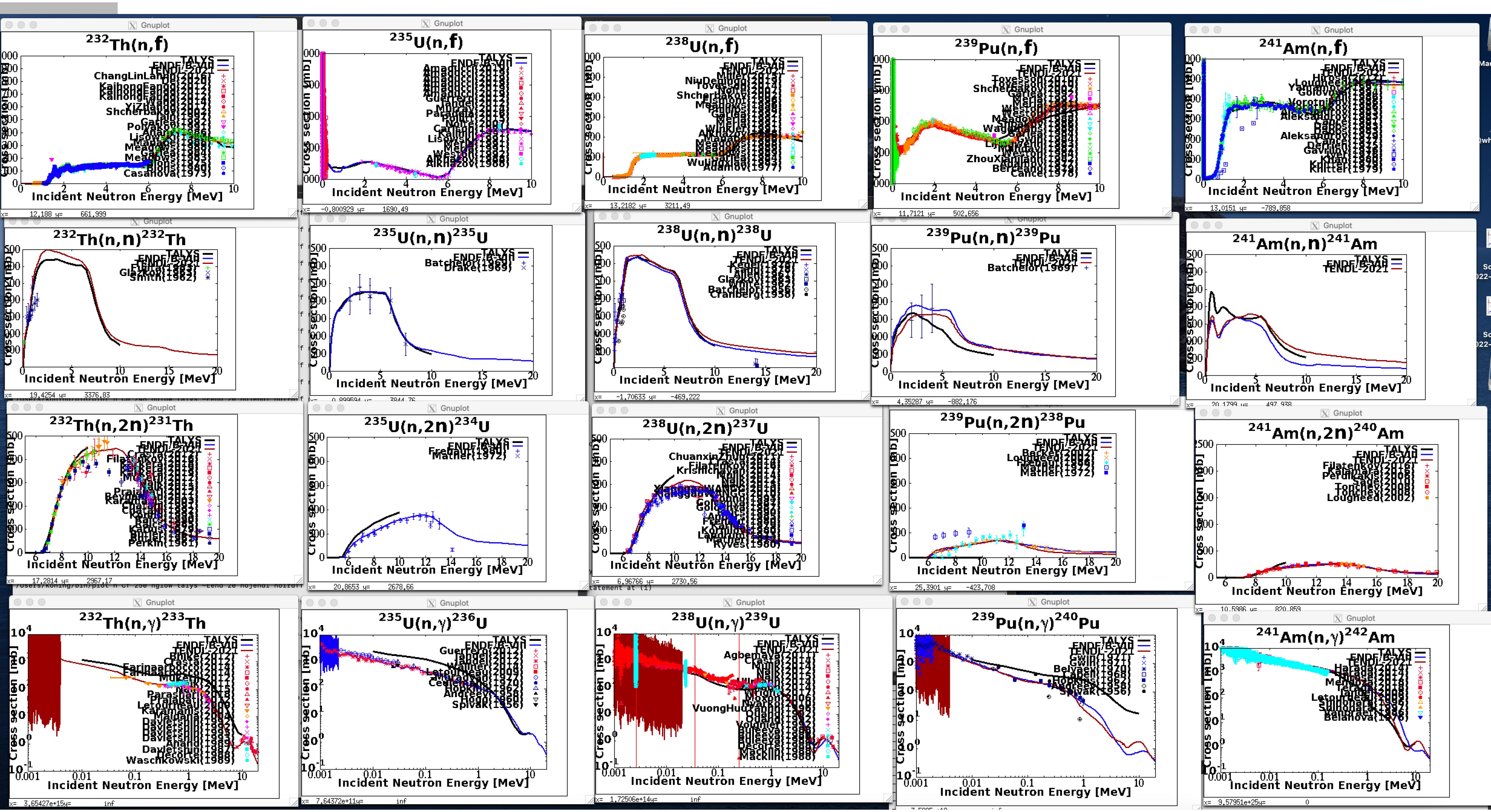
Global verification



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)

Fast neutron range: based on TALYS

- Global selection of models + isotopic adjustment



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Fast neutron range: based on TALYS

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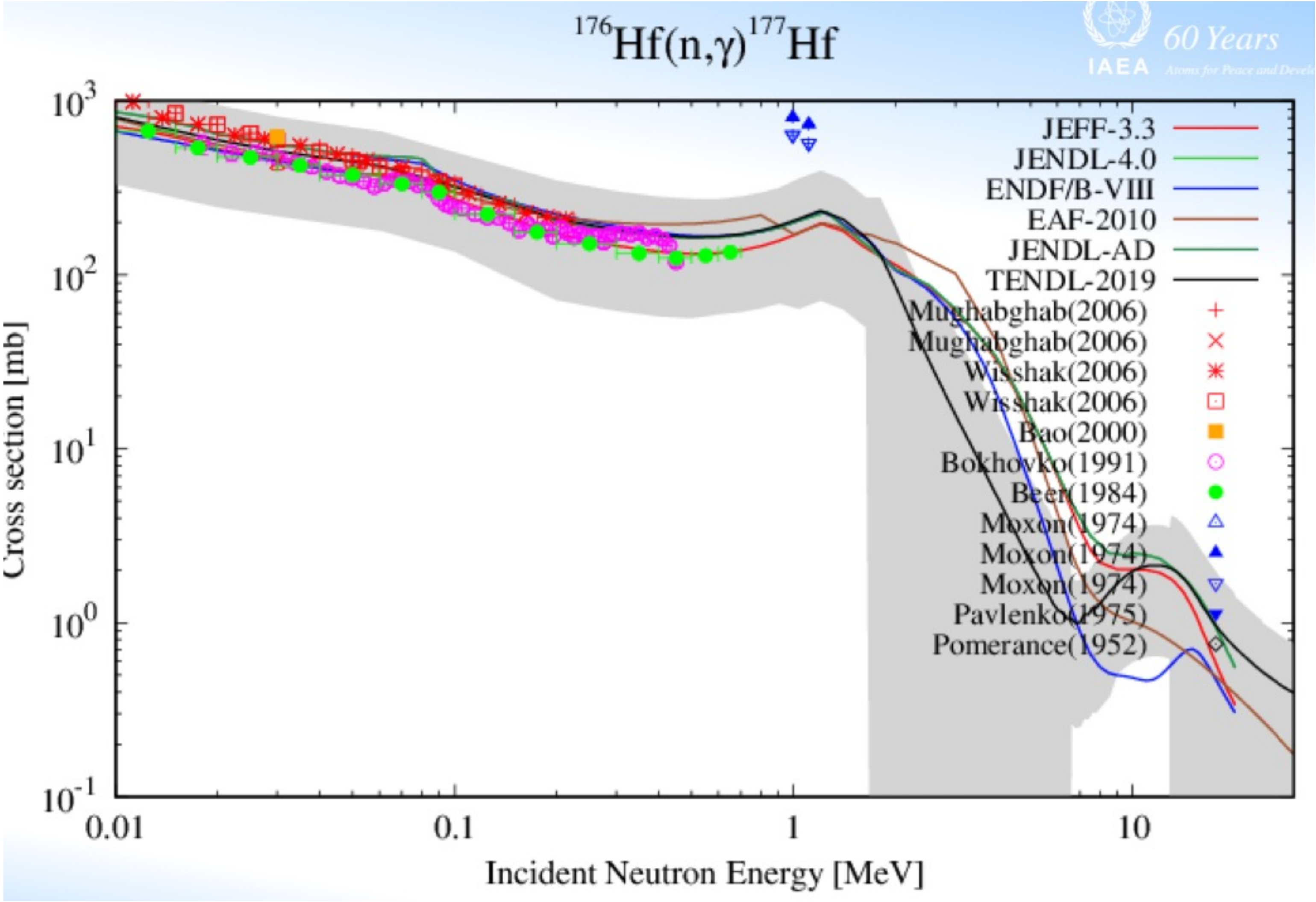

Feedback on bugs (page 1 of 567)

I've done some tests on T6 (I running the version used to create TENDL17, according the Arjan). Many nuclides run perfectly well, but do not produce endf files that match TENDL 2017 endf files. Other results crash, giving:

*** AUTOTALYS error: TEFAL crashes for U235

I found the bug. It is in Tares where I give a wrong NLS for MF32. Previous versions of NJOY didn't care, but njoy12.50 is checking this value... I'm going to modify Tares...

Arjan, Pu9 ?

After debugging, I think there is a bug in NJOY (ERRORR) for Multi Level Breit Wigner (MLBW). In TENDL, following the (good) advice of JC, we dropped Reich Moore (RM) in 2013 and switched to MLBW. Today, I've produce two similar files in MLBW and RM and process them with NJOY. The one with RM is giving me what I expect, and the one with MLBW

I have already checked the ENDF files for TENDL2015 for Th232 and I also see some extrange behaviour. For example if I see the MF 3 MT 5 (p,x) and MF 3 MT 37, some energy points are repeated or missing (when you compare with the same ENDF file available in TENDL2015 web page without the individual reaction channels). So maybe using this files as basis will lead to some extrange behaviour in ACE files.

Just talked witrh Steven, and he shopwed me the files are ijndeed wrong.
At leats I see it in Er168 and it may be a problem in every TENDL file. It looks loke the elastic peak has been folded into the spectra of MF6/MT5. You only see this with > 30 MeV tests and

Feedback on bugs (page 2 of 567)

Now… The bad one is that there is a BIG bug in stellarrate.f subroutine, in the integration procedure of the MACS. I found it out comparing TALYS astrorate.g output with the small code I wrote to estimate the MACS with the RRR.

I guess these are both more NJOY issues than TALYS errors, but maybe you can build a workaround in the TENDL files or send corresponding bug reports/fixes to some responsible people behind NJOY…

Most ridiculous TEFAL error ever:
TALYS and TEFAL say: above mass 216 there is fission, so we need nubar, pfns, etc.
W216 has no nubar in any library, so TEFAL starts searching until if finds the lowest Z,A combination with a nubar in a library. That is Th227 in JEFF3.2.

That looks good. But first of all: stop the presses, the photonuclear library for TENDL-2015 is wrong and should be changed. I discovered a terrible bug in the production system which affects the photonuclear data library. I am going to reproduce it, hoping

Recently we found a new problem on the ACE file of TENDL-2017 neutron sub-library. Please see the attached file about this new problem. If you have any questions, please tell me.

Feedback on bugs (page 567 of 567)

The secondary neutron spectrum data of mt=5 in TENDL-2017 are incorrect at 30MeV.

The calculated neutron spectra with 40 MeV neutrons are shown in Fig. 3 with the measured ones [6]. The calculated neutron fluxes with TENDL-2017 unphysically increase near 30 MeV, while those with

Bug found in TENDL data: wrong particle yields. Wait until TENDL 2012 (December)

I am having similar difficulties with TENDL 2015.

After writing a download script for TENDL-2017 (link to tendl-2017 script) and getting an NJOY with Boron 10 (link to issue) I started trying to use TENDL-2015

I have written a openmc-get-tendl-2015-data script (link to tendl-2015 script) which downloads the ace files and converts them to h5 (based on the nndc and JEFF scripts).

Problems on TENDL-2015 neutron sub-library and its ACE file

Konno, Chikara; Tada, Kenichi

The nuclear data library TENDL-2015 up to 200 MeV is being used as a standard nuclear data library worldwide, particularly in Europe. We found out the following three problems in the ENDF and ACE files in TENDL-2015 neutron sub-library; (1) no unresolved resonance data in most of the ACE files, (2) no secondary γ data in most of the ACE files, (3) No high-energy γ peaks in the capture reaction of a lot of the ENDF files. We examined effects of these problems and the followings were demonstrated; (1) insufficient self-shielding correction, (2) wrong γ spectra in neutron-γ coupling calculations and wrong DPA cross section data. Secondary γ data of the capture reaction and ACE files in TENDL-2015 neutron sub-library should be revised.

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TENDL evaluation: General observations

- First comment: the more we produce, the more bugs we distribute
- Second comment: in T6, problems can be related to T6, but also to ENDF format, to PREPRO, to NJOY, to MCNP, …
- Many users of TENDL: many aspects which are tested. Therefore more problems found
- Open new possibilities (complete ENDF/text files for charged particles): more troubles
- Need to skip ENDF format and go straight to GNDS or JSON
- Difficult to create a priority list (who pays ?): who says what is important ?
- Avoid latest “computer environment” packages: for portability, only simple scripts, commands.

Uncertainties: relation between evaluation and needs

- Two main related dilemma:
  1. Preliminary question: “Does general-purpose library exist ?”
     – It certainly can, but today all libraries are adjusted (even JENDL ??)
     – There are no correct/wrong covariances: only reflect the knowledge we put in
     – Same for cross sections

  2. From users, two typical questions/remarks are

“Why do you get 500 pcm uncertainty on k_{eff} ? We know it better, please do it again.”
“Are these correlations correct ?”

- Solution for the time being:
  – Produce two evaluated files: (1) without integral feedback
  (2) with integral feedback

  – The key point being: do it at the evaluation level !

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Making use of T6/TENDL: uncertainty propagation

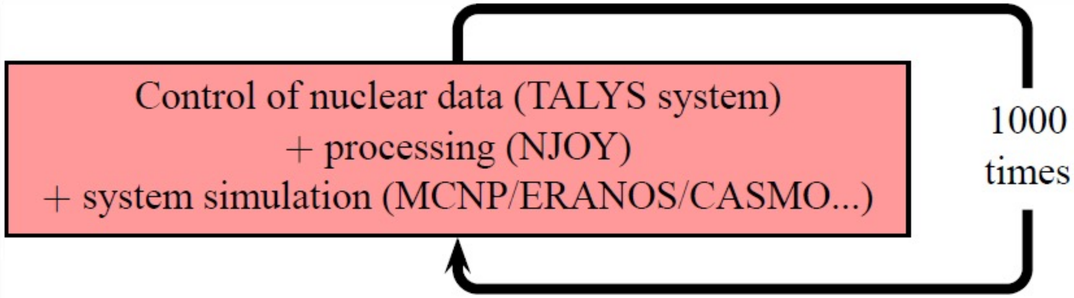
Three methods exist today:

1. Based on nuclear data covariance data
- So-called “Sandwich rule” = sensitivity times covariances ,
- Provide uncertainties, sensitivities

2. Based on nuclear data parameter covariance data:
- So-called TMC (Total Monte Carlo)
- Sampling of model parameters,
- Provide uncertainties,
- Does not provide sensitivities, but importance factors.

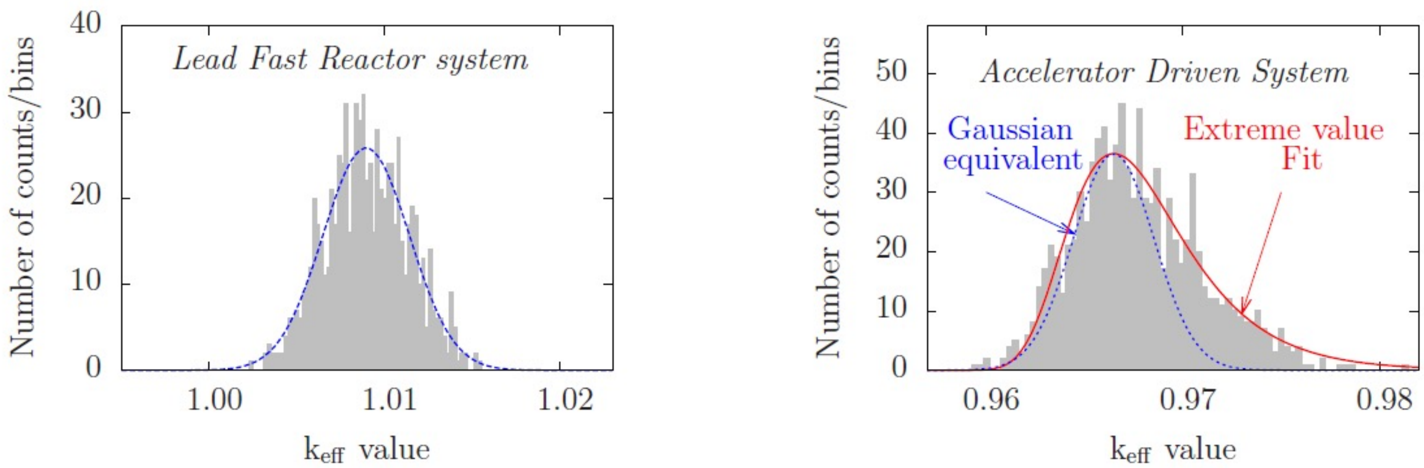
3. In between: based on nuclear data covariance data:
- Sampling of cross section data, based on nuclear data covariances
- Provide uncertainties,
- Does not provide sensitivities, but importance factors,
- Many software: XSUSA, ACAB, NUDUNA, NUSS, SANDY, SAMPLER…

Making use of T6/TENDL: uncertainty propagation with TMC



For each random ENDF file, the benchmark calculation is performed with MCNP. At the end of the *n* calculations, *n* different k_{eff} values are obtained.

$$\sigma^2_{total} = \sigma^2_{statistics} + \sigma^2_{nuclear\ data}$$



"Towards sustainable nuclear energy: Putting nuclear physics to work",
A.J. Koning and D. Rochman, ANE 35 (2008) 2024.

Uncertainty reduction with BMC

- <u>Step 1 - Preliminary work:</u> in-depth cross section evaluation (traditional method of parameters/models adjustment)

- <u>Step 2 - BMC</u>: Based on step 1,
  – Generate n=100 000 (or 1000) random files (TMC-way)
  – Calculate n times the benchmarks
  – Assign weights to all realizations *i* with a chi2 and update the parameter distributions

For a random file i and a set of p benchmarks:

$$\chi_i = \sum_j^p \left(\frac{\mathrm{k}_{\mathrm{eff,i}}^{(\mathrm{j})} - \mathrm{k}_{\mathrm{exp}}^{(\mathrm{j})}}{\Delta \mathrm{k}^{(\mathrm{j})}} \right)^2 \quad (1)$$

$$w_i = \exp(-\frac{\chi_i}{2}) \quad (2)$$

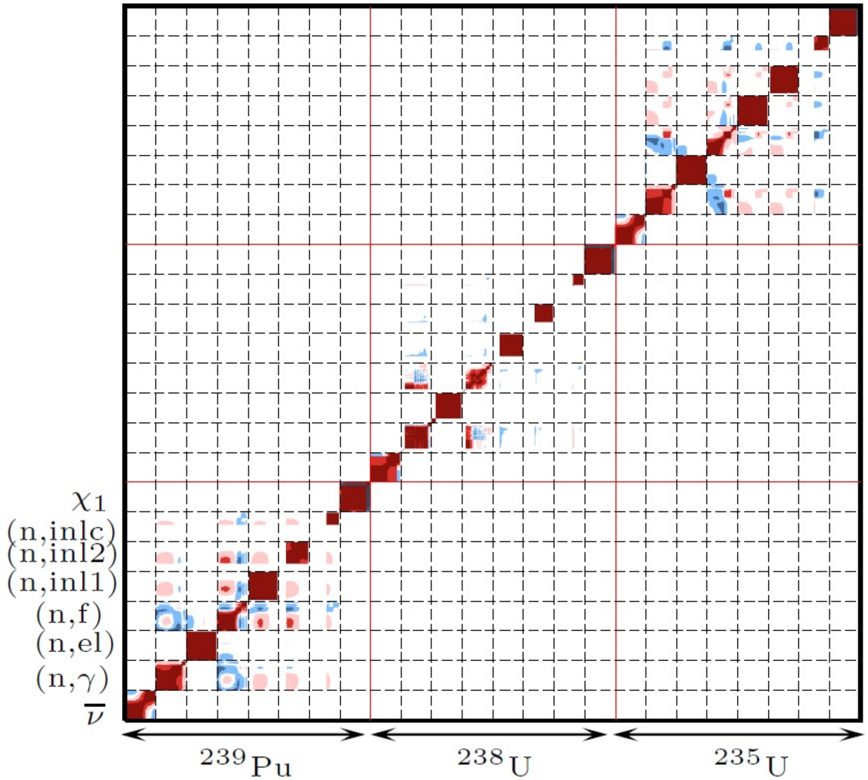
$$\begin{cases} \omega = \sum_i^n w_i \\ \omega_\sigma = \sum_i^n w_i \cdot \sigma_i / \omega \end{cases}$$

  – Update the cross sections with the weights.

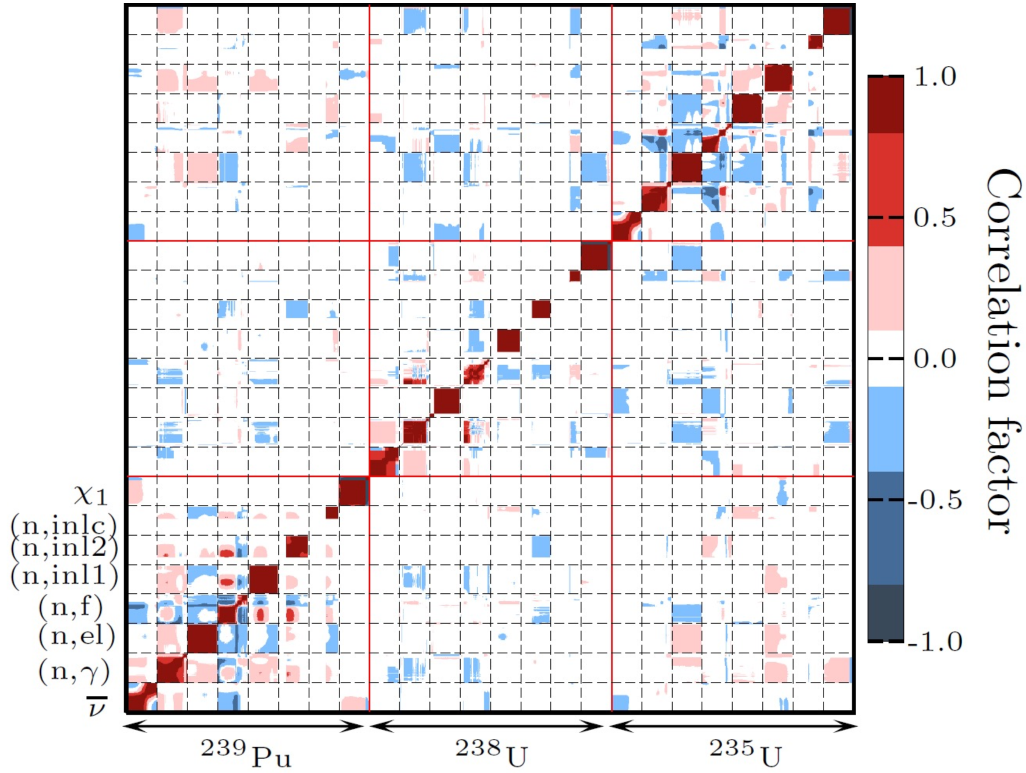
- Some BMC/BFMC references:
  – EPJ/A 51 (2015) 184, Nucl. Data Sheets 123 (2015) 201, EPJ/N 3, 14 (2017)

Example 2: Using integral data

- Fast range: 14 reactions together (k_{eff} and reaction rates) (EPJ/N **4** (2018) 7)



Prior



Posterior

More correlations → uncertainty reduction

Main references

- TENDL: Complete Nuclear Data Library for Innovative Nuclear Science and Technology, *Nucl. Data Sheets 155 (2019) 1*.
- Conception and software implementation of a nuclear data evaluation pipeline, *Nucl. Data Sheets 173 (2021) 239*.
- The joint evaluated fission and fusion nuclear data library, JEFF-3.3, *Eur. Phys. Jour. A 56 (2020) 181*.
- Multifaceted coded nuclear data libraries assemblage, verification and validation: TENDL-2019, *ICRS 14/RPSD 2020 conference, Seattle, Sept. 13-17, 2020*.
- A statistical analysis of evaluated neutron resonances with TARES for JEFF-3.3, JENDL-4.0, ENDF/B-VIII.0 and TENDL-2019, *Nucl. Data Sheets 163 (2020) 163*.
- From average parameters to statistical resolved resonances, *Annals of Nucl. Ene., 51 (2013) 60.*
- Radiative neutron capture: Hauser Feshbach vs. statistical resonances, *Physics Letters B 764 (2017) 109*.

Conclusion

- The TENDL library is improving year after year, TENDL-2021 being (hopefully) a better set

- The new T6 code package allows to produce TENDL, random files and to go further,

- Still, as proven by distributing T6, many improvements are necessary

- Open unexpected opportunities


photo courtesy of Gerry Hofstetter

Wir schaffen Wissen – heute für morgen