STATUS of TENDL

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Outline

- TENDL philosophy
- TENDL-2015
- Some examples
- Parameter uncertainties in TALYS
- Summary

WPEC-2016, 12-13 May 2016
NEA Data Bank, Paris
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TALYS-based evaluated nuclear data library

Home Reference & us Citations

TENDL-2015

By A.J. Koning[1], D. Rochman[2], J. Kopecky[3], J.Ch. Sublet[4], M. Fleming[4], E. Bauge[7], S. Hilaire[7], P. Romain[7], B. Morillon[7], H. Duarte[7], S.C van der Marck[6], S. Pomp[5], H. Sjostrand[5], R. Forrest[1], H. Henriksson[8], O. Cabellos[9], S. Goriely[10], J. Leppanen[11], H. Leeb[12], A. Plompen[13], and R. Mills[14]

[1] IAEA, [2] PSI,[3] JUKO Research, [4]CCFE, [5]Uppsala Univ., [6]NRG, [7]CEA,[8]Vattenfall, [9]NEA, [10]ULB, [11]VTT, [12]ATI, [13]IRMM, [14]NNL.

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

Random files

1. Random fission yields
2. Random thermal scattering

Sub-library files

1. neutron
Proton 2.
Deuteron 3.

TENDL-2015: (release date: 18 January 2016)

Last update: 2 May 2016

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 8th version is **TENDL-2015**, 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, and 2014).

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TENDL philosophy

- **Fundamental nuclear reaction data should NOT be assembled, or touched, at the level of individual isotopic evaluations of ENDF/B-VII, JEFF, JENDL, CENDL, ROSFOND or CIELO.**
- **Fundamental evaluated nuclear reaction data are:**
  - The EXFOR database with an associated table of weights per experiment
  - An evaluated set of resonance data
  - An input file with parameters for a nuclear model code of a precisely defined version (TALYS-1.8)
  - If necessary: “unphysical actions” like
    - “Fiddling” with data, fit by eye, GLS, other fitting
    - Adoption of MT numbers from existing libraries

    should be stored in scripts
- **TENDL considers ENDF-formatting as trivial and reproducible (future: same for GND)**
- **Result: fundamental data per isotope are not several Mb in MF1-MF40. The knowledge put into an isotope is represented (and actually is nothing more in practice!) by a few small files. Anything after that: ENDF-6 files, processed files, random files for Total Monte Carlo, etc. etc. is automated.**

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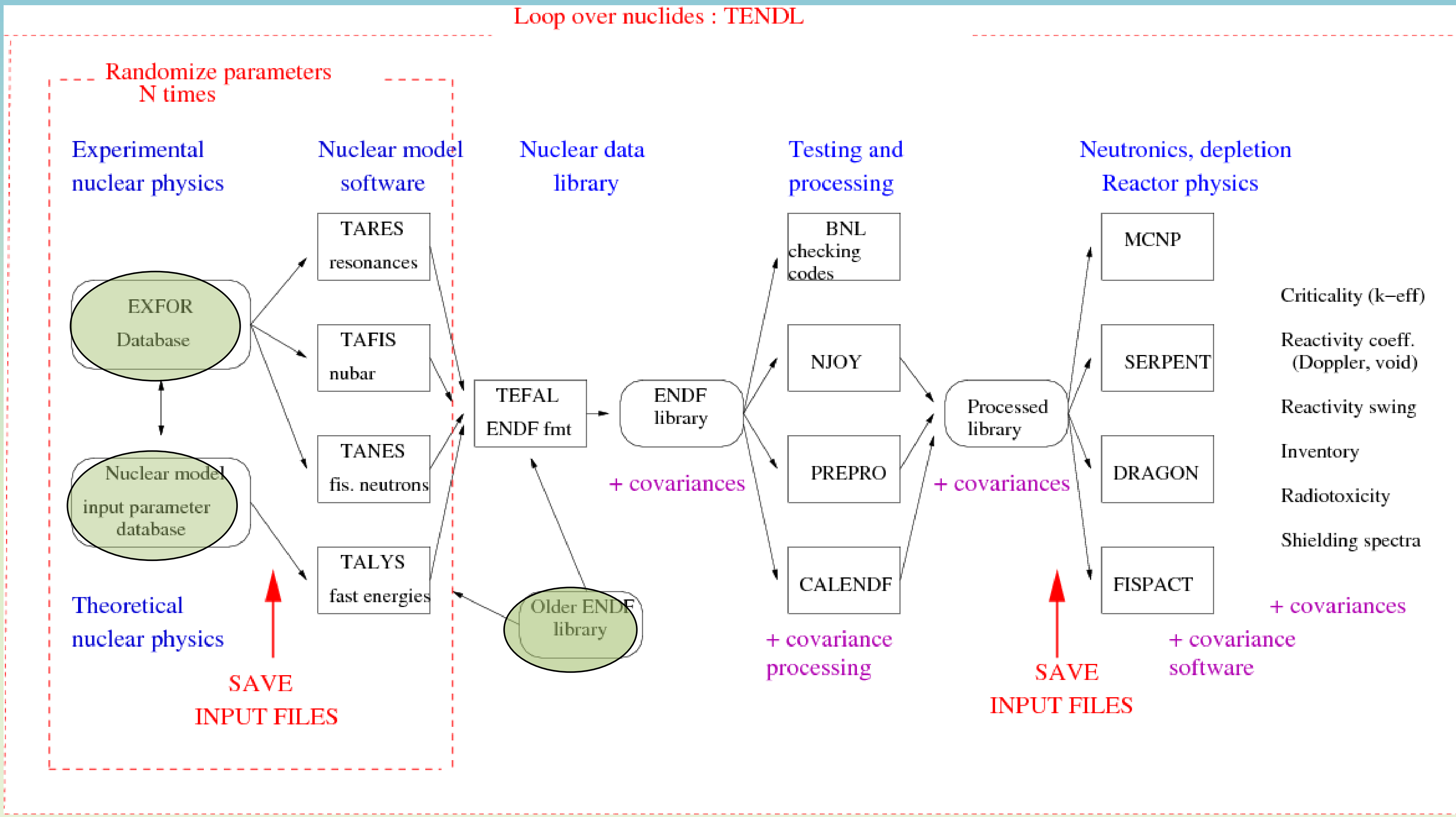
TENDL nuclear data library



A.J. Koning and D. Rochman ,"Modern nuclear data evaluation with the TALYS code system", Nuclear Data Sheets 113, 2841 (2012).

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TALYS Evaluated Nuclear Data Library: TENDL-2015

- Neutron, proton, deuteron, triton, Helium-3, alpha and gamma data libraries.
- 2808 targets (all isotopes with lifetime > 1 sec.)
- Complete reaction description in ENDF-6 format: MF1-MF40, up to 200 MeV
- MCNP-libraries ("ACE-files"), PENDF files and multi-group covariance data

Default: Global calculations by TALYS-1.8 and TARES (resonances), which are overruled by

Adjusted TALYS calculations (340 input files) and Resonance Atlas-based TARES calculations, which are overruled by

TALYS-normalization to ~200 (experimental) evaluated reaction channels from other libraries (e.g. IRDFF, light nuclides, main channels of "big 3")

For TENDL-2015, all nuclides have been evaluated by a Bayesian Monte Carlo procedure. **As usual**, this has resulted in complete covariance information as far as the ENDF-6 format allows: MF 31 (nubar) ,32 (resonances), 33 (cross sections), 34 (angular distributions, 35 (fission neutron spectra), 40 (isomeric information),

for those who are able to process and use all that.

Alternative for covariances: TENDL-2015 comes with 300 random ENDF-6 files per nuclide

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Thermal capture cross sections

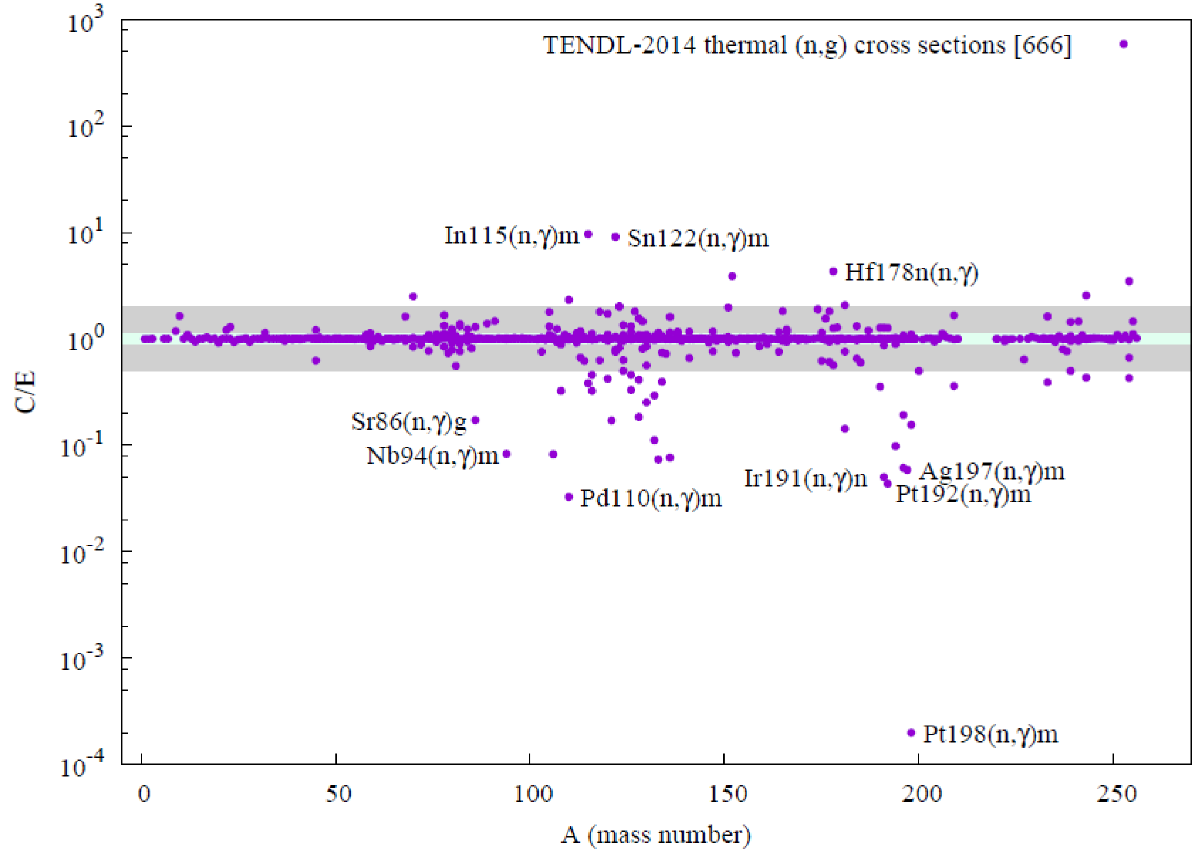

Figure 4: Distribution of TENDL-2014 (n,γ) thermal cross section C/E values against number of nucleons A. The bands represent regions of $\frac{1}{2}$<C/E<2 and |C-E|/E <10%.

Fleming et al, Probing experimental & systematic trends of the neutron -induced TENDL-2014 nuclear data library, UKAEA-R(15)30

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Thermal (n,alpha) cross sections

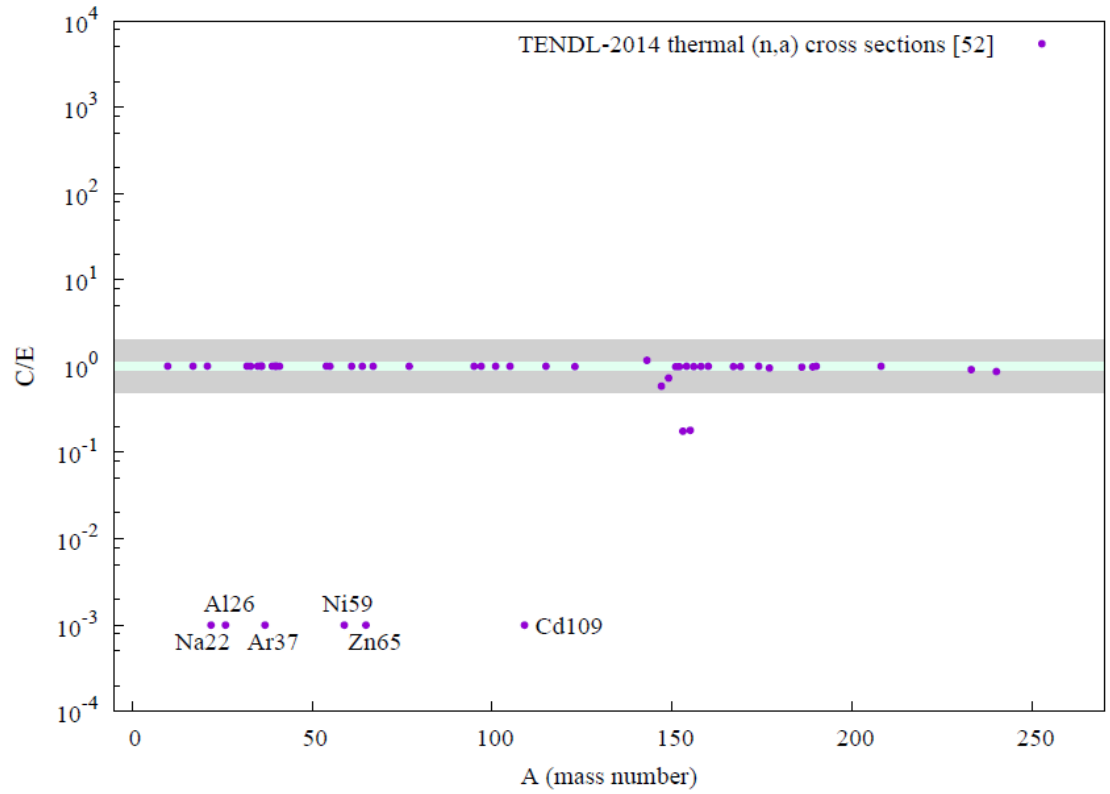

Figure 11: Distribution of TENDL-2014 (n,α) thermal cross section C/E values against number of nucleons A. The bands represent regions of $\frac{1}{2}$<C/E<2 and |C-E|/E <10%.

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Maxw. Av. capture cross sections

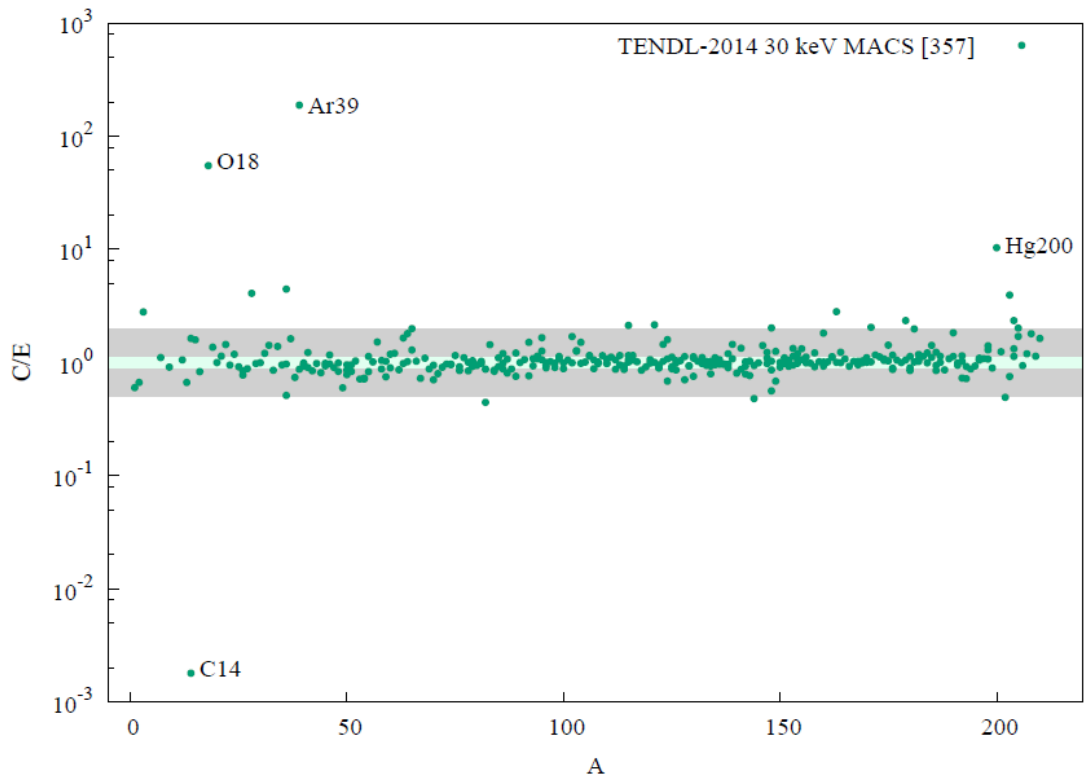

Figure 8: Comparison of all 357 KADoNiS 30 keV cross sections with TENDL-2014 values calculated with maxwav. A few nuclides are isolated which require an adjustment of over one order of magnitude. The bands represent regions of $\frac{1}{2}$<C/E<2 and |C-E|/E <10%.

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MACS comparison with other libraries

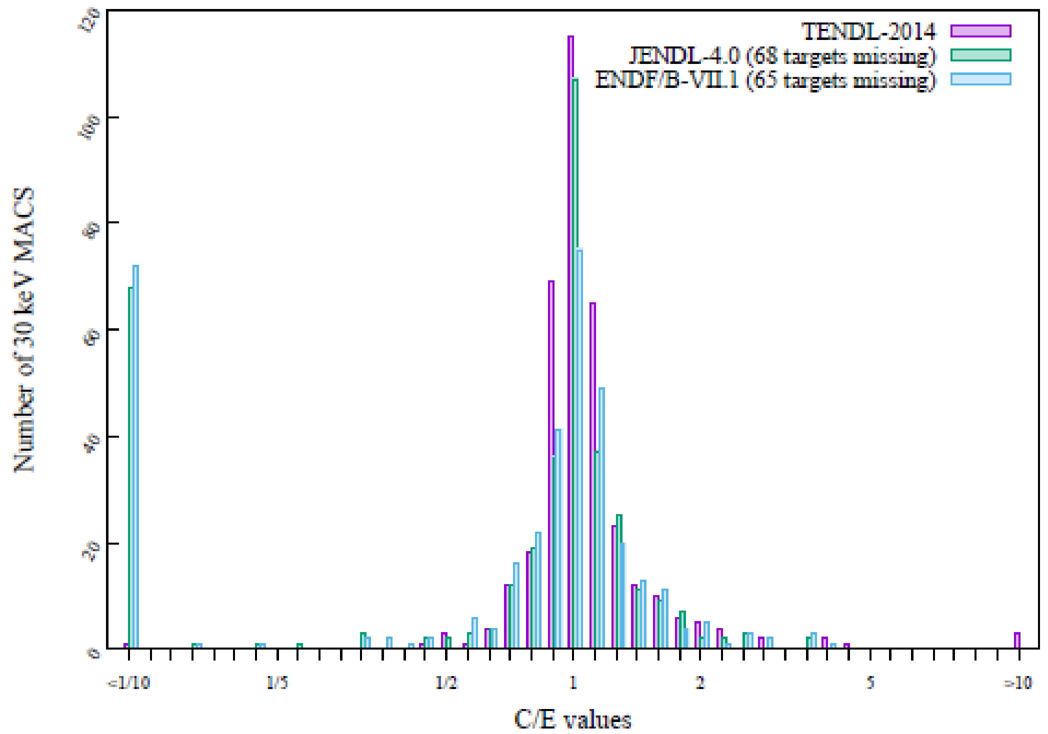

Figure 8: Comparison of C/E distributions overal all 357 KADoNiS 30 keV cross sections with TENDL-2014, JENDL-4.0 and ENDF/B-VII.1 values calculated with maxwav. C/E values for missing nuclides in JENDL-4.0 and ENDF/B-VII.1 are tallied in the <1/10 bin.

Sublet and Fleming, Maxwellian-averaged neutron-induced cross sections for kT=1 keV to 100 keV, KADoNiS, TENDL-2014, ENDF/B-VII.1 and JENDL-4.0u nuclear data libraries UKAEA-R(15)29

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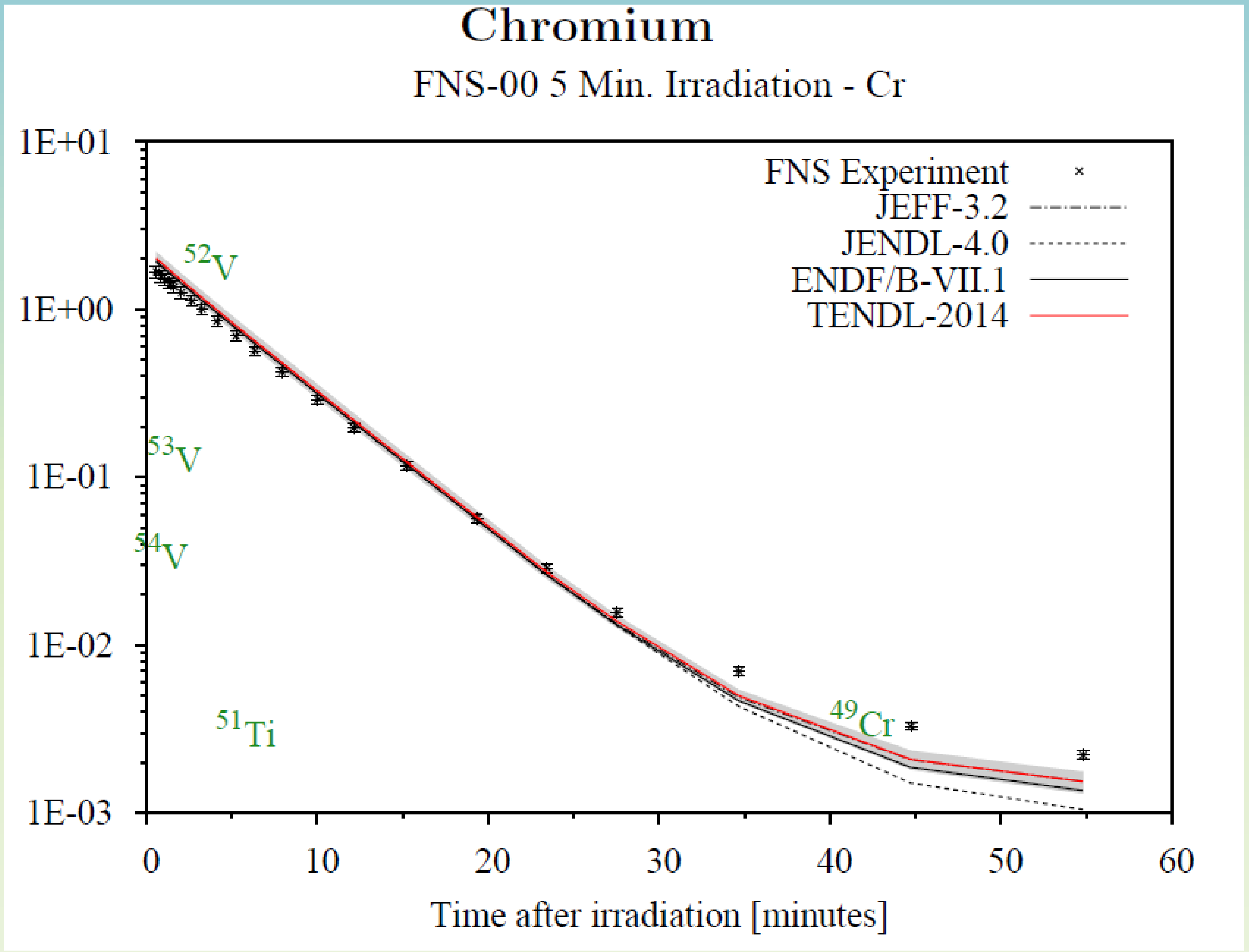
J.C. Sublet and M. Gilbert, Decay heat validation CCFE-R(15)25, january 2015.



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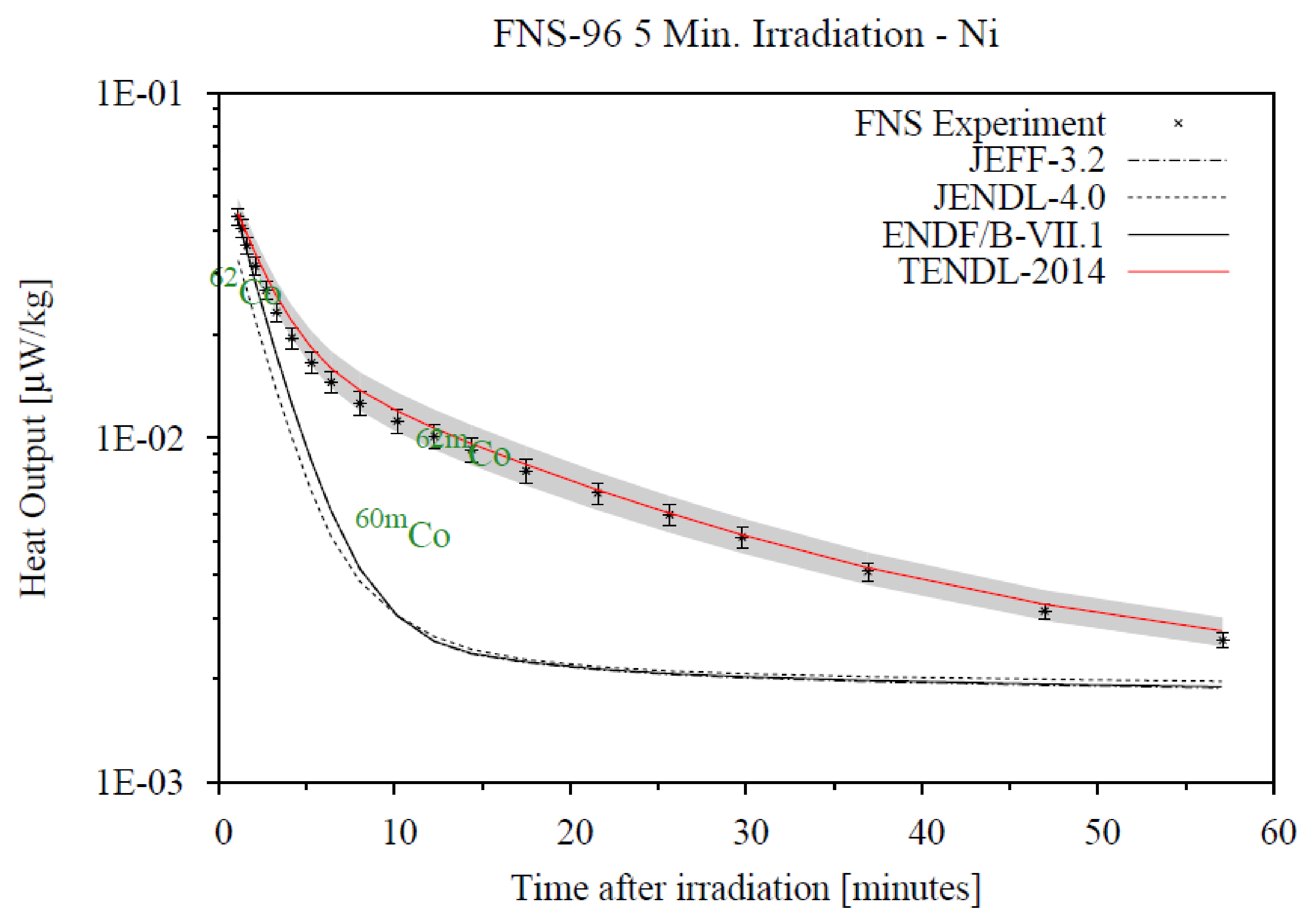

Decay heat should only be analyzed with General Purpose Libraries

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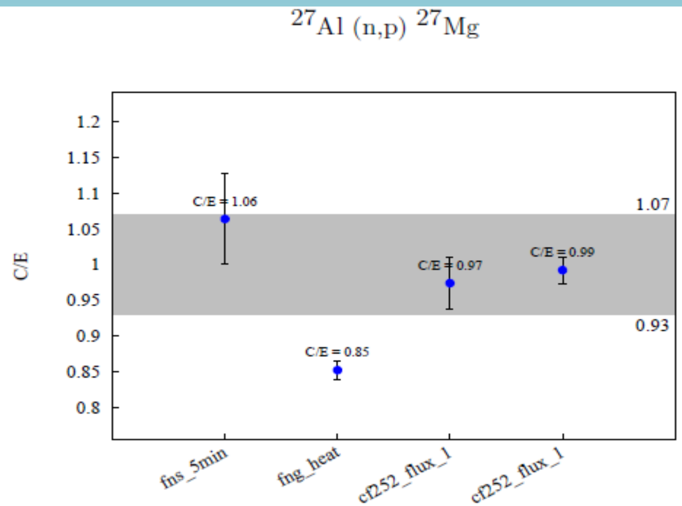

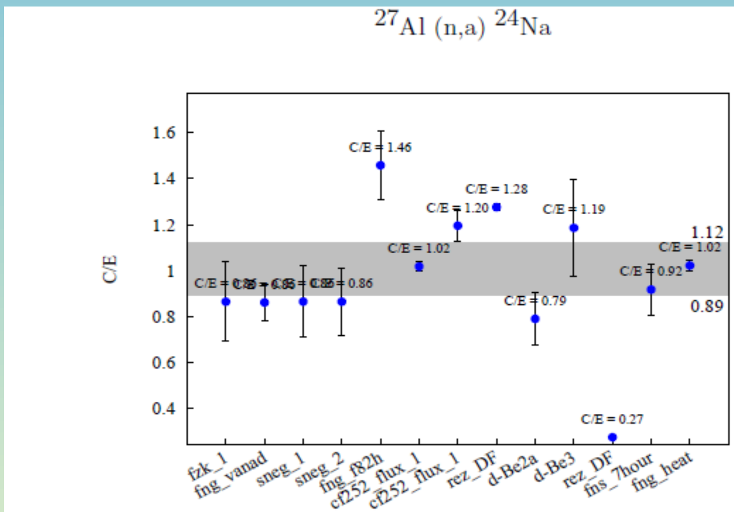

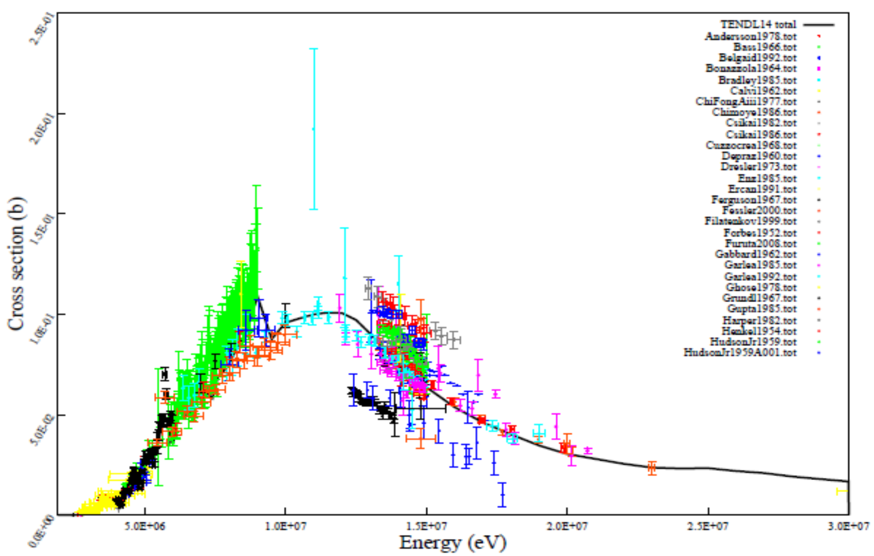

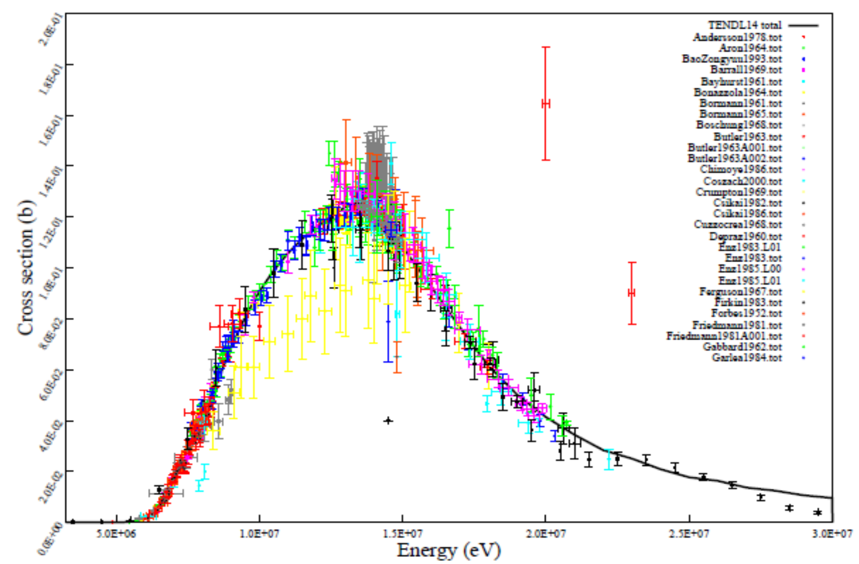

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Improvements of activation cross sections for fusion

- Dzysiuk and Koning F4E-GRT-168.02 Task 5.3 Progress Report, May 2016. Improve 42 important activation cross sections for TENDL.

Table 2. Integral Data

	Reaction	Spectrum	σ(b)	C/E (EAF)	C/E (TENDL 2012)	C/E (TENDL 2014)	C/E (TENDL 2016**)
1	$^{16}O(n,p)N^{16}$	fns_5min	3.23E-02	1.016	1.040	1.060	1.009*
2	$^{23}Na(n,p)Ne^{23}$	fns_5min	3.03E-02	1.190	1.189	1.190	1.163
3	$^{24}Mg(n,p)Na^{24}$	fns_5min	1.57E-01	1.165	1.000	–	0.984*
		cf252_flux_1	1.94E-03	1.347	1.238	–	1.107*
		cf252_flux_1	2.01E-03	1.300	1.283	–	1.068*
4	$^{32}S(n,t)P^{30}$	d-Be	4.13E-03	0.608	0.655	2.770	1.032
5	$^{34}S(n,\alpha)Si^{31}$	fns_5min	0.1160	1.019	1.019	0.940	1.001
6	$^{34}S(n,p)P^{34}$	fns_5min	0.0723	0.971	0.996	3.700	1.000
7	$^{37}Cl(n,p)S^{37}$	fns_5min	0.0179	1.368	0.871	0.970	0.971
8	$^{37}Cl(n,\alpha)P^{34}$	fns_5min	0.0275	0.980	1.305	0.940	1.011
9	$^{40}Ca(n,t)K^{38}$	d-Be	4.94E-03	0.338	0.571	–	1.007
10	$^{41}K(n,p)Ar^{41}$	fns_5min	3.63E-02	1.176	1.205	–	1.132

Etc.

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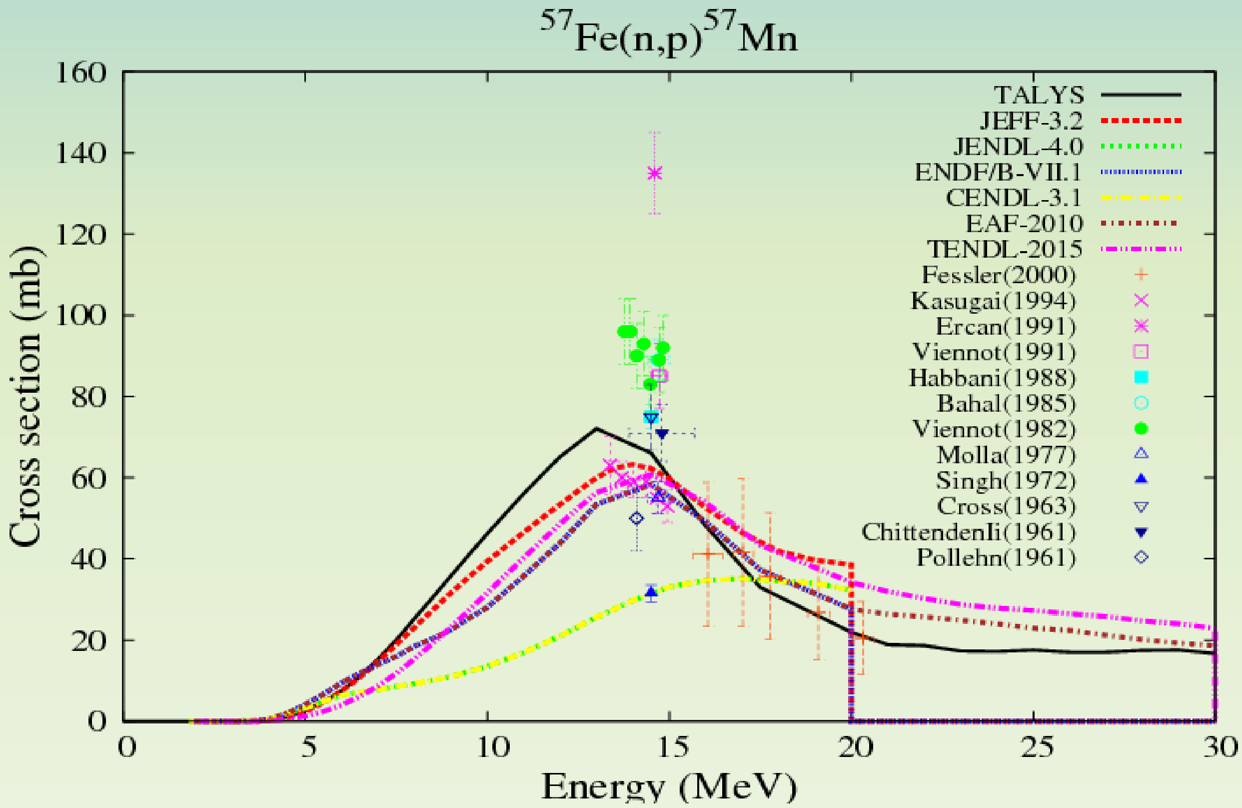
Improvements of activation cross sections for fusion

- Improve Koning's best set of TALYS parameters by carefully weighting experimental data



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Starting point: "Expert" (Gaussian) parameter uncertainties

(A.J. Koning and D. Rochman, ``Modern nuclear data evaluation with the TALYS code system'', Nucl. Data Sheets 113, 2841 (2012).) Origin: *Fingerspitzengefühl*

Parameter	uncertainty (%)	Parameter	uncertainty (%)
	Optical model		
r_V^n	2	d_1^n	10
a_V^n	2	d_2^n	10
v_1^n	2	d_3^n	10
v_2^n	3	r_{SO}^n	10
v_3^n	3	a_{SO}^n	10
v_4^n	5	v_{so1}^n	5
w_1^n	10	v_{so2}^n	10
w_2^n	10	w_{so1}^n	20
r_D^n	3	w_{so2}^n	20
a_D^n	4		
r_V^p	4	d_1^p	20
a_V^p	4	d_2^p	20
v_1^p	4	d_3^p	20
v_2^p	6	r_{SO}^p	20
v_3^p	6	a_{SO}^p	20
v_4^p	10	v_{so1}^p	10
w_1^p	20	v_{so2}^p	20
w_2^p	20	w_{so1}^p	40
r_D^p	6	w_{so2}^p	40
a_D^p	8	r_C^p	10
λ_V	5	λ_{V1}	5
λ_W	5	λ_{W1}	5
λ_{Vso}	5	λ_{Wso}	5

	Level density		
a	11.25-0.03125.A	σ^2	30
γ	30	δW	$\pm$ 1 MeV
α	30	β	30
R_σ	30	γ	30
E_0	20	E_M	20
T	10	δ	$\pm$ 2 MeV
K_{rot}	80		
C_{HFM}	30	δ_{HFM}	30
	Gamma-ray strength		
Γ_γ	20	$\sigma_{E\ell}$	20
$\Gamma_{E\ell}$	20	$E_{E\ell}$	10
$E_{\rm nor}$	20	$E_{\rm shift}$	$\pm$ 0.8 MeV
	Fission		
B_f	10	$\hbar\omega_f$	10
	Pre-equilibrium		
M^2	30	$R_{\pi\pi}$	30
$R_{\nu\pi}$	30	$R_{\pi\nu}$	30
$R_{\nu\nu}$	30	R_γ	50
g_ν	11.25-0.03125.A	$E_{\rm surf}$	20
g_π	11.25-0.03125.A	$C_{\rm break}$	80
$C_{\rm knock}$	80	$C_{\rm strip}$	80

Multiply these uncertainties by 5 and sample ~200 parameters from uniform distribution

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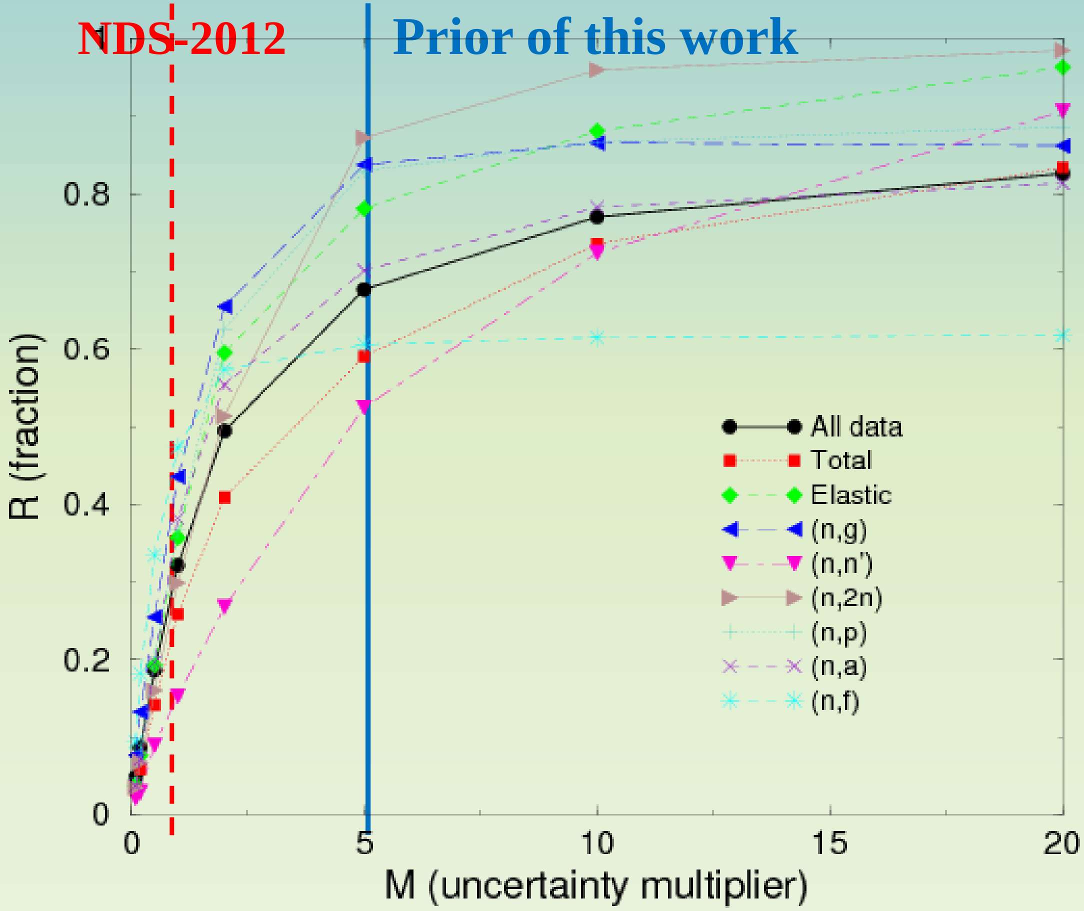
Fraction of EXFOR data inside 1-sigma uncertainty band



Random TALYS calculations for all nuclides compared with 23490 experimental data sets = 2.7 million data points

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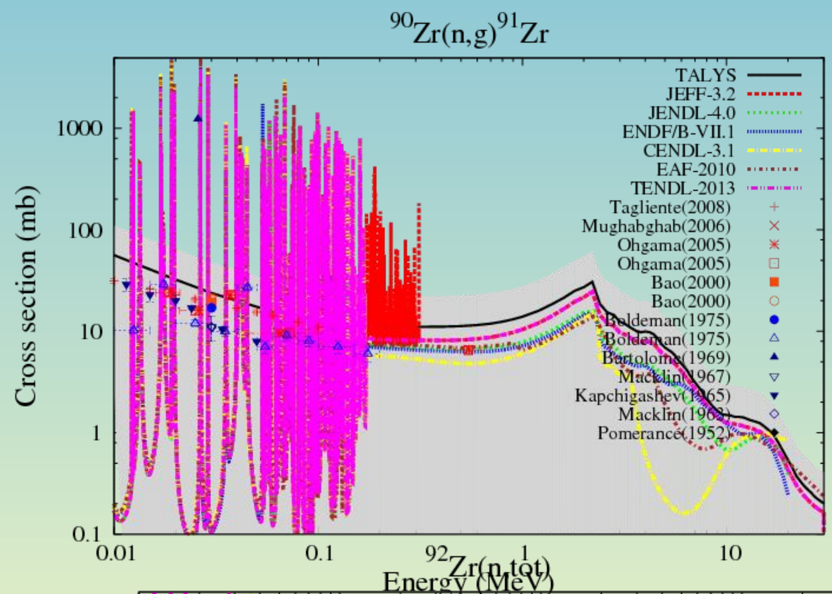
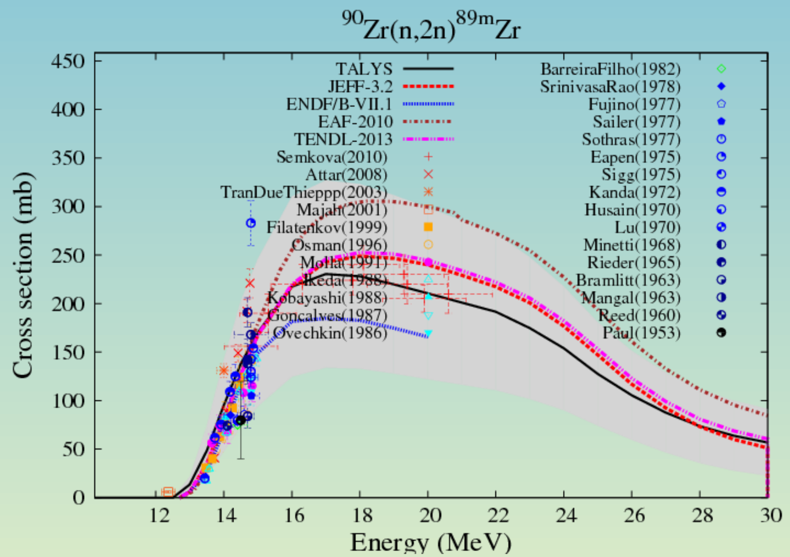
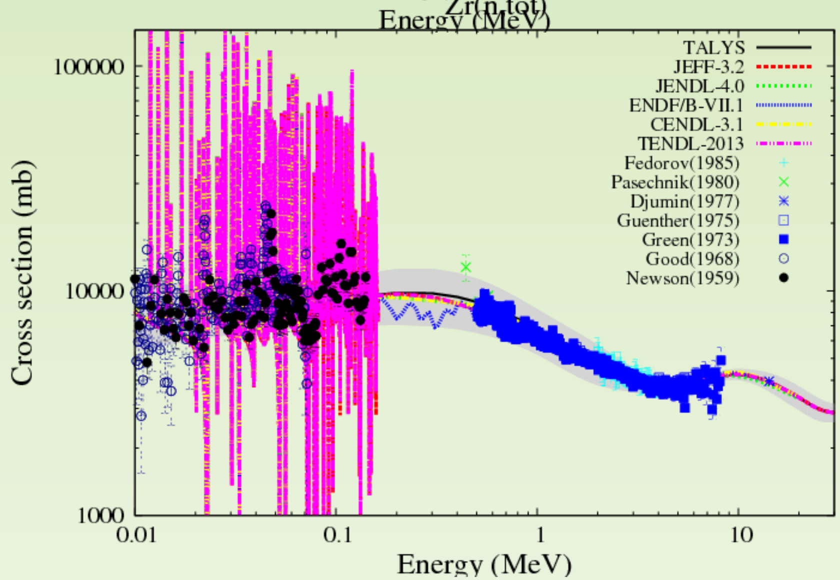
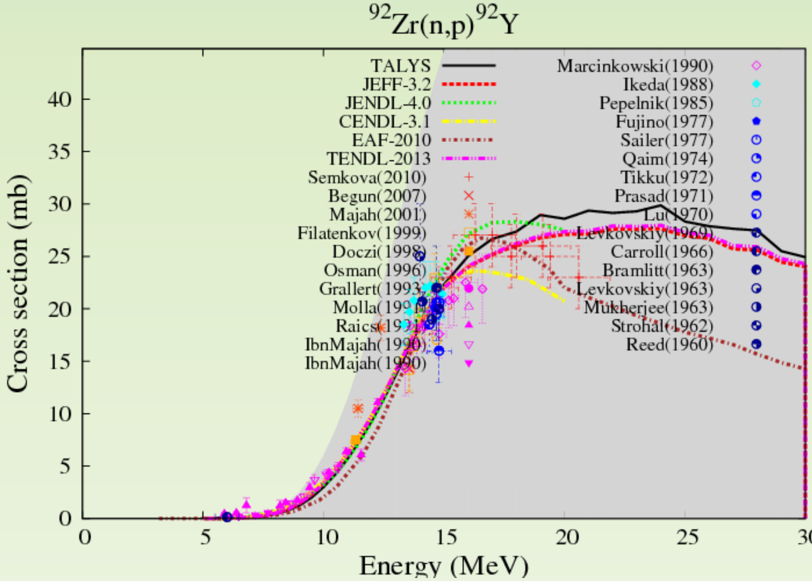
“Knowing nothing”: Random TALYS parameters from initial parameter pdf: uniform distribution with uncertainty multiplier = 5









Initial probability distribution for cross sections

- **Perform 1 global, unadjusted TALYS calculation for the entire periodic table of elements**
- **Compare the results with all EXFOR data: 23490 experimental data sets = 2.7 million data points**
- **Determine the average deviation between TALYS and experiment.**
- **Use the results as knowledge ("pseudo-experimental data") in a Bayesian Monte Carlo updating scheme.**

- **A.J. Koning, "Bayesian Monte Carlo method for nuclear data evaluation", EPJ A51(12), p1-16 (2015)**

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19

TALYS predictive power

Table 7. Global cross section uncertainties per reaction channel from default TALYS calculations; average deviation and parameters for energy-dependent variation, see eq. (20).

Reaction	$s^{glob}_{c,ave}$ in %	$s^{glob}_{c,min}$ in %	a	b	c	d	E_{cent}
(n, tot)	6	8	0.6	0.3	0	12	6
(n, el)	10	12	0.6	0.3	0	12	6
(n, non)	10	12	0.6	0.3	0	12	6
(n, inl)	50	12	1	1	1	12	5
(n, γ)	62	40	0.6	0.3	0	20	20
(n, 2n)	25	24	1	1	1	15	6
(n, 3n)	150	40	1	1	1	12	6
(n, f)	110	50	1	1	1	12	6
(n, p)	53	34	1	1	1	12	6
(n, α)	120	45	1	1	1	12	6

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Energy dependent predictive power

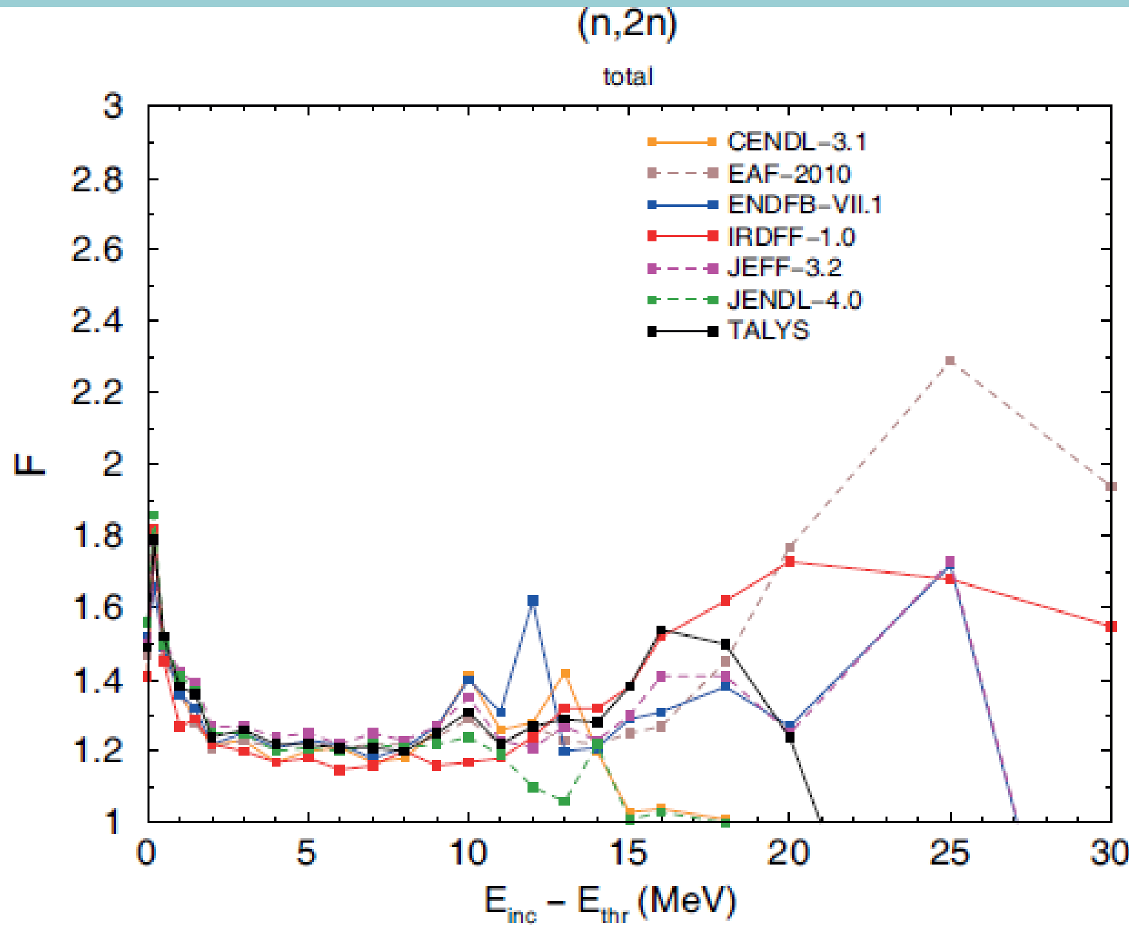

Fig. 3. Energy dependent deviation of all calculated (n, 2n) cross sections compared to the values in EXFOR. For reference, also the values for other world libraries are given.

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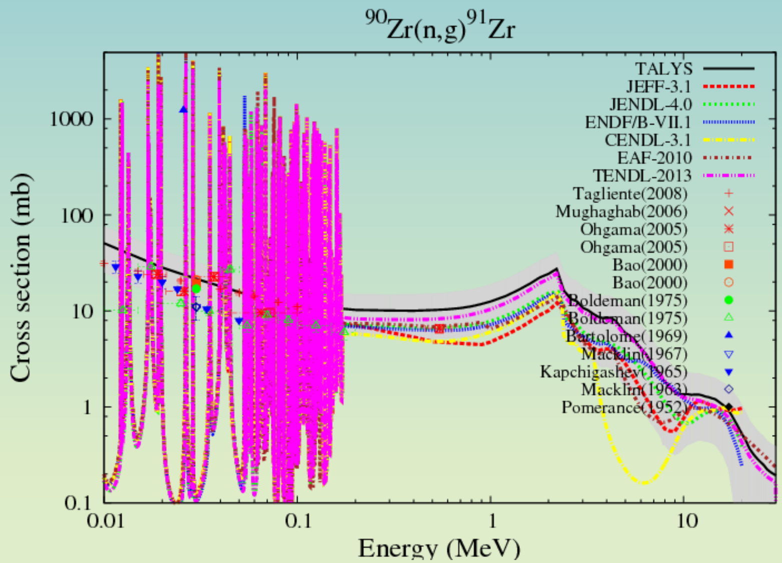
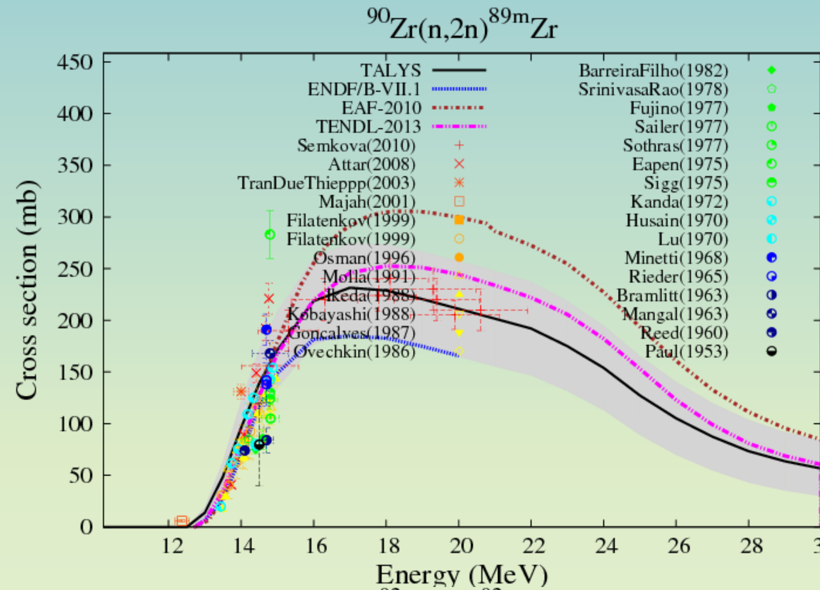
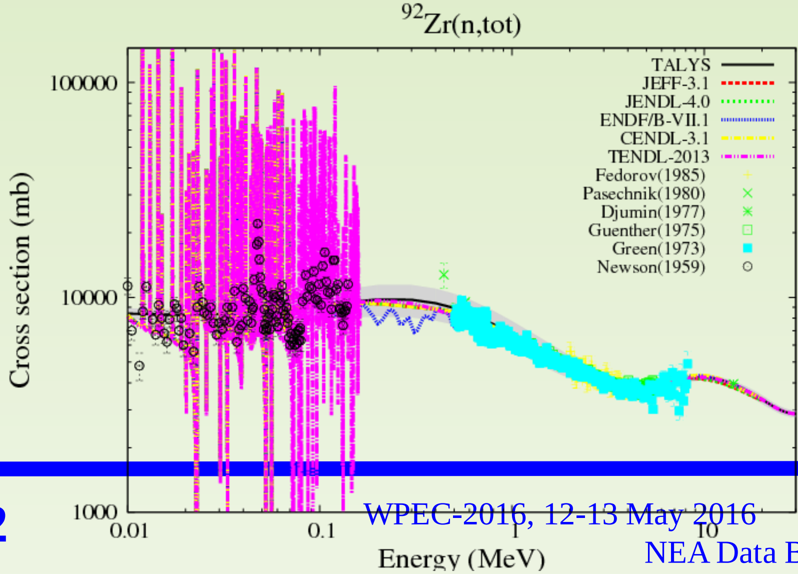
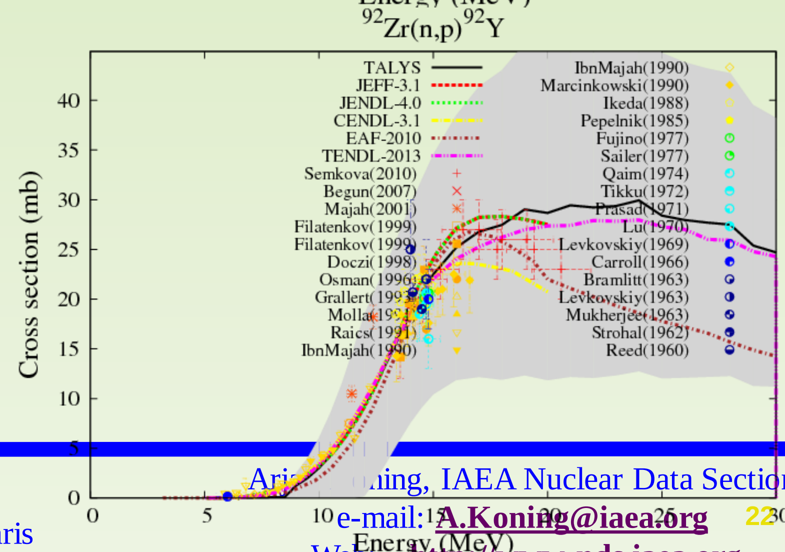
Initial probability distributions for cross sections

Starting point: global TALYS central values and uncertainties based on cross sections for all nuclides









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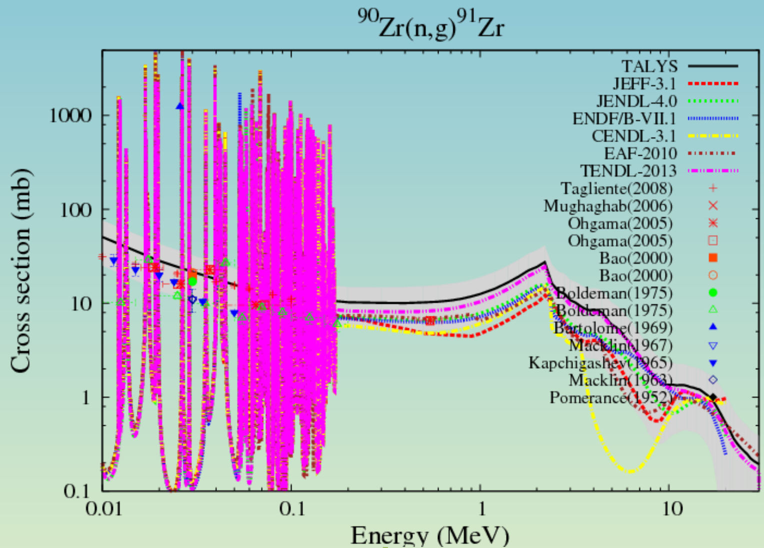
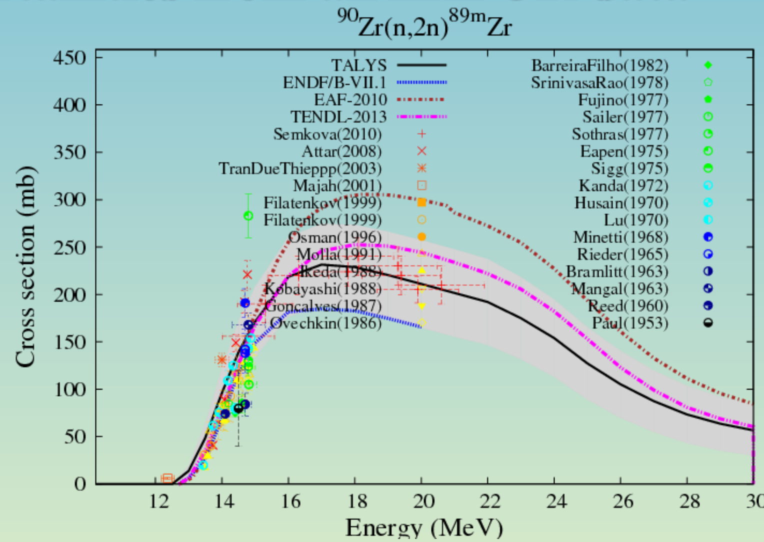
Zooming in

Prior: Global TALYS – uncertainties from all EXFOR data

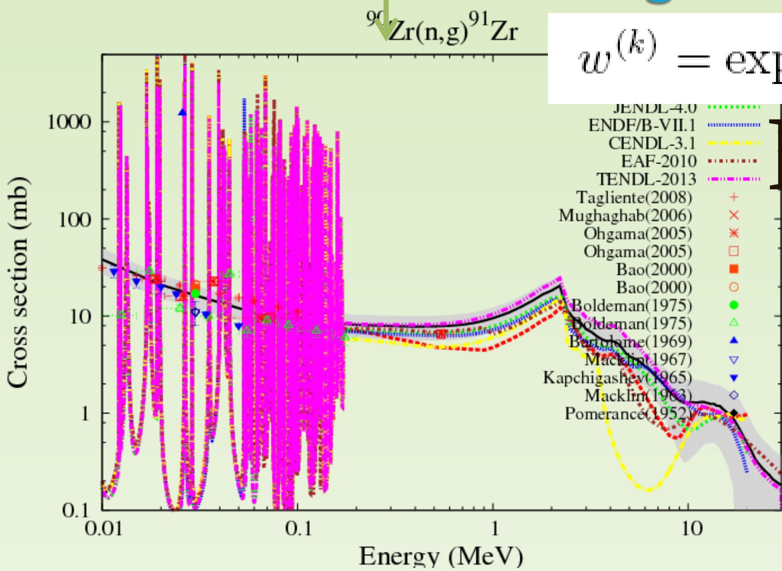


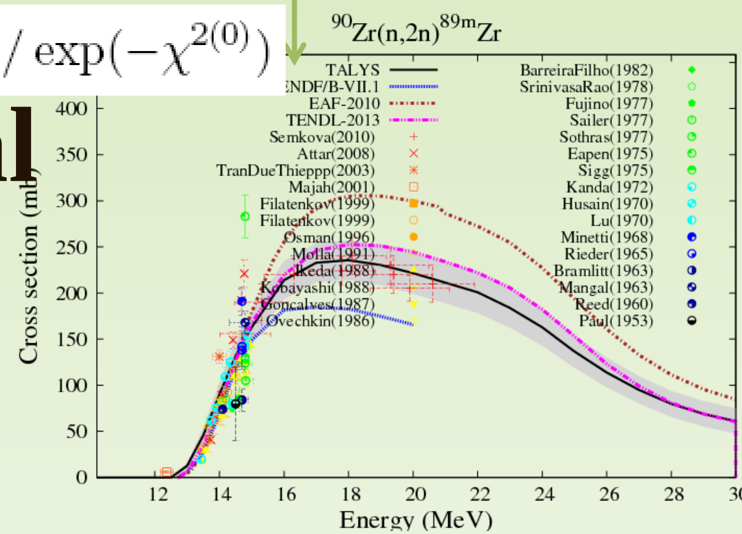


Use weights based on EXFOR for ^{90}Zr

$$w^{(k)} = \exp(-\chi^{2(k)}) / \exp(-\chi^{2(0)})$$

Final





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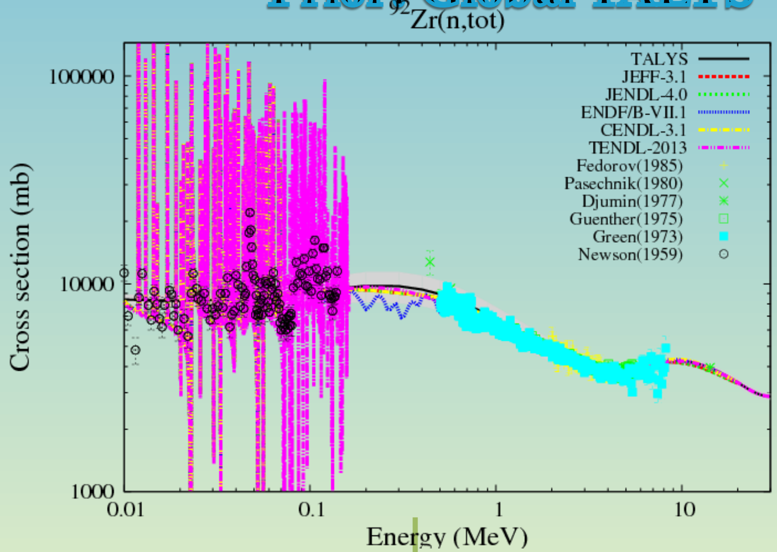
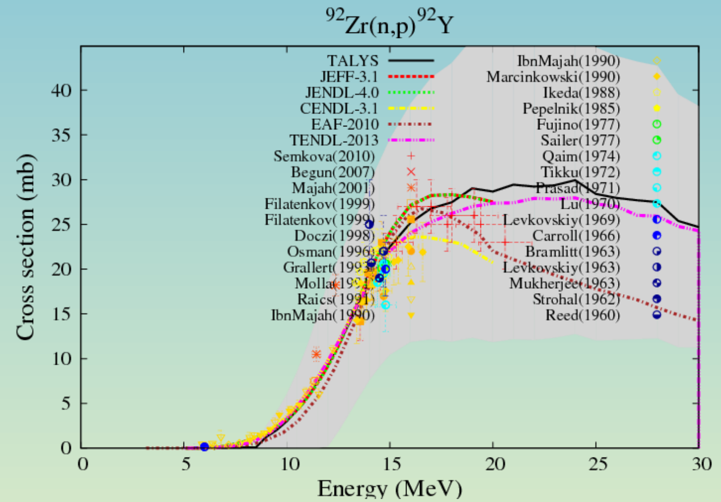
Zooming in

Prior: Global TALYS – uncertainties from all EXFOR data

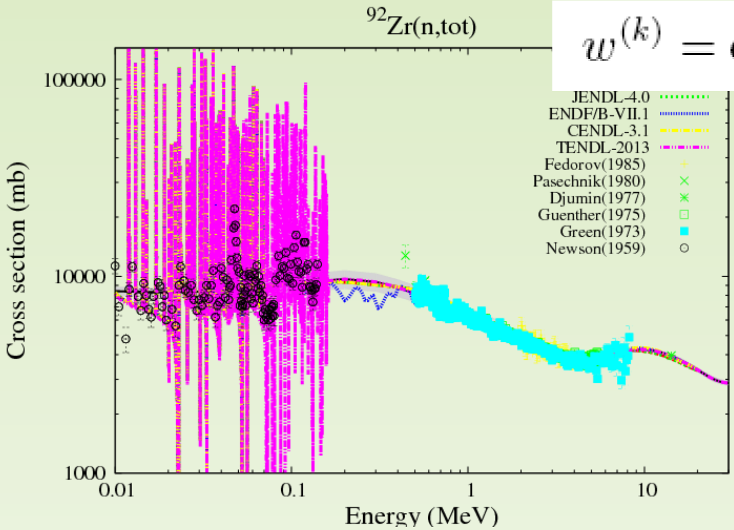


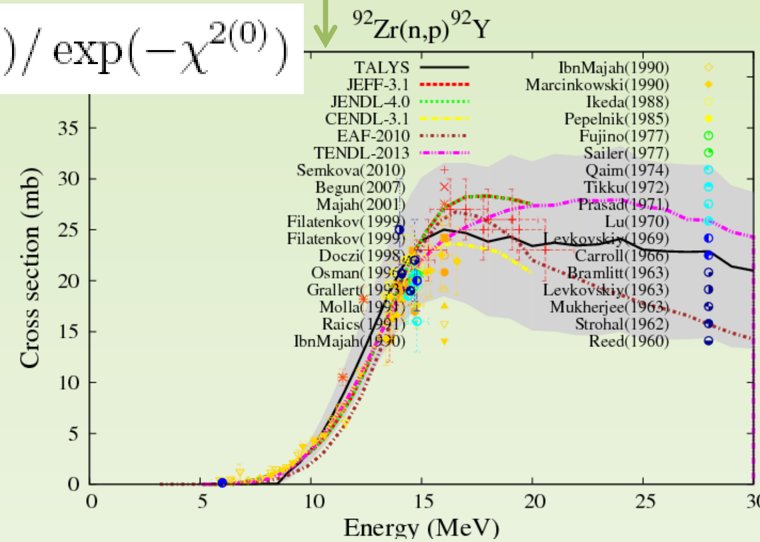


Use weights based on EXFOR for ^{90}Zr

$$w^{(k)} = \exp(-\chi^{2(k)}) / \exp(-\chi^{2(0)})$$

Final





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Towards TALYS-2.0

- Full rewrite in Fortran-90/95/03/08:
  - Work already underway.
- Integration of TASMAN:
  - Statistics, optimization (parameter search), sensitivities, covariances, and Total Monte Carlo
- Integration of TEFAL:
  - Complete ENDF-6 formatting from MF1 to MF40
- Latest current version: TALYS-1.8 (2015):
  - Pointwise resonance data (Atlas++ and PREPRO routines)
  - Full integration of GEF (Schmidt and Jurado) for FY, nubar, PFNS, PFGS etc.
  - Implementation of Avrigeanu models for alpha OMP and deuteron break-up
- TALYS-2.0: Now that I have done it all, I know how I should have done it, so let’s do that: even more modular all-in-one package.

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Conclusions

- **Emphasis for TENDL now equally on differential development and integral testing.**
- **New "best" TALYS input files for each isotope, based on comparison with experimental data: thermal, RI, MACS, all other EXFOR data and integral activation measurements.**
- **Optimization continues until comparison with (differential and integral) experiments is at least as good as other libraries: again, after 2015 more nuclides fall in this category. (Note that a TENDL isotopic file is always more complete than any other library, measurement or no measurement). This process goes from less important (easy) to important (challenging) nuclides.**
- **Completeness (MF1-40) and processibility (PREPRO, NJOY): no real competitor left.**
- **TENDL keen to adopt (essential parts of) CIELO nuclides.**
- **TENDL team now scattered over more places, but aims to continue.**

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26