Status of TENDL: TENDL-2013 and 2014

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NRG Petten

The Netherlands

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WPEC meeting
NEA Data Bank

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- **General philosophy of TENDL**
- **TENDL-2013:**
  - General trends
  - Integral testing
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  - Zooming in on particular nuclides
- **Some final thoughts: TALYS, comparison with other libraries**
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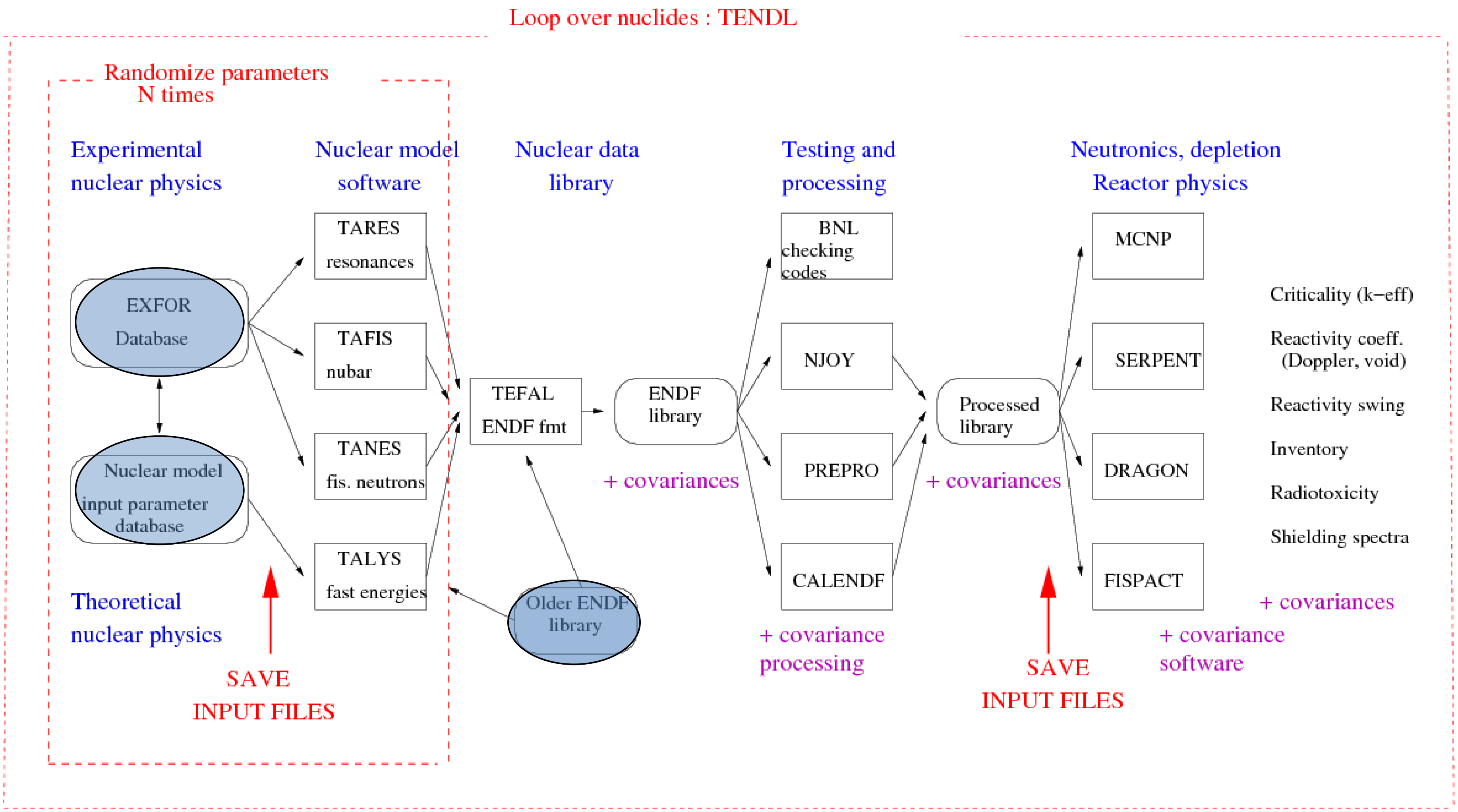
TENDL nuclear data library



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

TALYS Evaluated Nuclear Data Library: TENDL-2013

- Neutron, proton, deuteron, triton, Helium-3, alpha and gamma data libraries.
- 2626 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-1.60 and TARES (resonances)

which are overruled by

Adjusted TALYS calculations (340 input files) and Resonance Atlas-based TARES calculations

which are overruled by

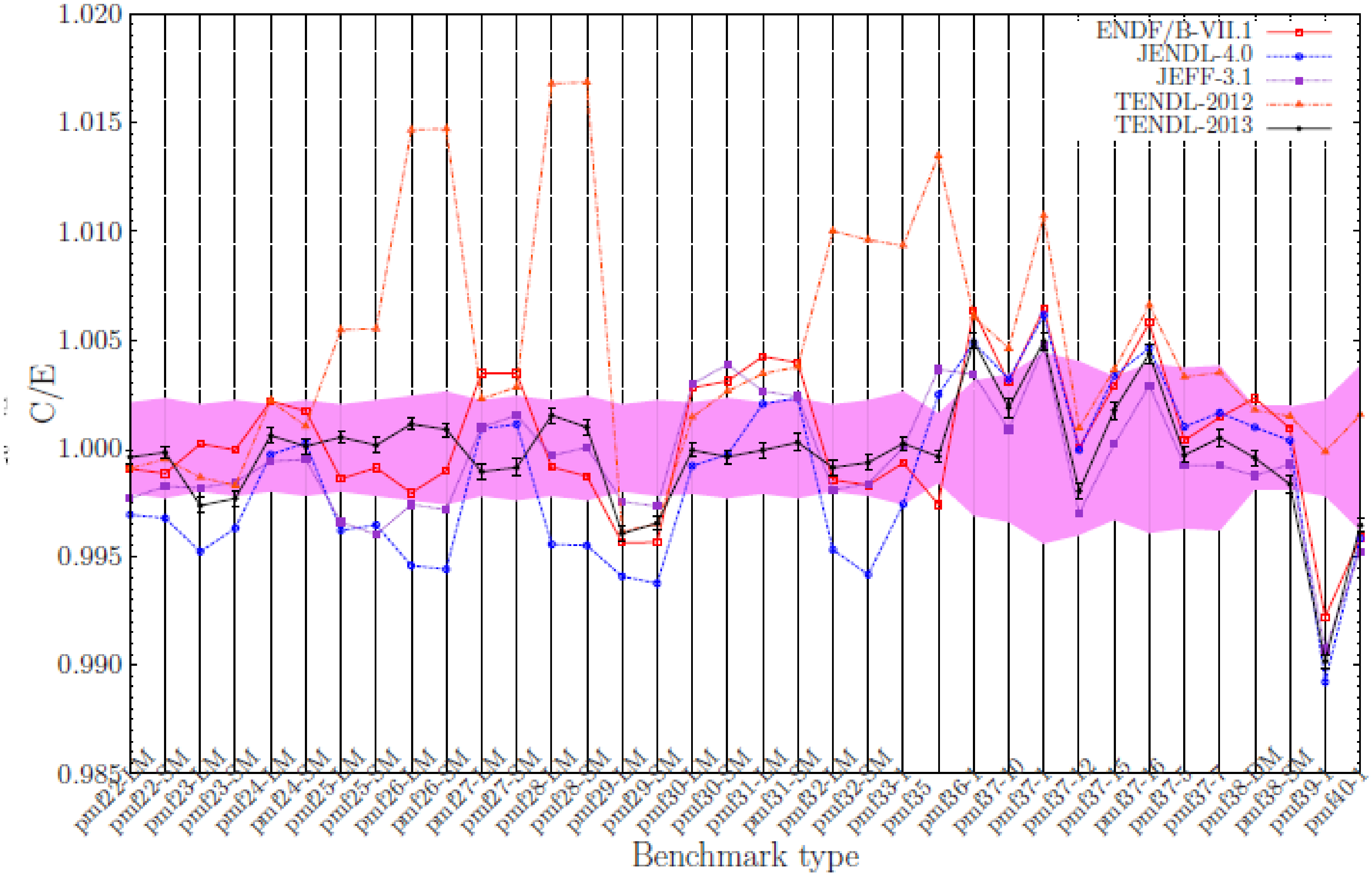
TALYS-normalization to ~200 (experimental) evaluated reaction channels from other libraries (e.g. IRDFF, light nuclides, main channels of "big 3")

Integral activation validation for Fusion for Energy

Preliminary work obtained by adjusting TALYS parameters and using the above mentioned references.

reaction	Spectrum	C/E EAF-2010	C/E TENDL-2014
^{48}Ca(n,2n)	fns_7hour	0.88	1.08
^{45}Sc(n,2n)	fns_5min	1.07	0.95
	fns_ScSmGd	1.63	1.45
^{90m}Zr(n,p)	fns_heat5	1.2	1.2
	Cf252_flux1	1.37	1.15
^{94}Zr(n,p)	fns_5min	1.03	1.00
^{124m}Sn(n,2n)	fns_5min	1.15	1.04
	fns_Sn	0.88	0.88
^{150}Sm(n,p)	fng_ScSmGd	1.24	0.92
^{158}Gd(n,p)	fng_ScSmGd	1.17	0.90
^{158}Gd(n,γ)	fng_ScSmGd	2.00	1.34
^{156}Dy(n,2n)	fng_Dy	1.12	1.08

TENDL-2013 for fast Pu benchmarks



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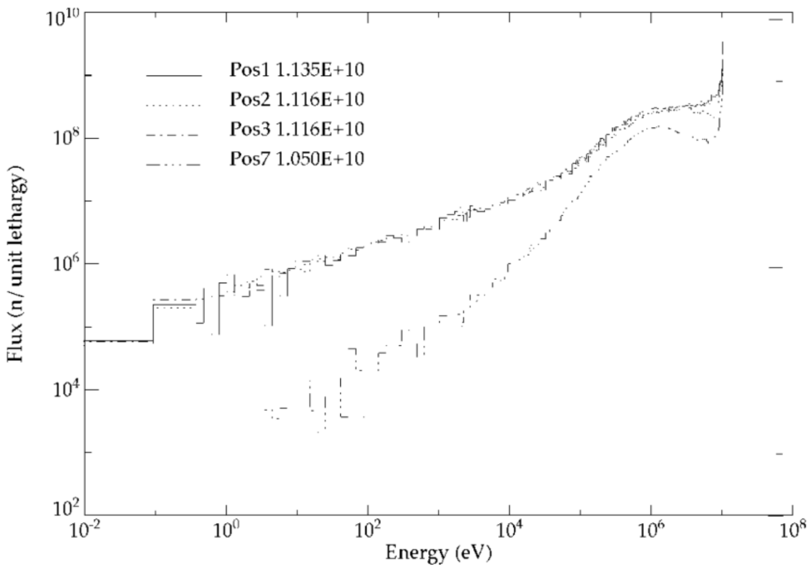
JAEA FNS Assembly; decay heat

14 MeV neutrons are generated by a 2 mA deuteron beam impinging on a stationary tritium bearing titanium target; Fusion Neutron Source

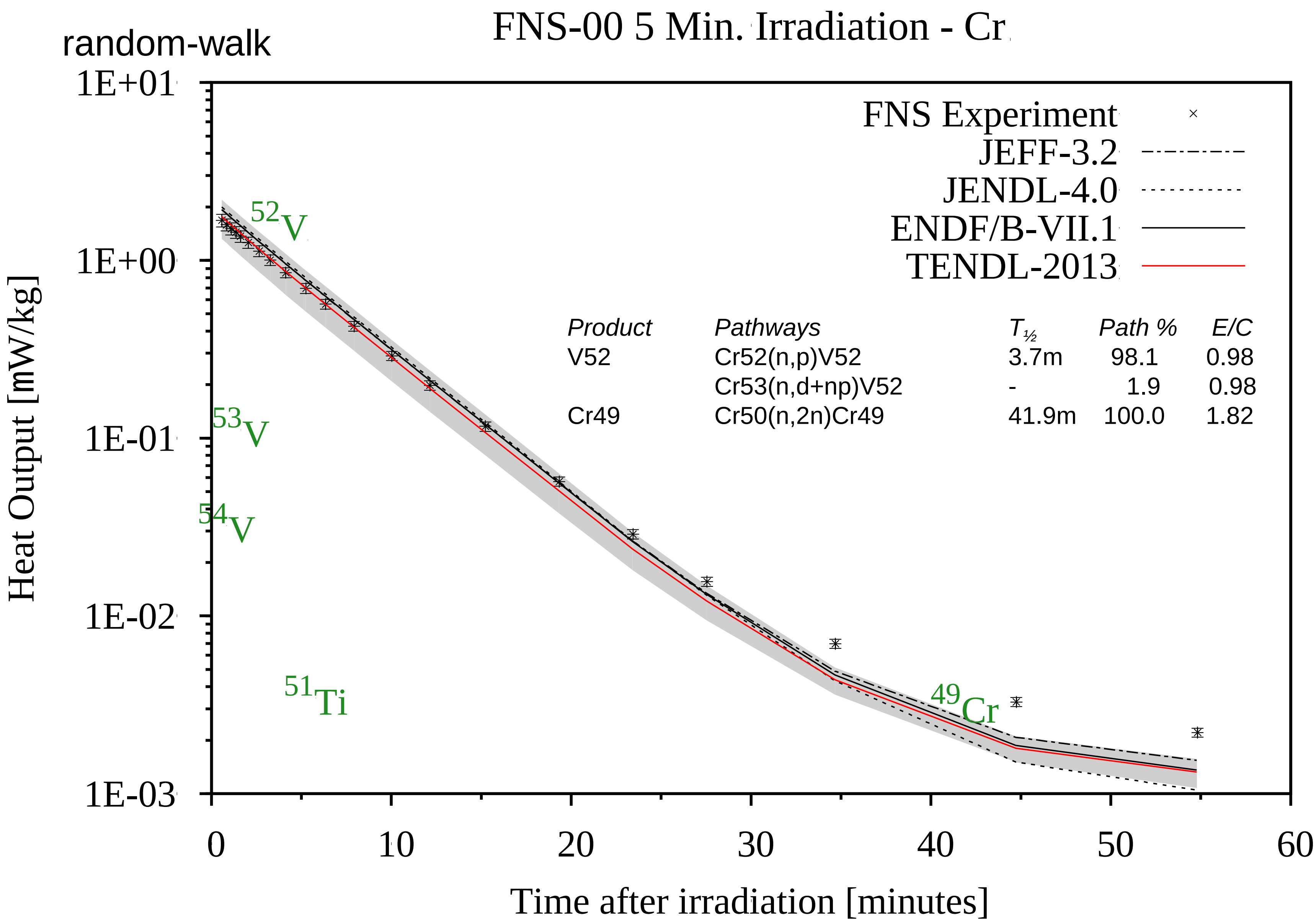


FNS Neutron spectra, neutron fluence monitored by ^{27}Al(n,a)Na^{24}

Two experimental campaigns:
1996 and 2000; 74 materials

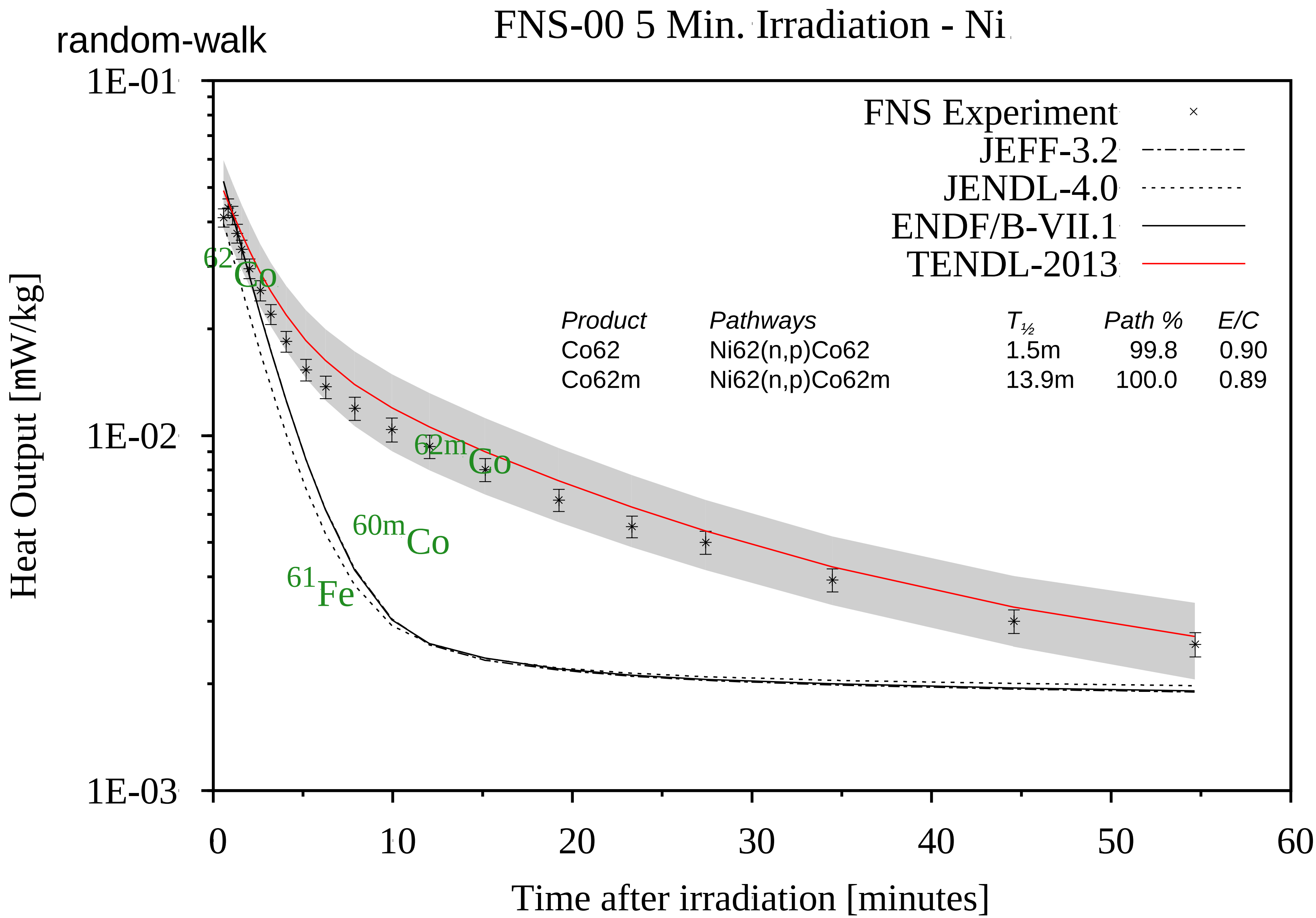
Z	Element	Form	Z	Element	Form
9	F	CF2	49	In	Metallic Foil
11	Na	Na2CO3	50	Sn	SnO2
12	Mg	MgO	51	Sb	Metallic Powder
13	Al	Metallic Foil	52	Te	TeO2
14	Si	Metallic Powder	53	I	IC6H4OH
15	P	P3N5	55	Cs	Cs2CO3
16	S	Powder	56	Ba	BaCO3
17	Cl	C2H2Cl2	57	La	La2O3
19	K	K2CO3	58	Ce	CeO2
20	Ca	CaO	59	Pr	Pr6O11
21	Sc	Sc2O3	60	Nd	Nd2O3
22	Ti	Metallic Foil	62	Sm	Sm2O3
23	V	Metallic Foil	63	Eu	Eu2O3
24	Cr	Metallic Powder	64	Gd	Gd2O3
25	Mn	Metallic Powder	65	Tb	Tb4O7
26	Fe	Metallic Foil	66	Dy	Dy2O3
27	Co	Metallic Foil	67	Ho	Ho2O3
28	Ni	Metallic Foil	68	Er	Er2O3
29	Cu	Metallic Foil	69	Tm	Tm2O3
30	Zn	Metallic Foil	70	Yb	Yb2O3
31	Ga	Ga2O3	71	Lu	Lu2O3
32	Ge	GeO2	72	Hf	Metallic Powder
33	As	As2O3	73	Ta	Metallic Foil
34	Se	Metallic Powder	74	W	Metallic Foil
35	Br	BrC6H4COOH	75	Re	Metallic Powder
37	Rb	Rb2CO3	76	Os	Metallic Powder
38	Sr	SrCO3	77	Ir	Metallic Powder
39	Y	Y2O3	78	Pt	Metallic Foil
40	Zr	Metallic Foil	79	Au	Metallic Foil
41	Nb	Metallic Foil	89	Hg	HgO
42	Mo	Metallic Foil	81	Tl	Tl_2O
44	Ru	Metallic Powder	82	Pb	Metallic Foil
45	Rh	Metallic Powder	83	Bi	Metallic Powder
46	Pd	Metallic Foil	Alloy	SS-304	Metallic Foil
47	Ag	Metallic Foil	Alloy	SS-316	Metallic Foil
48	Cd	Metallic Foil	Alloy	NiCr	Metallic Foil
49	In	Metallic Foil	Alloy	Inc600	Metallic Foil

Decay power: FNS JAERI Cr



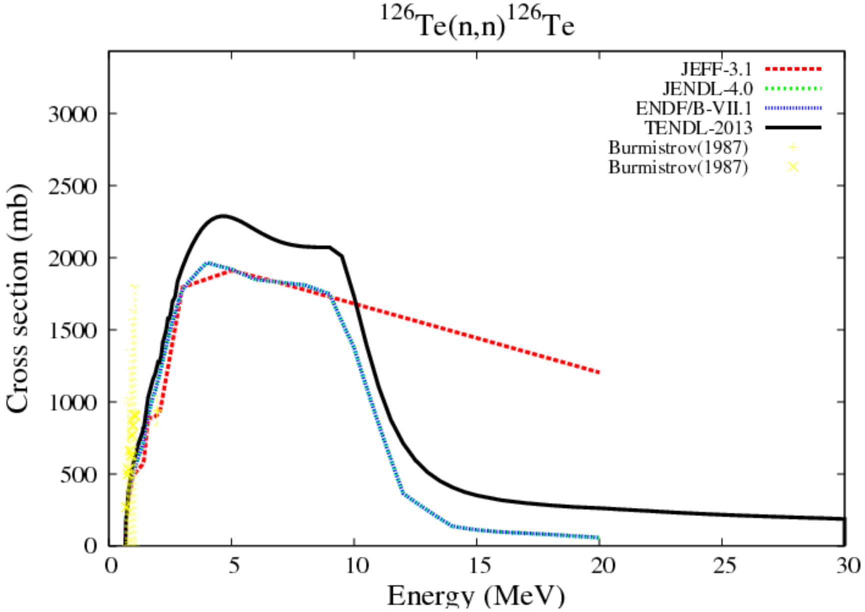
Product	*Pathways*	$T_{½}$	*Path %*	*E/C*
V52	Cr52(n,p)V52	3.7m	98.1	0.98
	Cr53(n,d+np)V52	-	1.9	0.98
Cr49	Cr50(n,2n)Cr49	41.9m	100.0	1.82

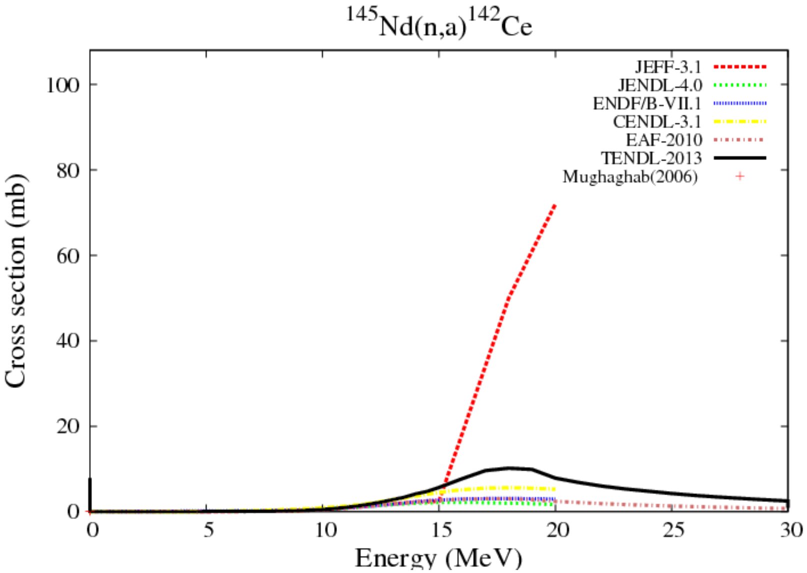
Decay power: FNS JAERI Ni

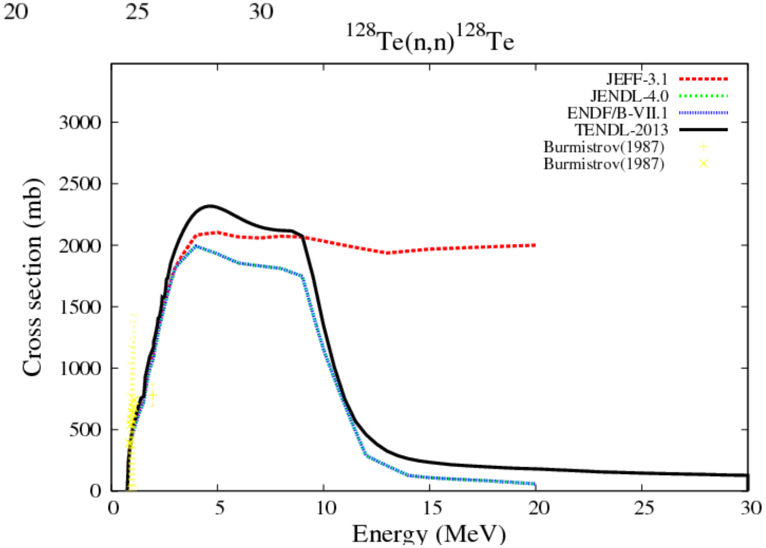


Further cleaning of JEFF

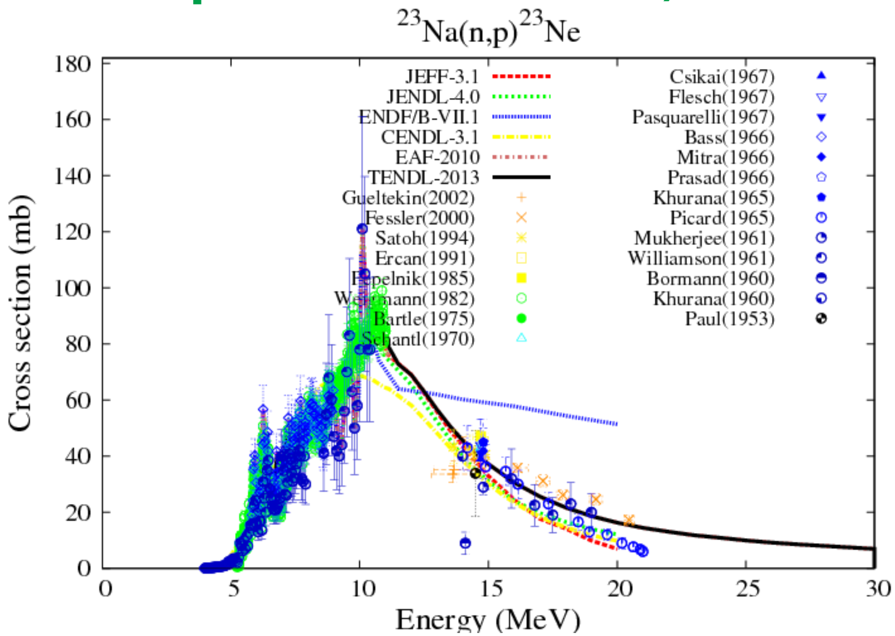
- **JEFF-3.2: 472 isotopes, 151 are from TENDL-2012**
- **More "clear" candidates for replacement, Te, Nd, etc.**

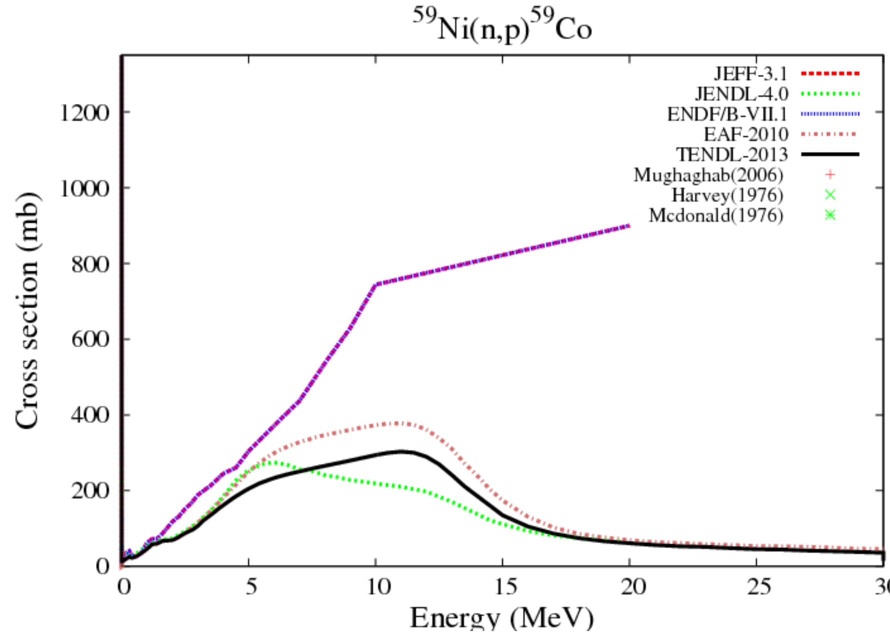


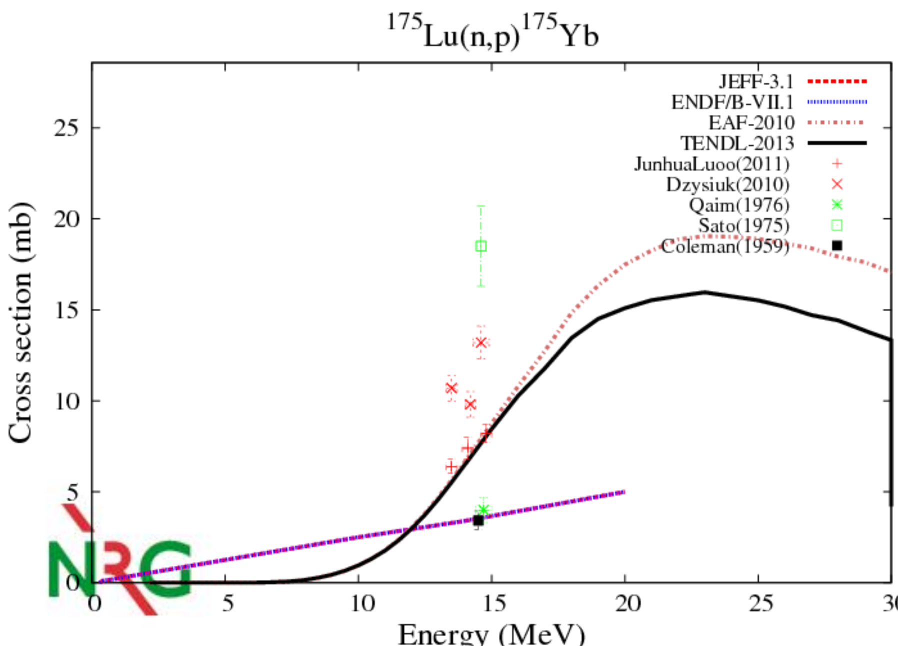


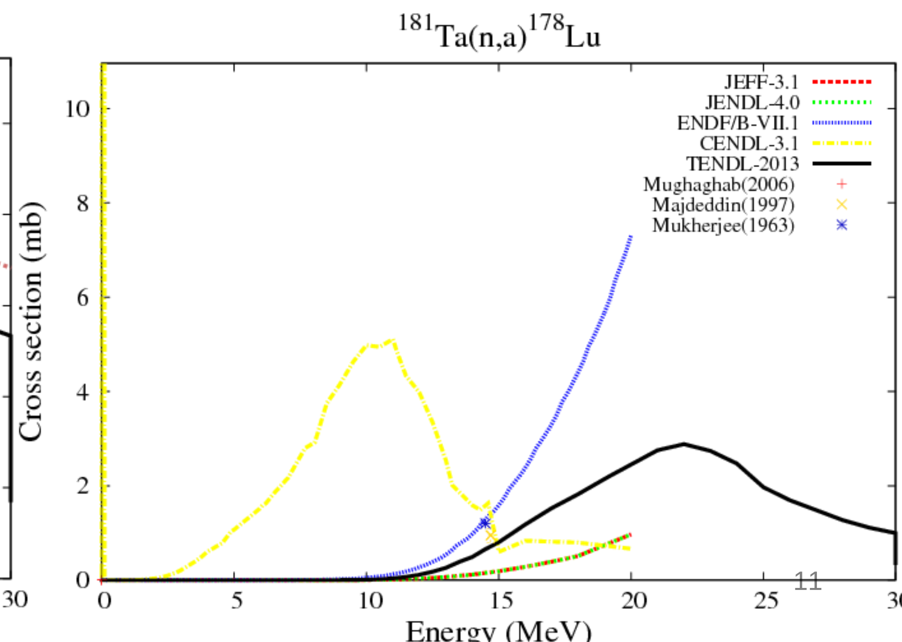


To compensate for JEFF, some suspicious plots of other libraries









Bayesian Monte Carlo:
Initial probability distribution for cross sections

- **Perform a global, unadjusted TALYS calculation for the entire periodic table of elements**
- **Compare the results with all EXFOR data**

Reaction	All	Reaction	Number	Reaction	Number	Reaction	Number
Composite	5791	Total	4493	Elastic	1118	Non-elastic	425
(n,γ)	5699	(n,γ) (tot)	4932	(n,γ)g	287	(n,γ)m	480
(n,f)	1259						
(n,n')	579	(n,n') (tot)	303	(n,n')g	7	(n,n')m	269
(n,n'$_k$)	1162	(n,n'$_1$)	517	(n,n'$_2$)	160	(n,n'$_3$)	64
(n,2n)	2866	(n,2n) (tot)	1677	(n,2n)g	402	(n,2n)m	787
(n,p)	2561	(n,p) (tot)	1878	(n,p)g	219	(n,p)m	464
(n,α)	1400	(n,α) (tot)	1081	(n,α)g	96	(n,α)m	223
part prod	515	(n,xn)	20	(n,xp)	94	(n,xα)	181
Other	665	(n,3n)	127	(n,nα)	83	(n,np)	116
Total	23490	= 2,7 million data points (Thanks Viktor, Naohiko and Emmeric!)					

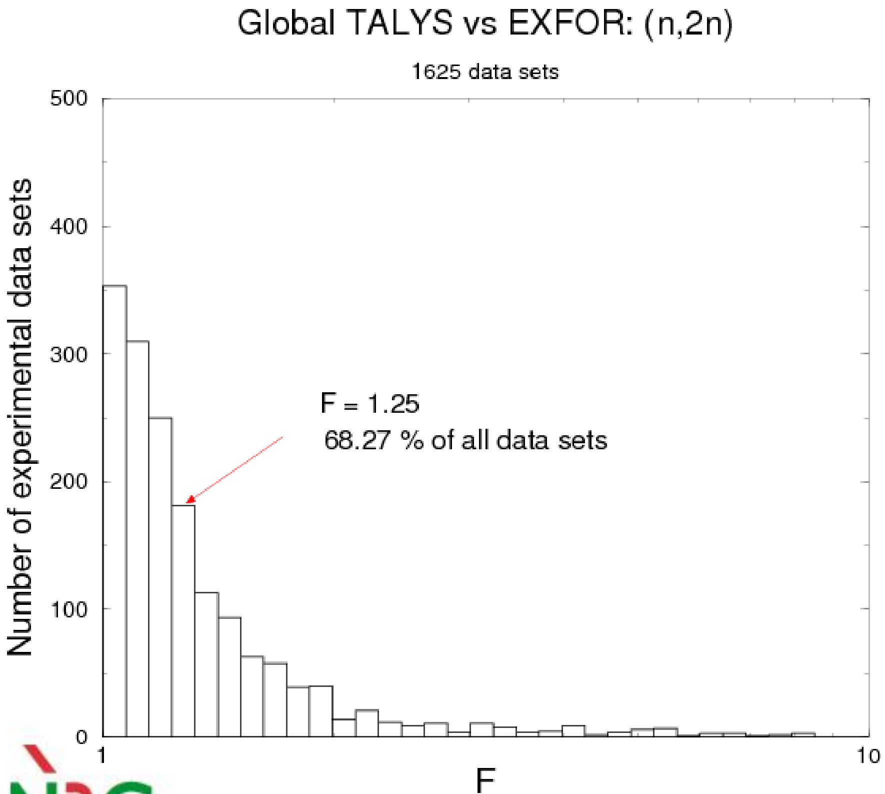
Table 1: Total number of neutron-induced *cross section* subentries available in XC4 format.

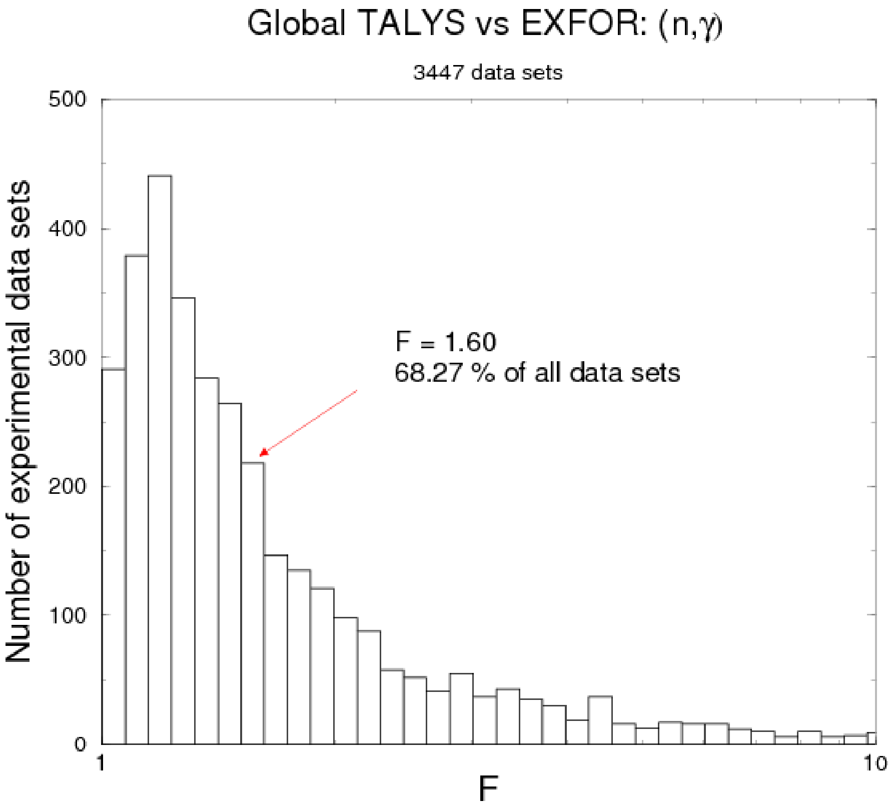
Initial probability distribution for cross sections

- **Use F-factor for each experimental data set:**

$$F = 10^{\sqrt{\frac{1}{N}\sum_{i}^{N}\left(\log\frac{\sigma_T^i}{\sigma_E^i}\right)^2}}$$

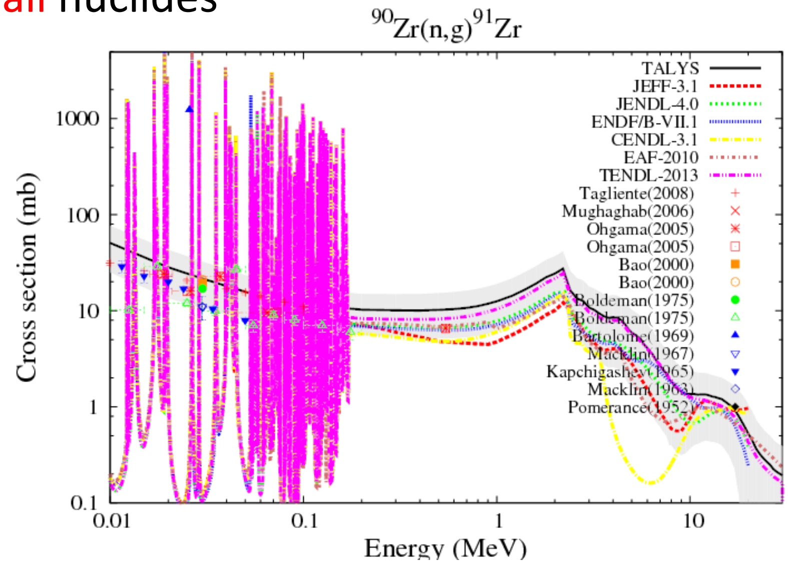
WPEC SG-30 on quality assessment of EXFOR

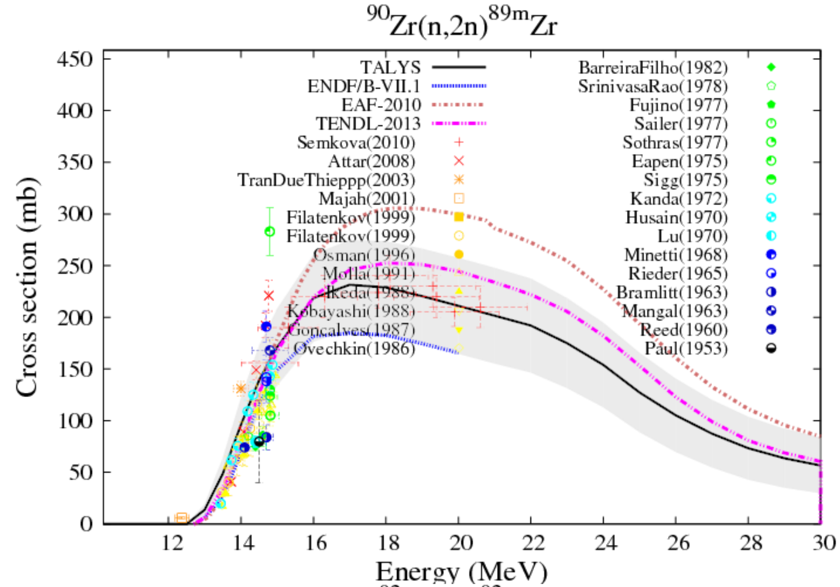


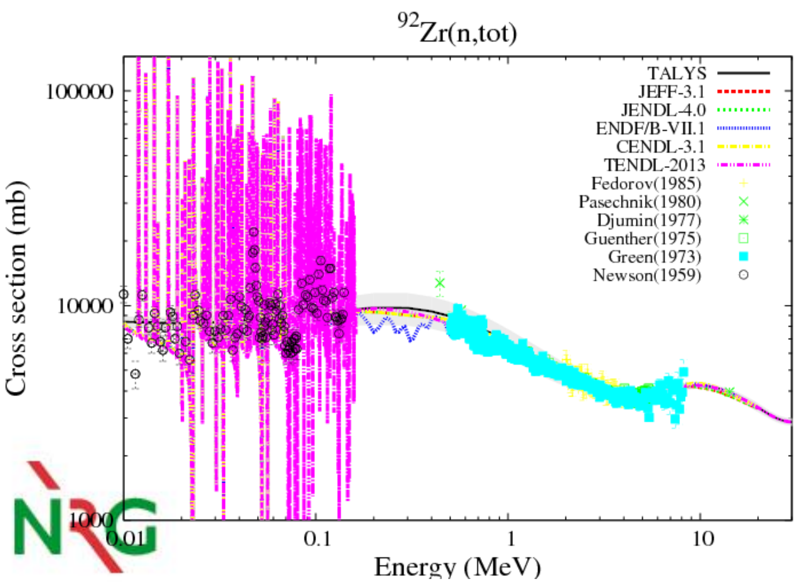


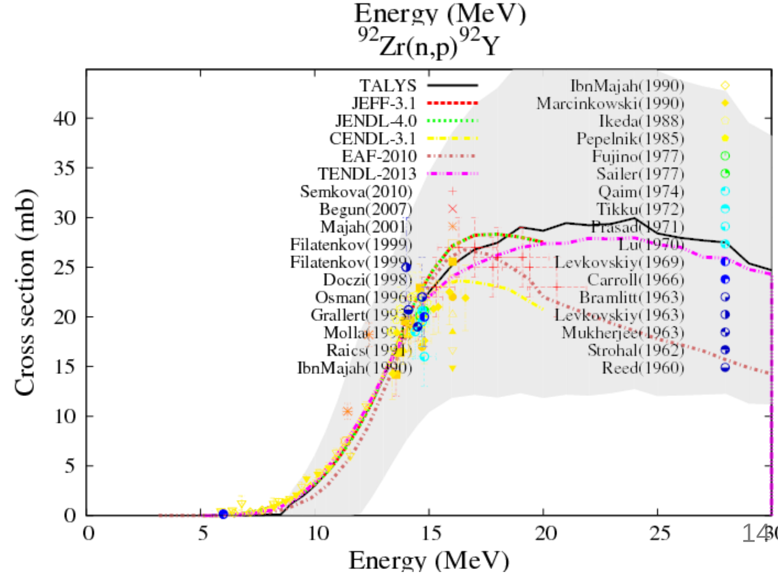
Prior probability distributions for cross sections

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









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

Create new parameter distributions using weights based on EXFOR

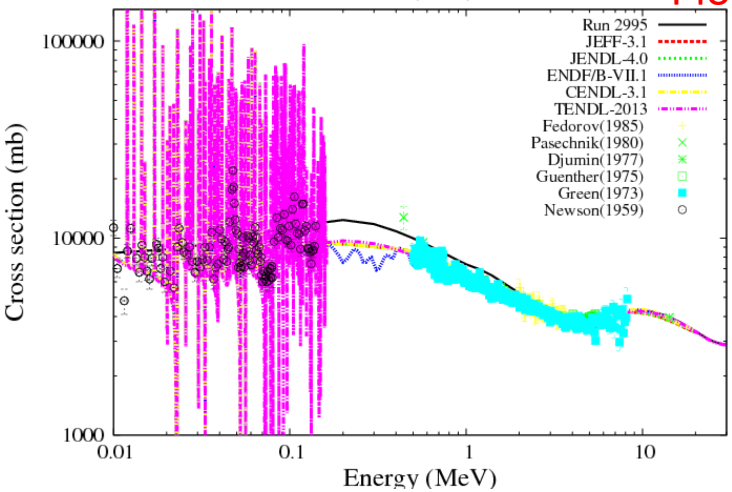
Each random data set k has a weight

Bauge: BFMC, Capote-Trkov: UMC-B

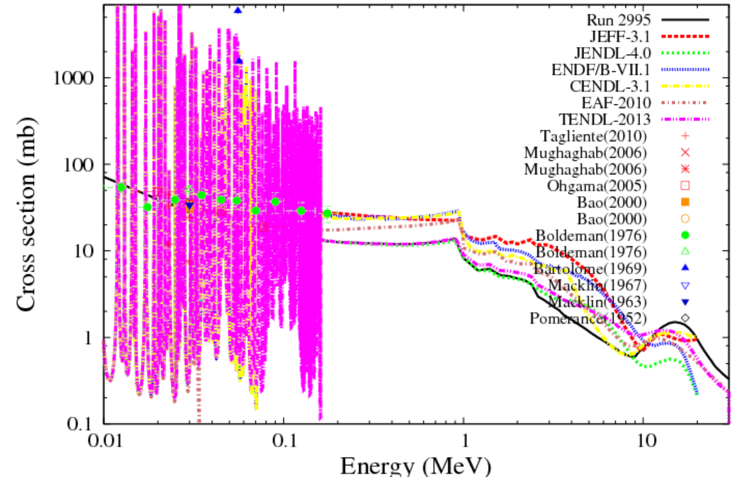
$$w^{(k)} = \exp(-\chi^{2(k)}) / \exp(-\chi^{2(0)})$$

Plots: Random run 2995

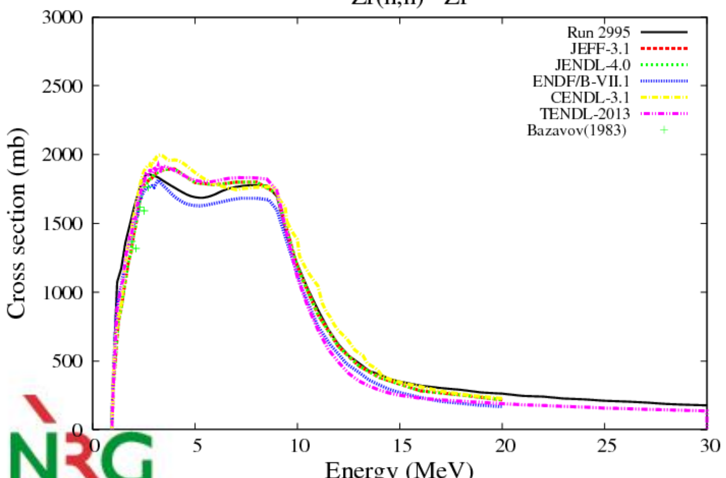
^{92}Zr(n,tot)



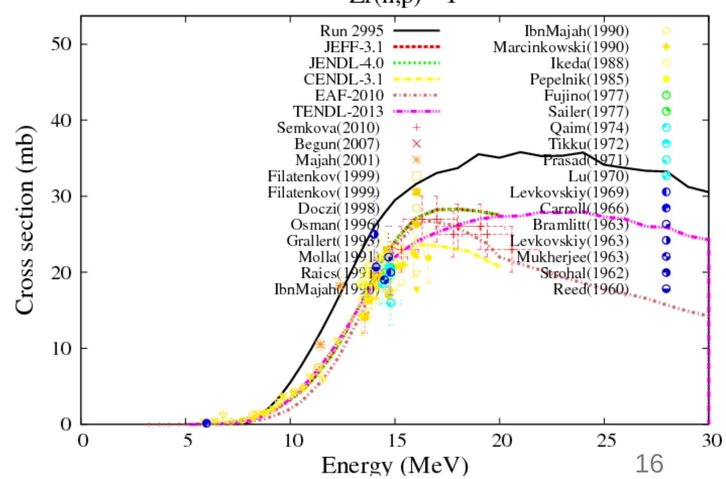
^{92}Zr(n,g)^{93}Zr



^{92}Zr(n,n)^{92}Zr

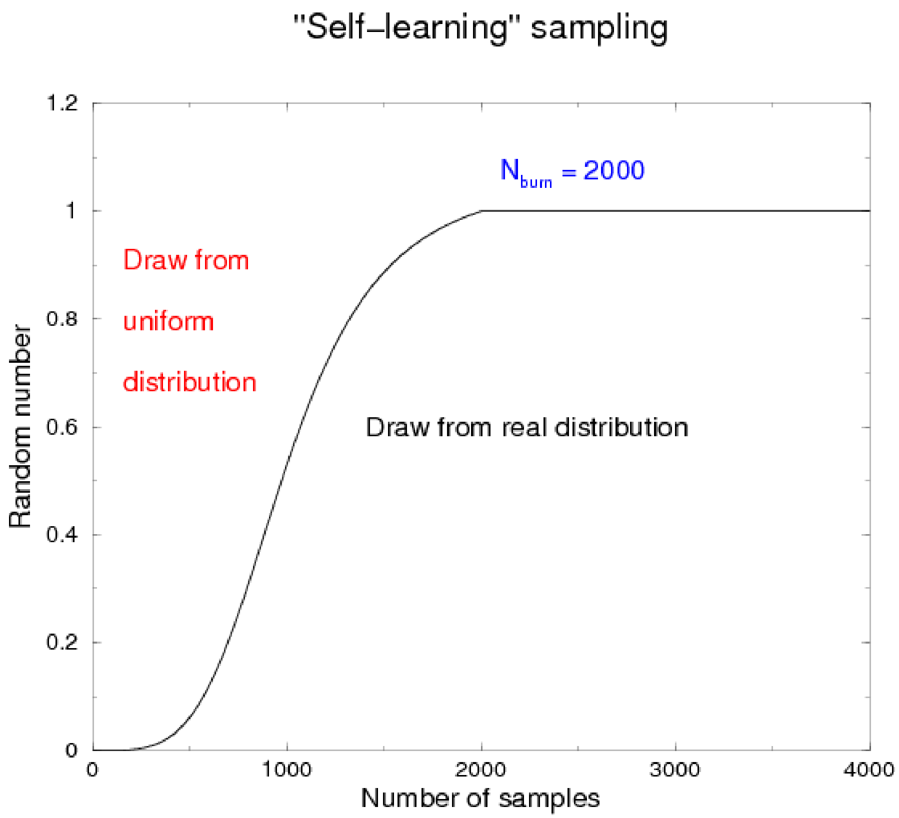


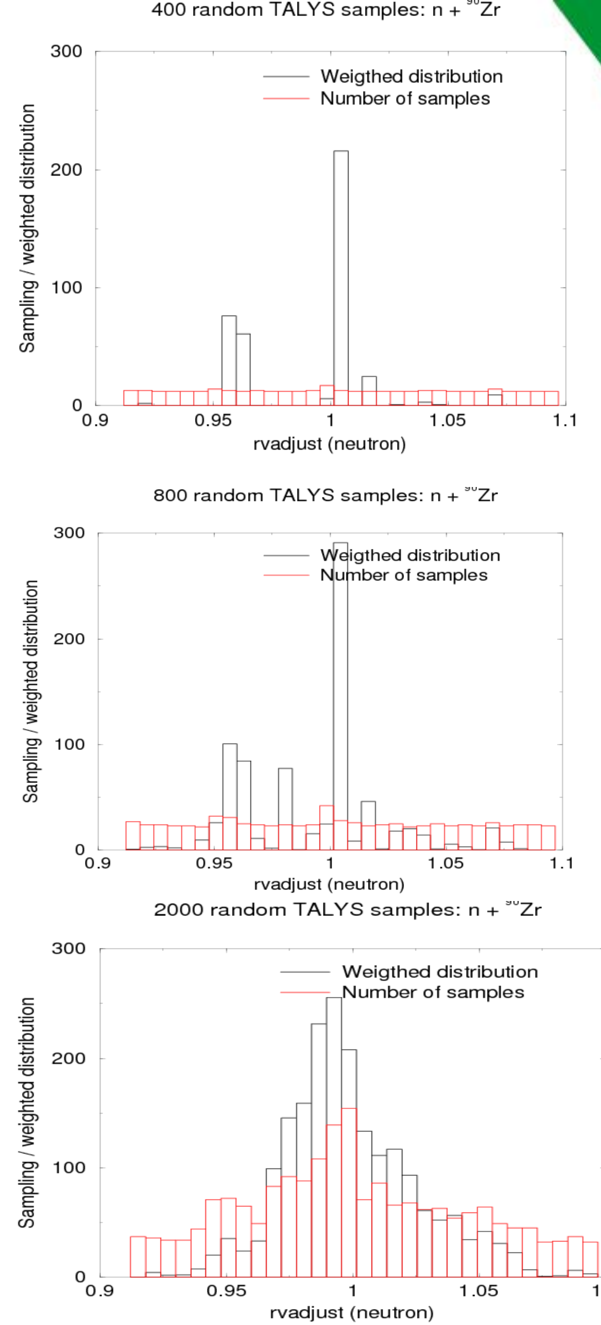
^{92}Zr(n,p)^{92}Y



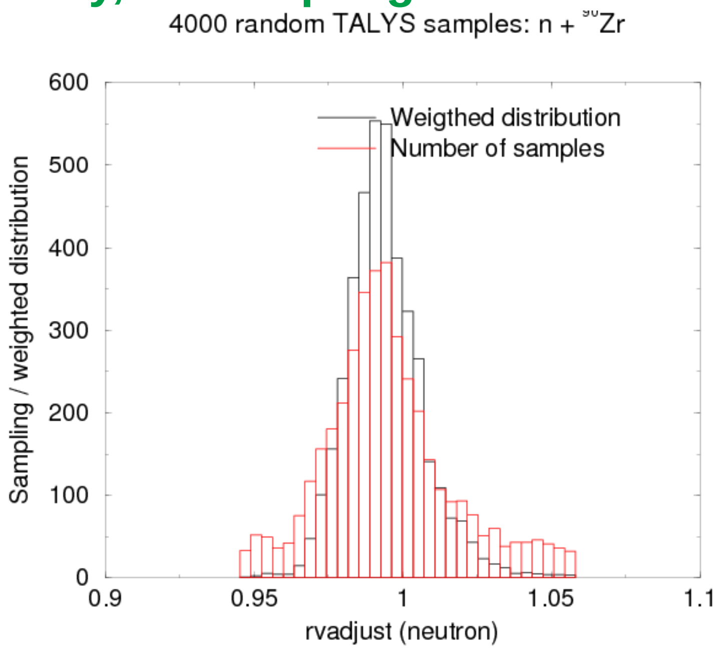
Create new parameter distributions using weights based on EXFOR

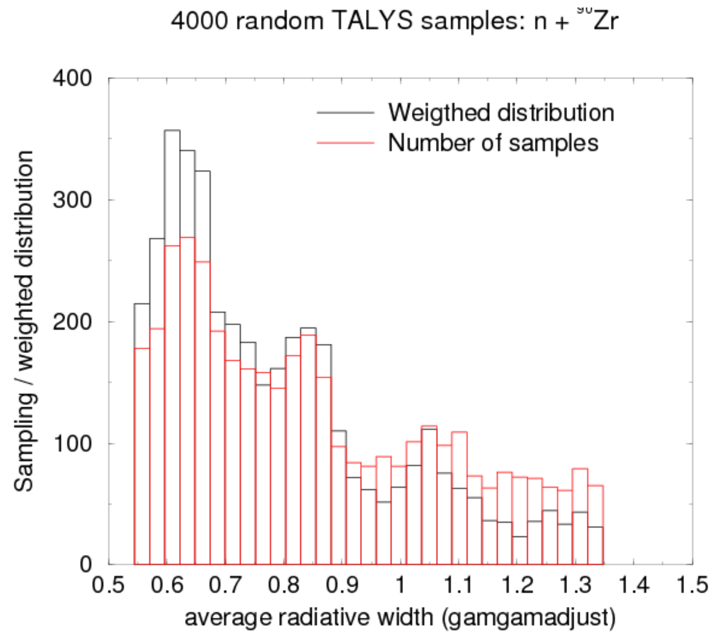
Assign the weight $w^{(k)}$ of random data set k to all TALYS parameters of that run

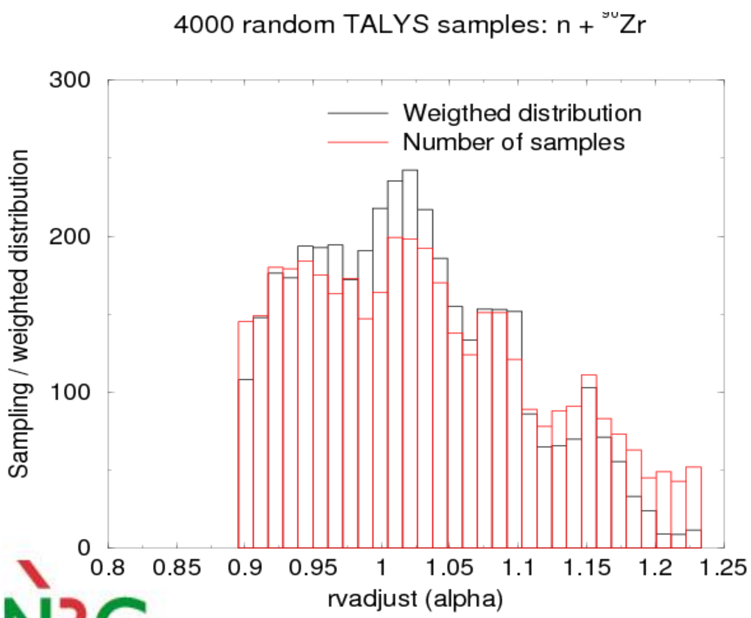


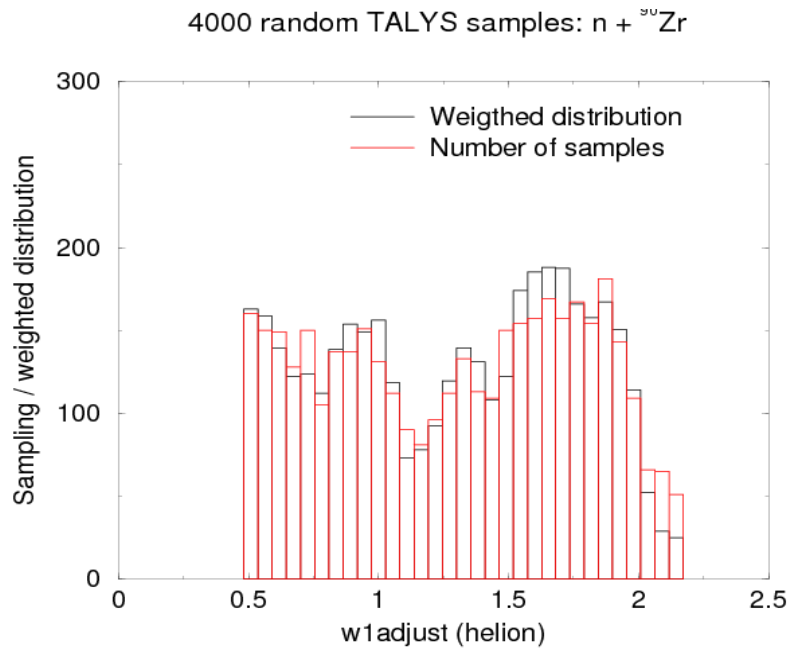


Finally, all sampling is done from the real weighted parameter distributions









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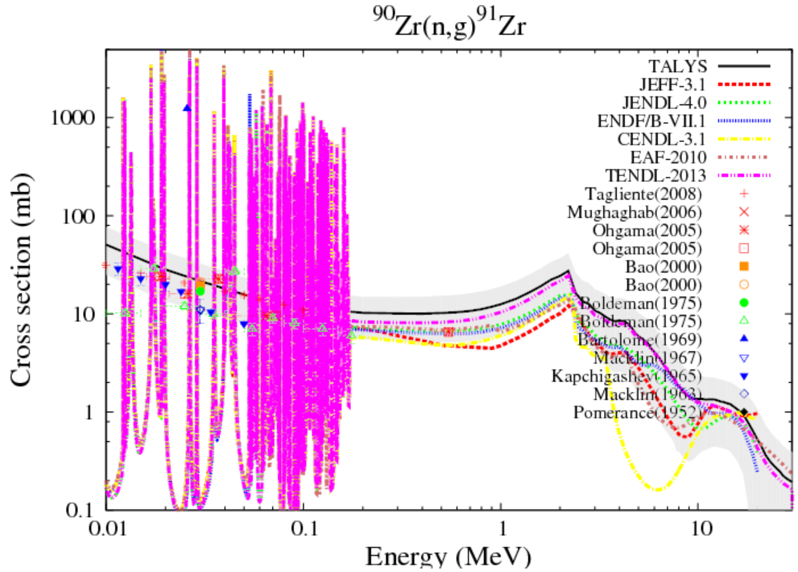
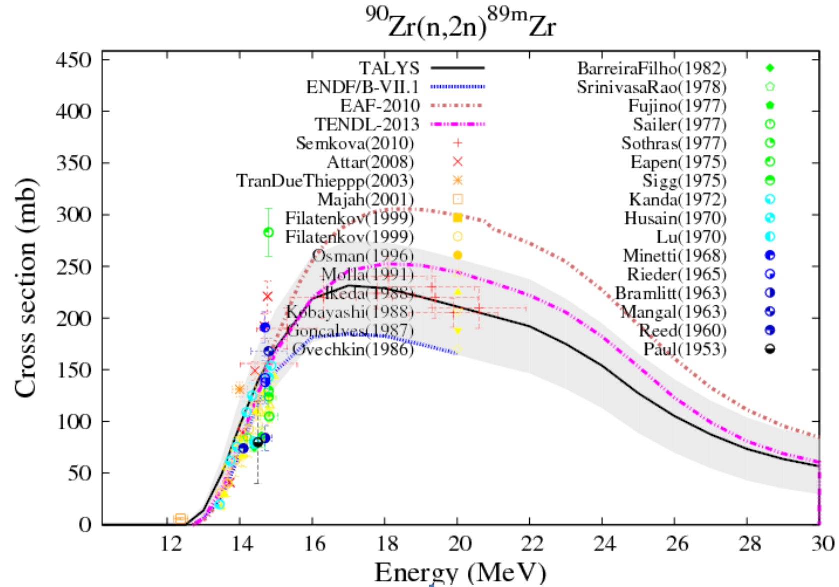
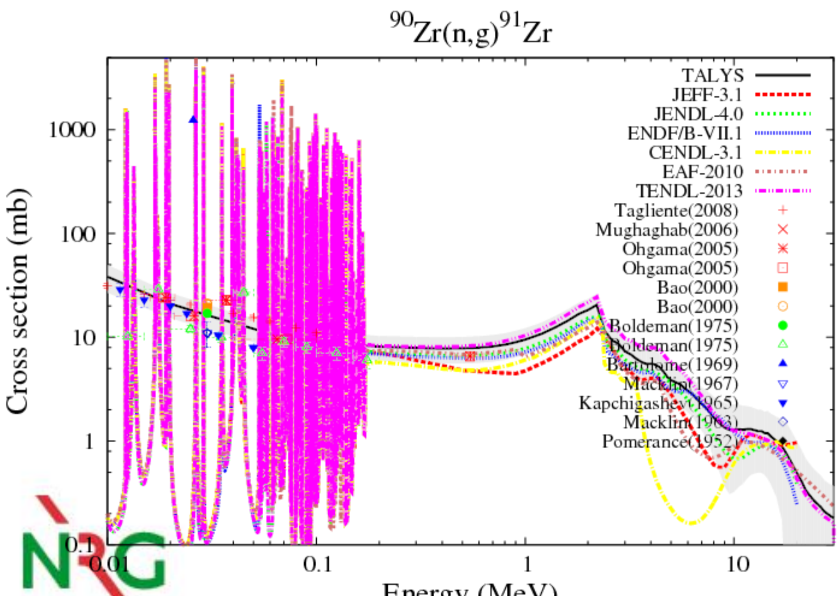
Prior: Global TALYS – uncertainties from all EXFOR data

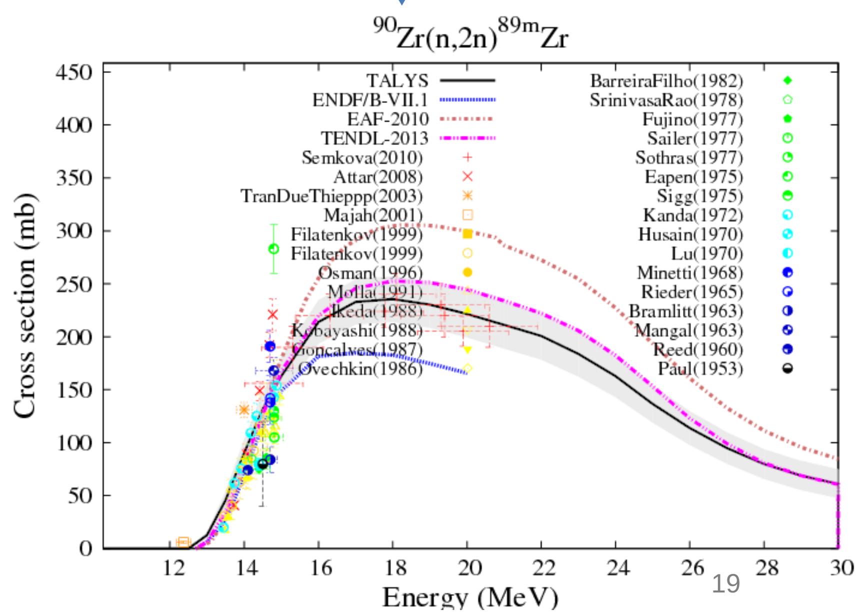




Use weights based on EXFOR for ^{90}Zr

Final





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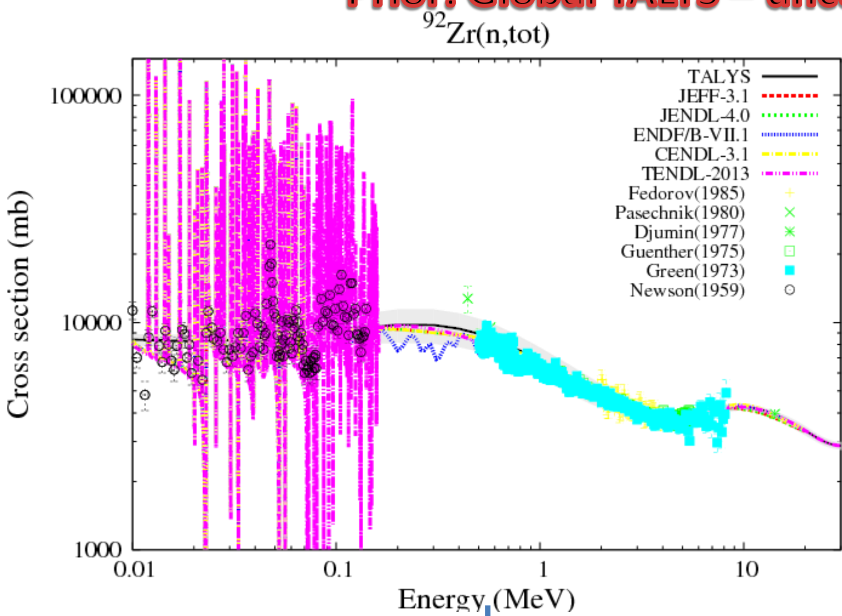

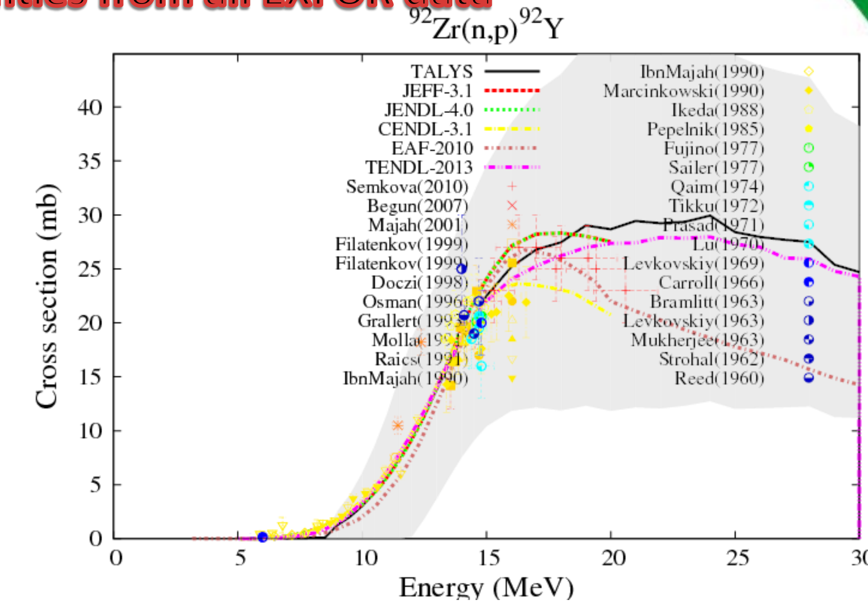

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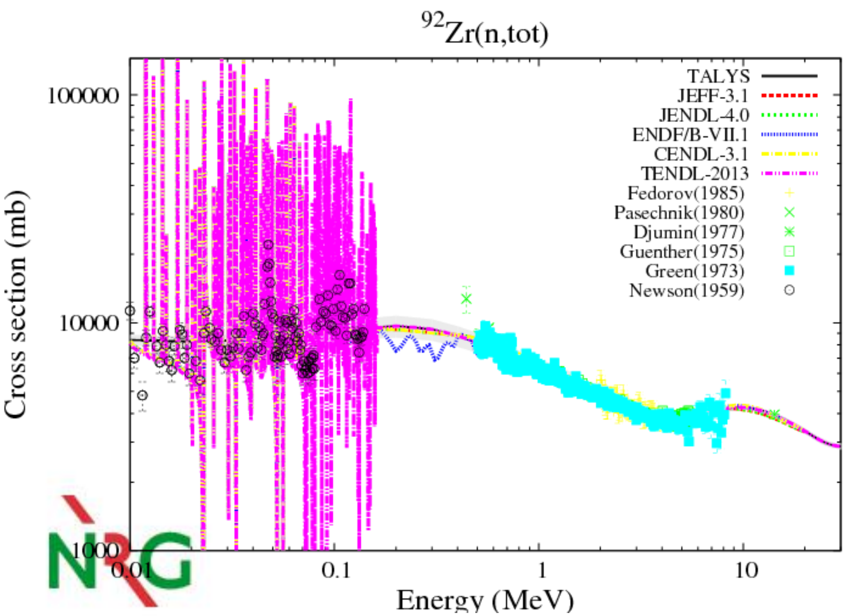

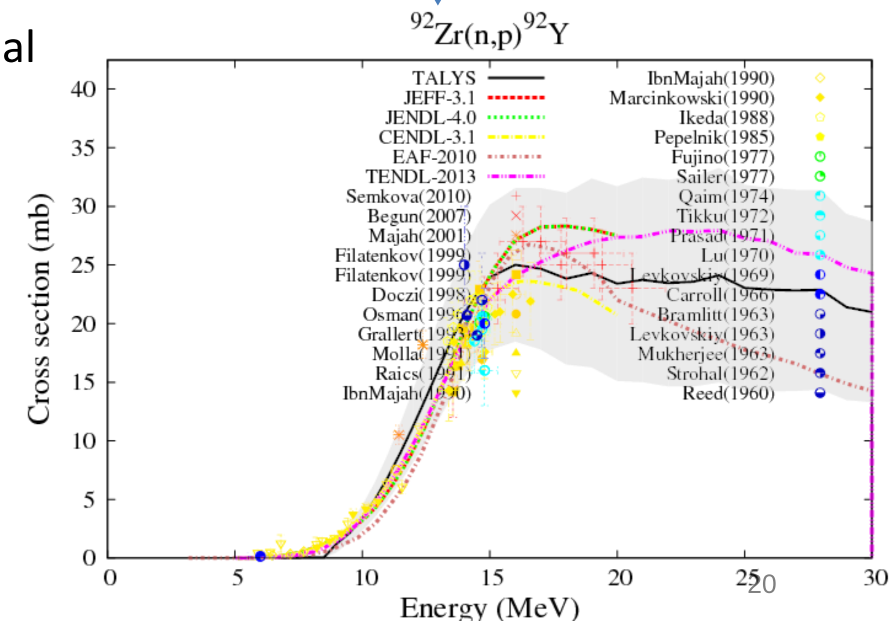

Practical approach: Start from “best” TALYS input files

- Automatic optimization to EXFOR + integral data requires a lot of pre-selection of data
- Minimal chi-square does often not match expectations (known problem from the OMP)
- For TENDL-2014 we have new “best” files for more than 300 isotopes, which give a visual optimal description of EXFOR + thermal c.s. + RI + MACS + integral activation data (EASY)
- Practical approach: Start from “best” file and update with EXFOR-based weights

Zr-90

```
#
# General
#
ldmodel 2
#
# (n,tot), (n,el), (n,inl)
#
rvadjust n 1.0 4. 8. 6. 0.99
rvadjust n 1.0 12. 16. 14. 0.995
#
# (n,p), (n,2n), (n,np)
#
#
# (n,a)
#
#
# (n,g)
#
gamgamadjust 40  91 0.75 0.10 #t#
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
#
branch 40 89 17 1 4 1.0
branch 40 89 20 1 4 1.0
branch 40 89 23 1 4 1.0
branch 40 89 25 1 4 1.0
branch 40 89 26 1 4 1.0
branch 40 89 30 1 4 1.0
```

Zr-92

```
#
# General
#
ldmodel 2
#
# (n,tot), (n,el), (n,inl)
#
rvadjust n 1. 0.01 1.5 0.7 0.99
rvadjust n 1. 3. 7. 5. 0.99
#
# (n,p), (n,2n), (n,np)
#
gnadjust 40 93 1.03
gpadjust 40 93 1.03
#
# (n,a)
#
rvadjust a 1.05
avadjust a 1.05
cstrip a 0.4 0.40 #t#
cknock a 0.4 0.40 #t#
#
# (n,g)
#
gamgamadjust 40 93 0.85 0.20 #t#
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
#
```

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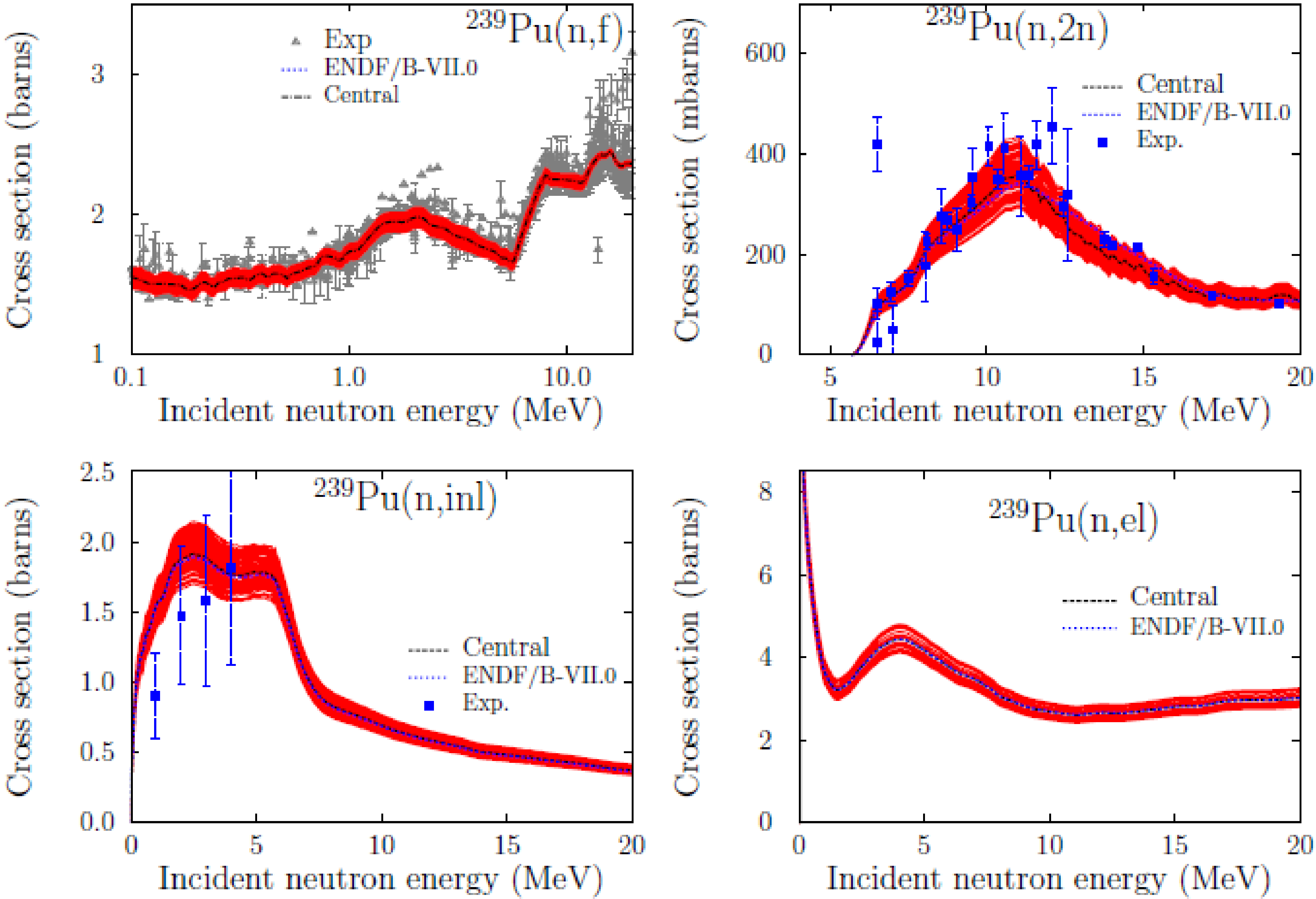
which are overruled by

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

For TENDL-2014, all nuclides will be evaluated by the Bayesian Monte Carlo procedure just described. **As usual**, this will result 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.

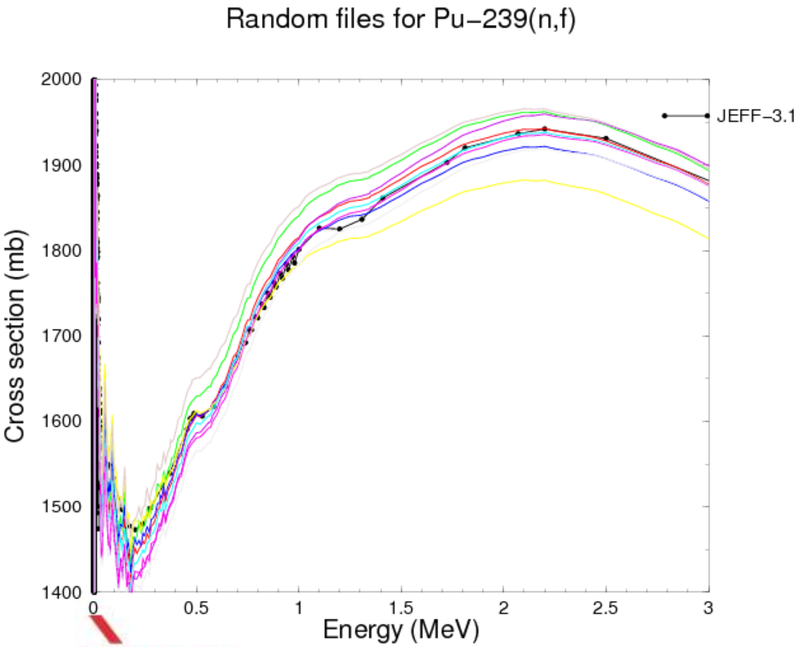
NRG

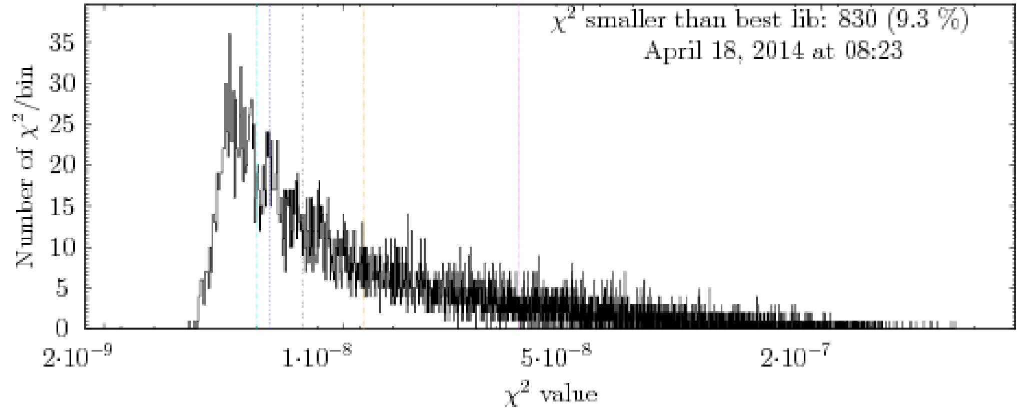
Random cross sections for ^{239}Pu

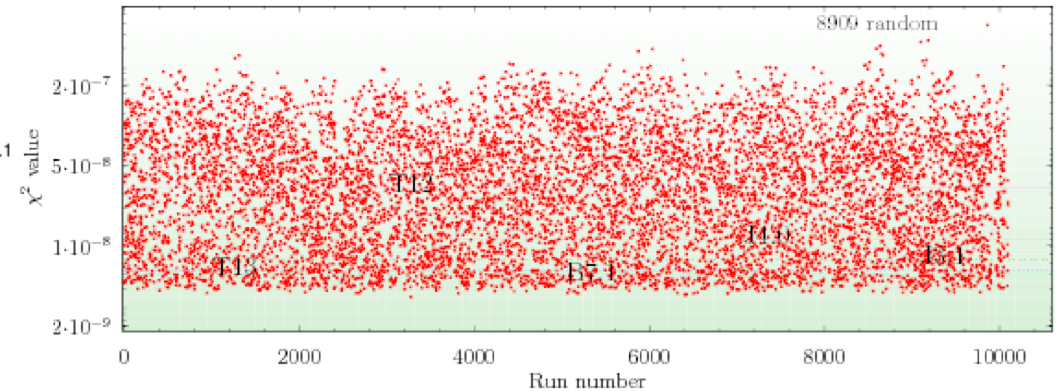


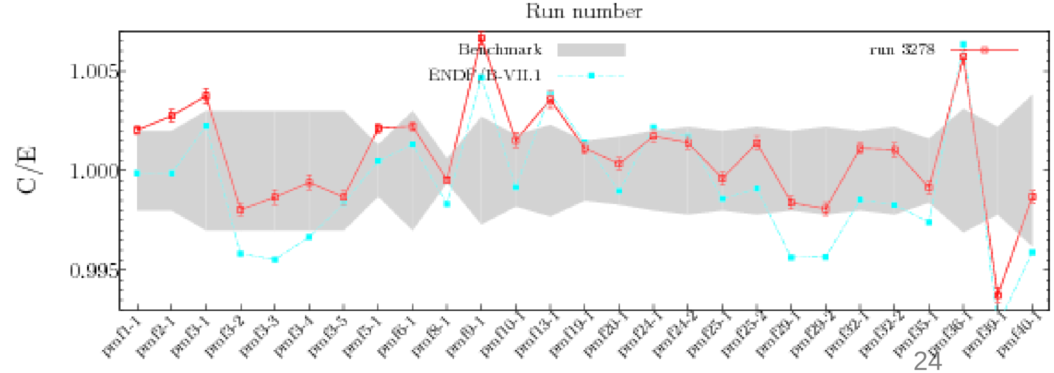
The Petten method: Monte Carlo optimization to integral benchmarks

- 10 000 random libraries for ^{239}Pu
- Run them all with MCNP through Steven van der Marck's ICSBEP criticality database
- Judge C/E quality for all of them
- Weights for your favorite system can be applied

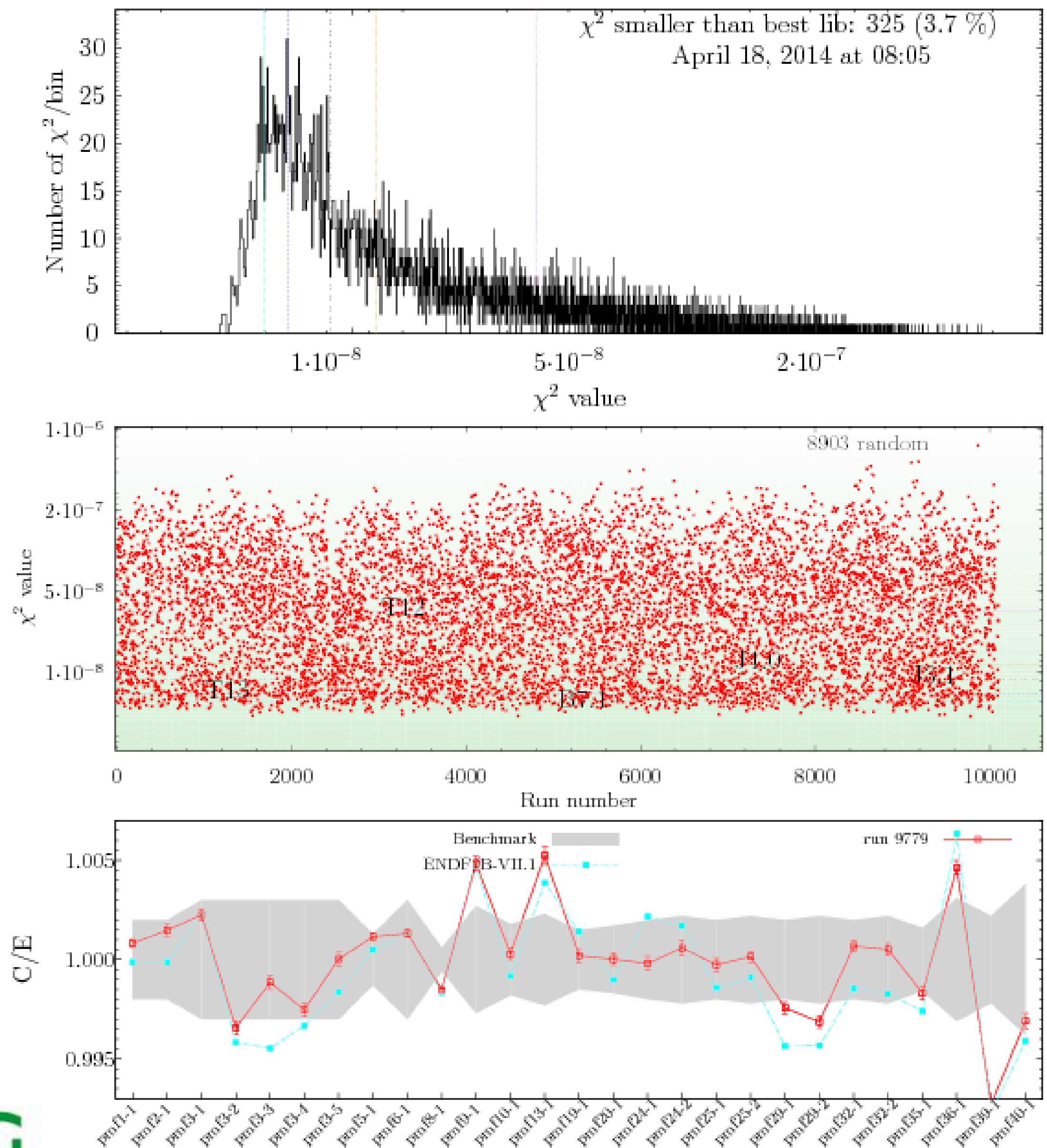








Applying a weight of 5 to PMF2



Killing the field:

1. First fast, then thermal
2. First (pure) Pu-239, U-235
3. Next U-238, O-16, H-1
4. Next the rest: Fe-56,….
5. (Optional) Goto 1

…but don't worry, we may have the tools, but not all required knowledge and computer power.

Still, expect results in future versions of TENDL

Towards TALYS-2.0

- Full rewrite in Fortran-90/95/03/08:
  - Work has already started: input and create_nucleus(Z,A)
- Integration of TASMAN:
  - statistics
  - optimization (parameter search)
  - sensitivities
  - uncertainties
  - covariances
  - Total Monte Carlo
- Integration of TEFAL:
  - Complete ENDF-6 formatting from MF1 to MF40
- TALYS-1.0 and1.2: First completeness then quality
- TALYS-1.4 and 1.6: Completeness and quality
- TALYS-2.0: Now that I have done it all, I know how I should have done it, so let's do that.

“Objective” quality assessment of data libraries

General	Specific	ENDF/B-VII.1	JENDL-4.0	JEFF-3.2	CENDL-3.1	TENDL-2014
Acceptance	Citations Software					
Integral Data	ICSBEP Shielding (fusion) Activation (EASY) Decay heat Reactor exps.					
Differential Data	Thermal xs Resonance Integral MACS (30 keV) Other EXFOR data					
Completeness	Covariances Gamma production Second. E-A dist. Isomers Recoils 200 MeV Nuclides Processability					

Use ✓ or numbers (C/E or chi-2) to fill boxes

Per nuclide or for the whole data library

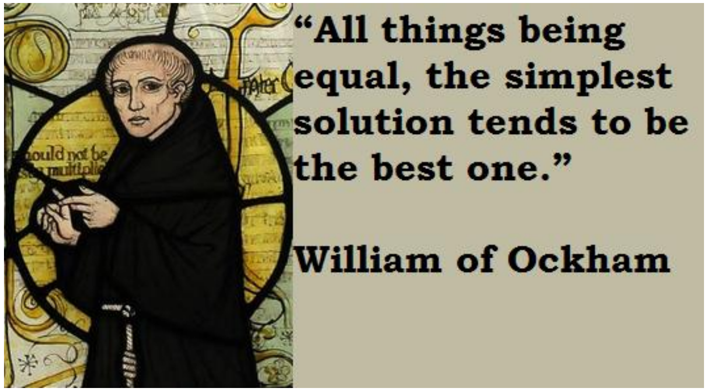
Conclusions

- **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 at least as good as other libraries.**
- **Completeness (MF1-40) and processibility (PREPRO, NJOY): no real competitor left.**
- **For “big 3”: ICSBEP included in the optimization (this has advanced most for Pu-239)**

Conclusions

- **Bayesian Monte Carlo for uncertainties:**
  - The methods are more and more reduced to sampling and counting.

**Among competing hypotheses,
the one with the fewest assumptions
should be selected.**



Ockham's razor - William of Ockham (c. 1287 - 1347):

  - The largest challenge is the proper definition of the weight in terms of (generalized) chi-square, taking into account a proper pre-selection of experimental data.
- **In 2014 nuclear data libraries will be consistently constructed using TALYS + sampling using EXFOR-based weights + the "best" TALYS input files:**
  - As usual, collapse of all random variations into covariance matrices (MF31-40)
  - N random nuclear data libraries per isotope for TMC: differential, integral and combined weight w(k), for each random file k, printed in MF1