Status of TENDL: TENDL-2014 and beyond

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The Netherlands

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WPEC meeting
NEA Data Bank

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- **TENDL-2014:**
  - General trends
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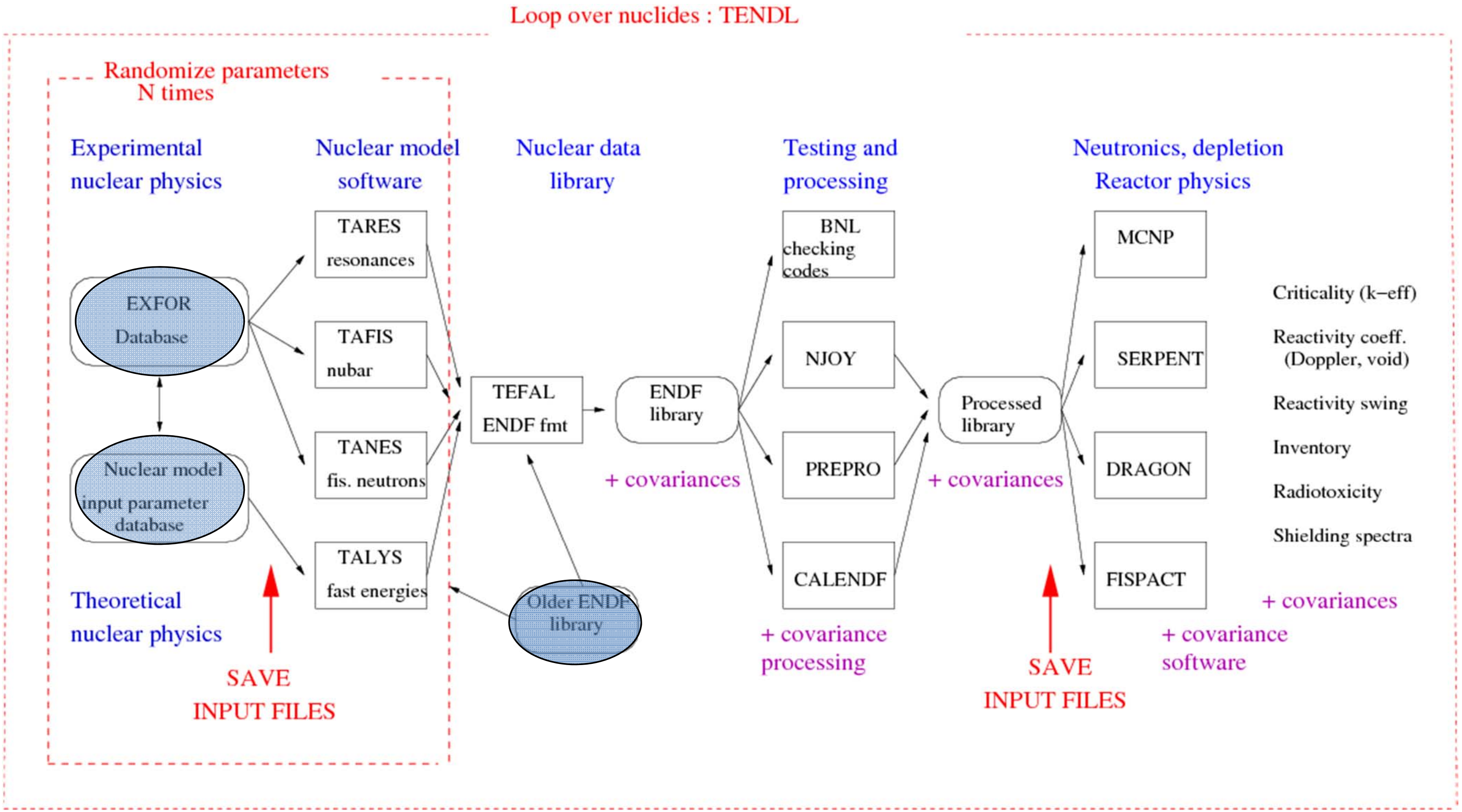
  - Update procedure using weights
  - Zooming in on particular nuclides
- **Towards TALYS-1.8 and TALYS-2.0**
- **Conclusions**

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-2014

- Neutron, proton, deuteron, triton, Helium-3, alpha and gamma data libraries.
- 2629 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-1.7 (not generally released) and TARES (resonances)

which are overruled by

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

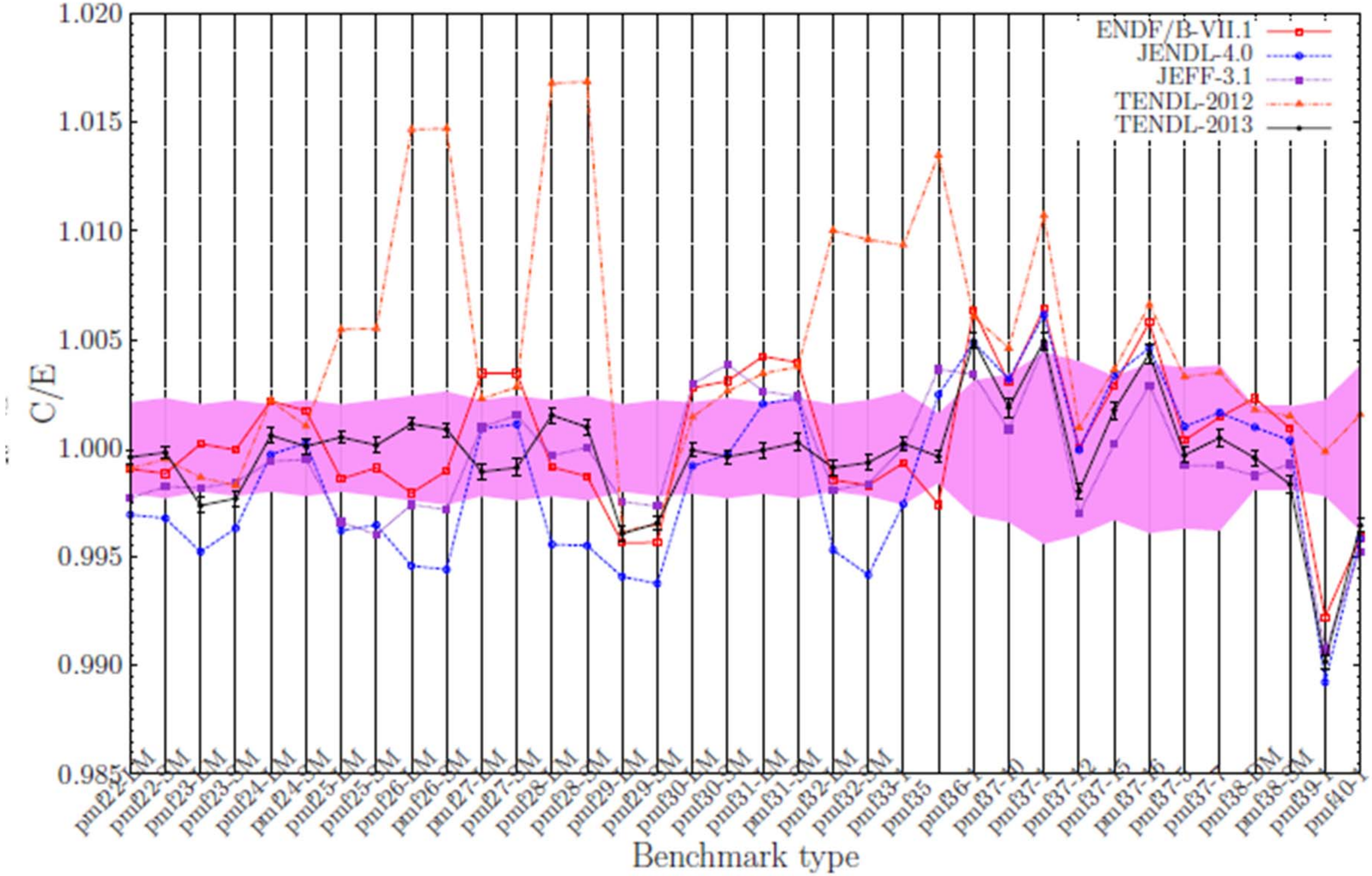
which are overruled by

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

For TENDL-2014, 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),

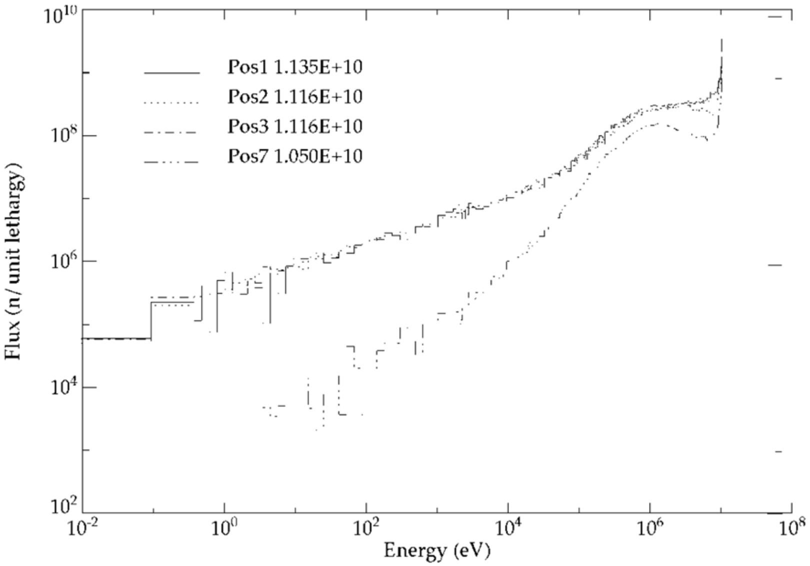
for those who are able to process and use all that.

TENDL-2013 for fast Pu benchmarks



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

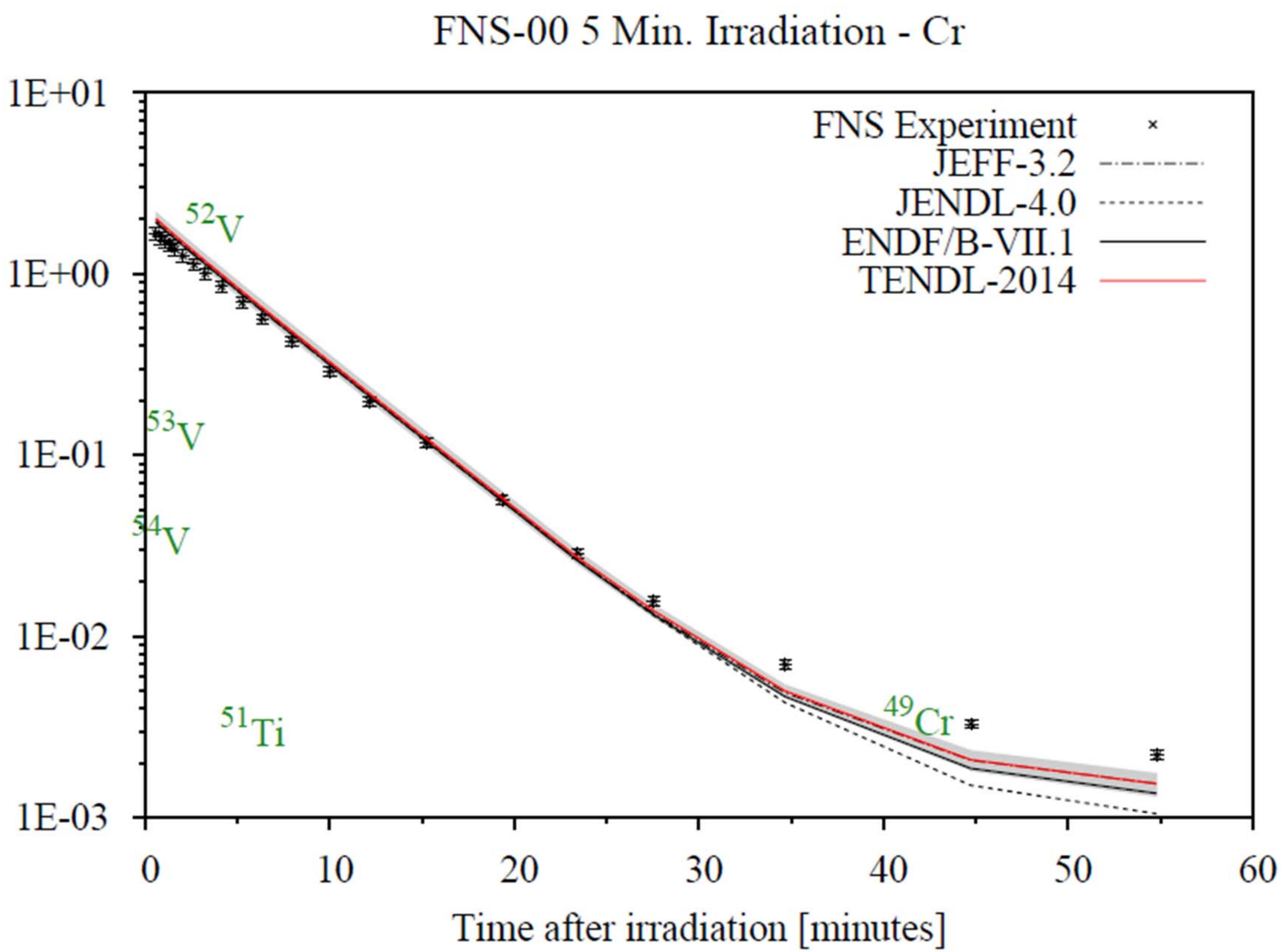


FNS Neutron spectra, neutron fluence monitored by $^{27}Al(n,a)Na^{24}$

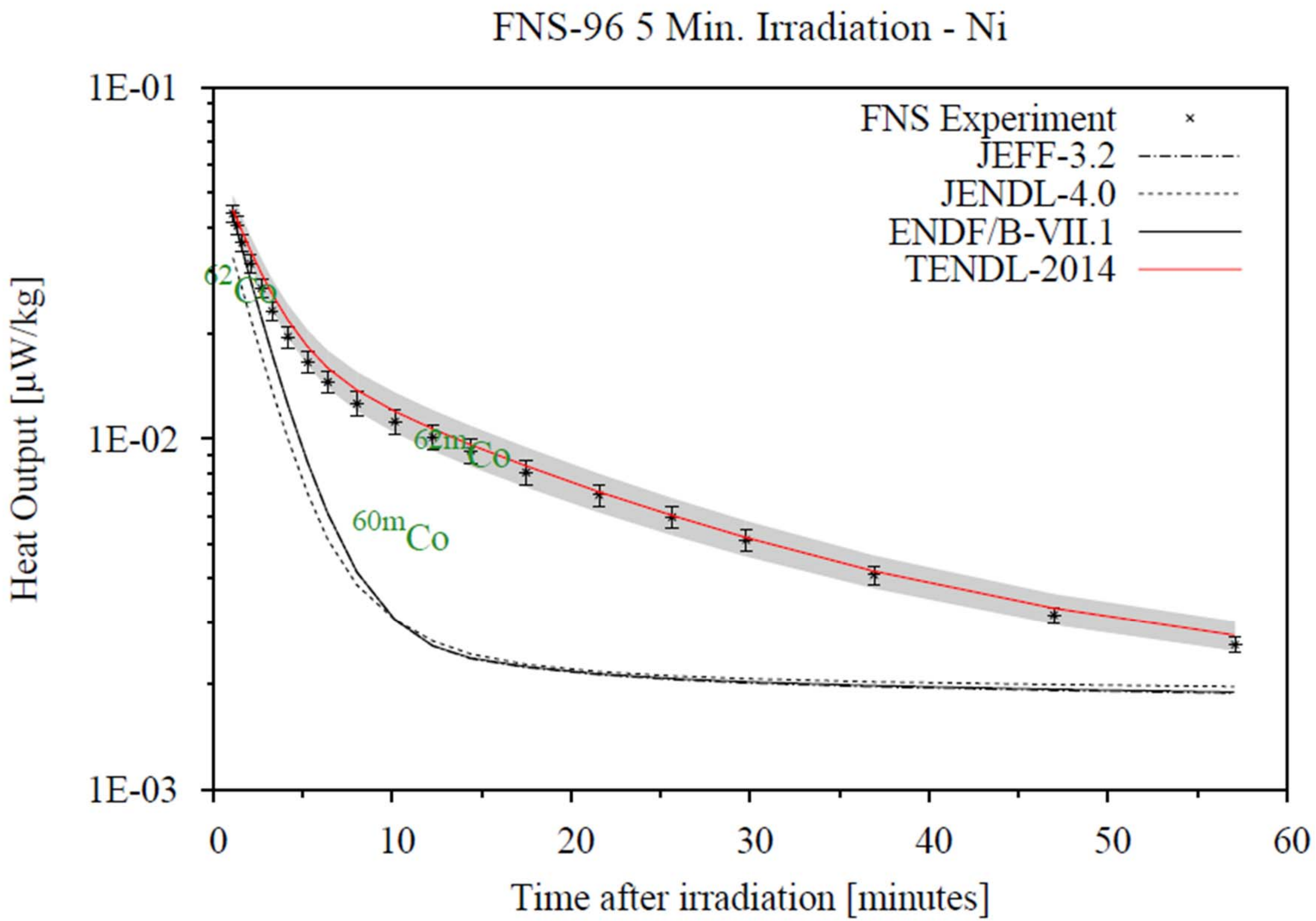
Two experimental campaigns: 1996 and 2000; 74 materials

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

Chromium

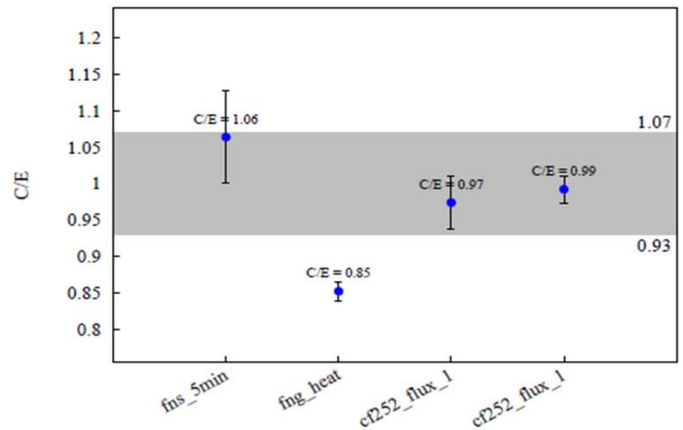

FNS-00 5 Min. Irradiation - Cr
FNS Experiment
JEFF-3.2
JENDL-4.0
ENDF/B-VII.1
TENDL-2014
^{52}V
^{53}V
^{54}V
^{51}Ti
^{49}Cr
1E+01
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60
Time after irradiation [minutes]

Decay power: FNS JAERI Ni

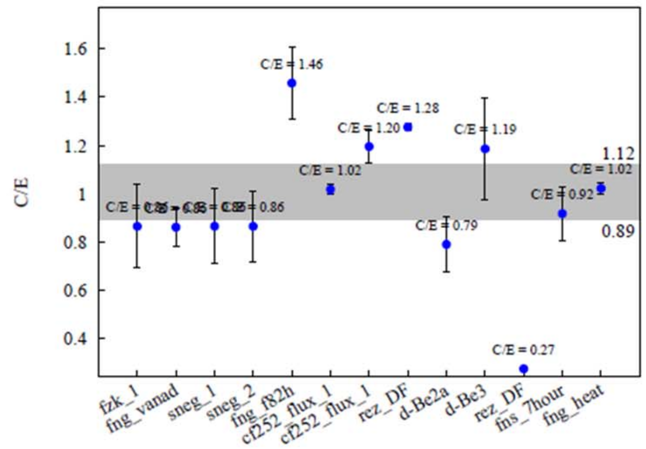


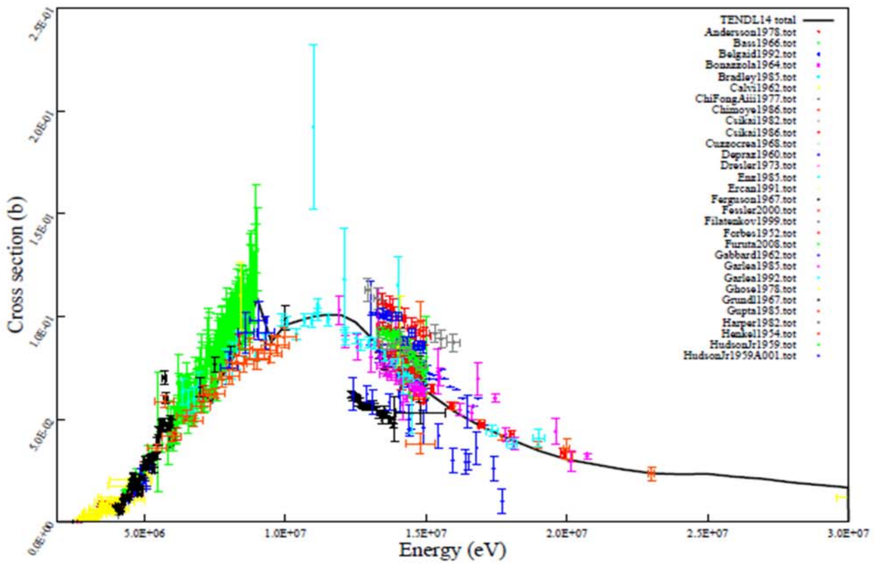
Decay heat should only be analyzed with General Purpose Libraries

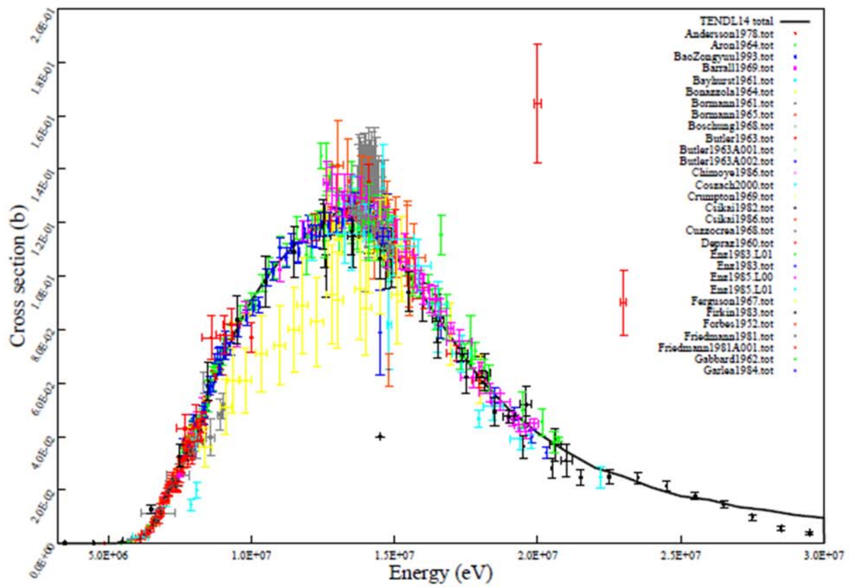
^{27}Al (n,p) ^{27}Mg



^{27}Al (n,a) ^{24}Na







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

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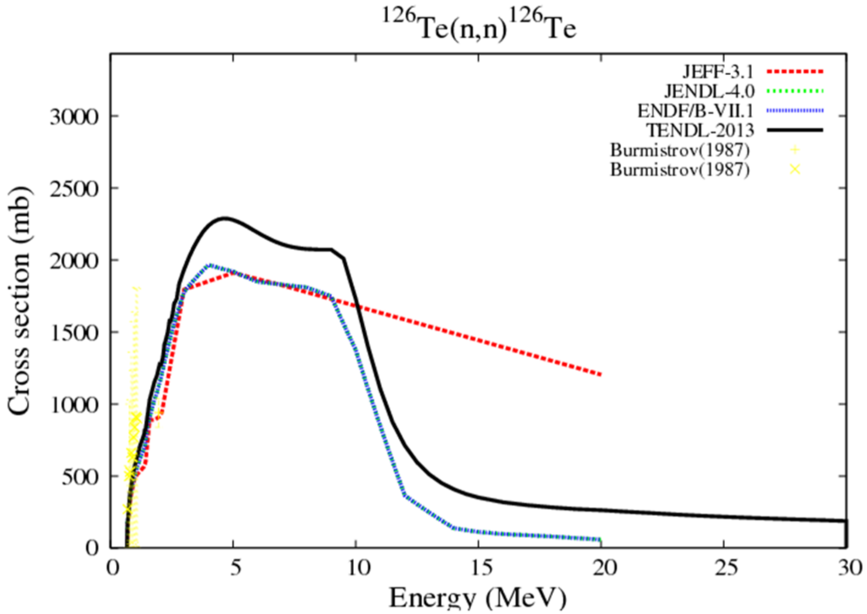
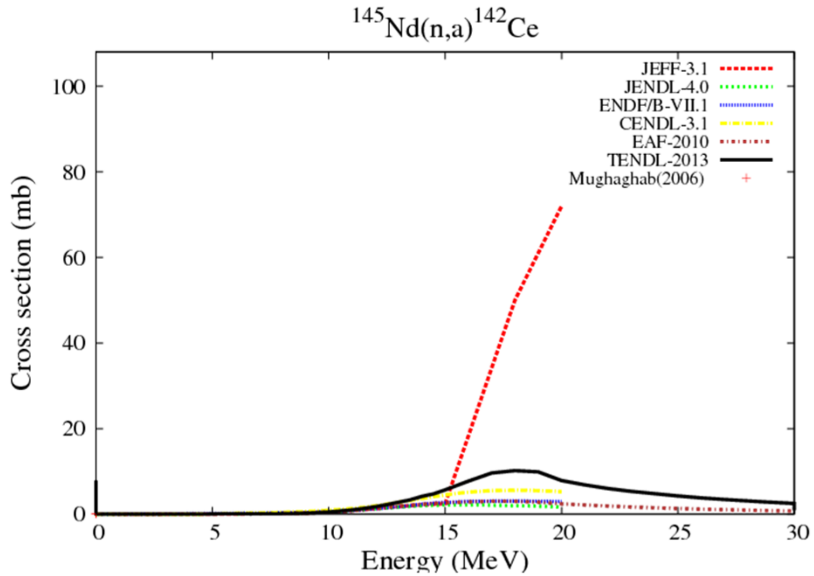
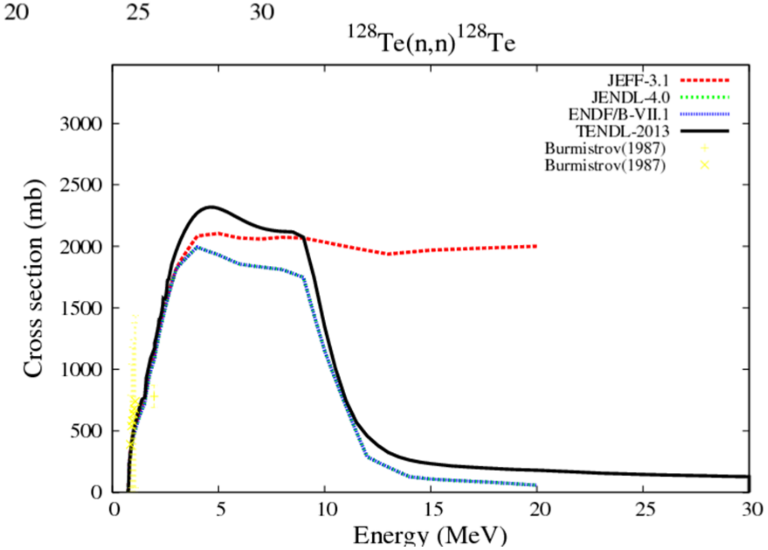
Further cleaning of JEFF

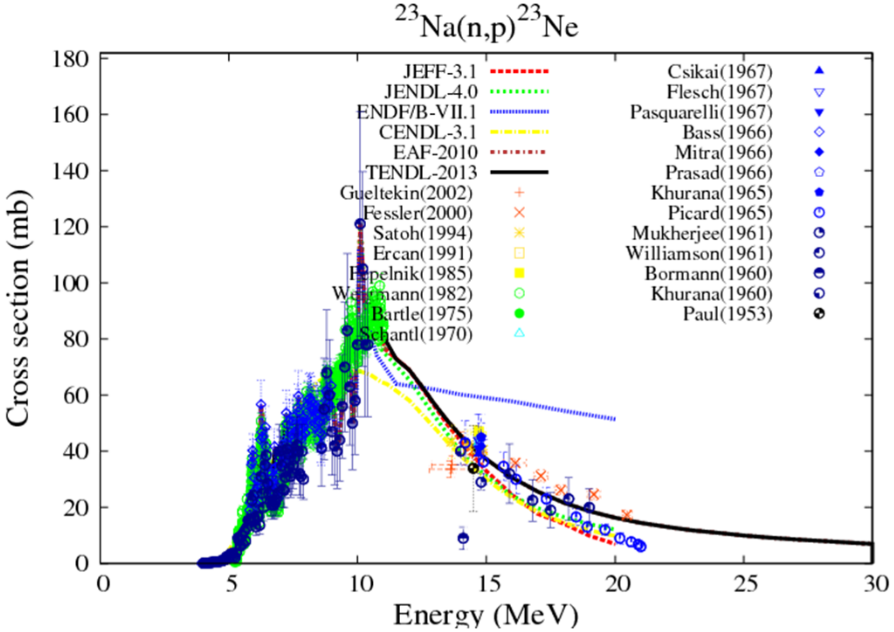
- **JEFF-3.2: 472 isotopes, 151 are from TENDL-2012**
- **More "clear" candidates for replacement, Te, Nd, etc.**

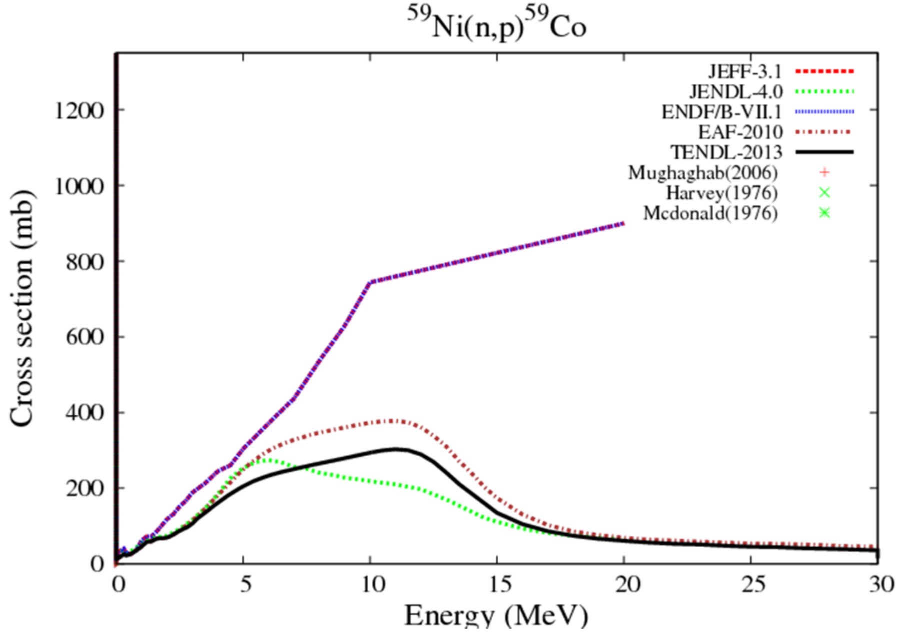


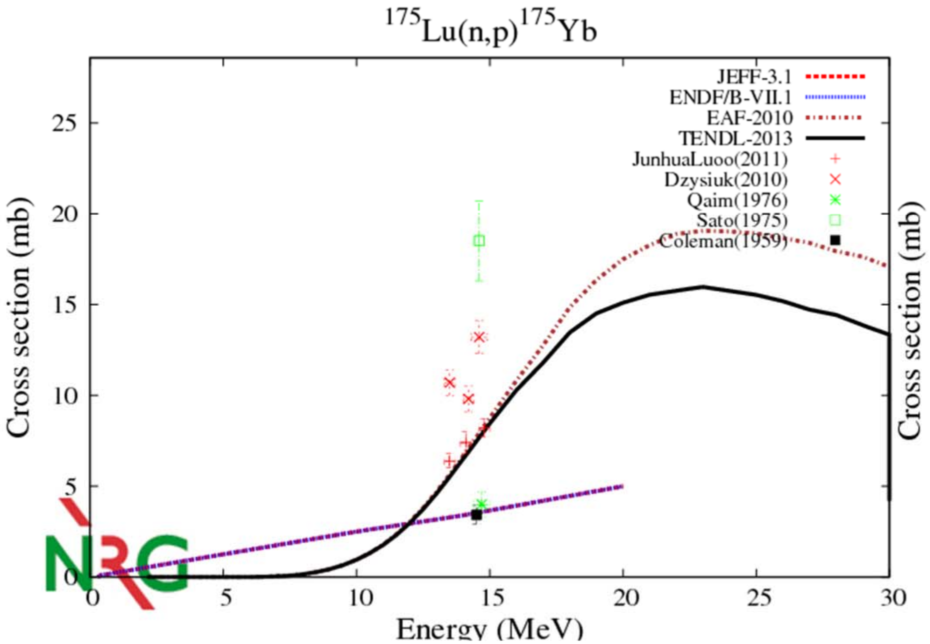


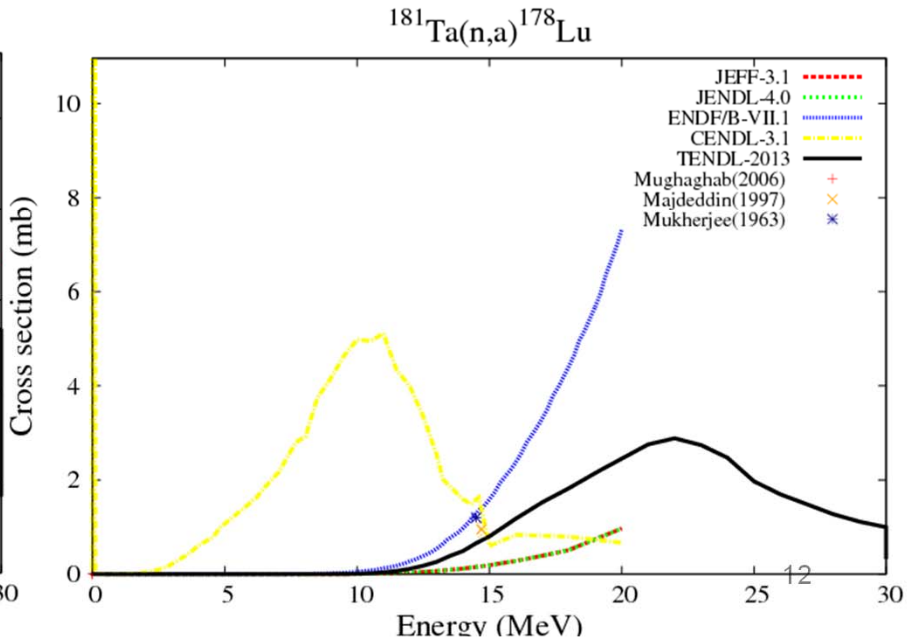


TENDL is also available to clean up other libraries









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!)					

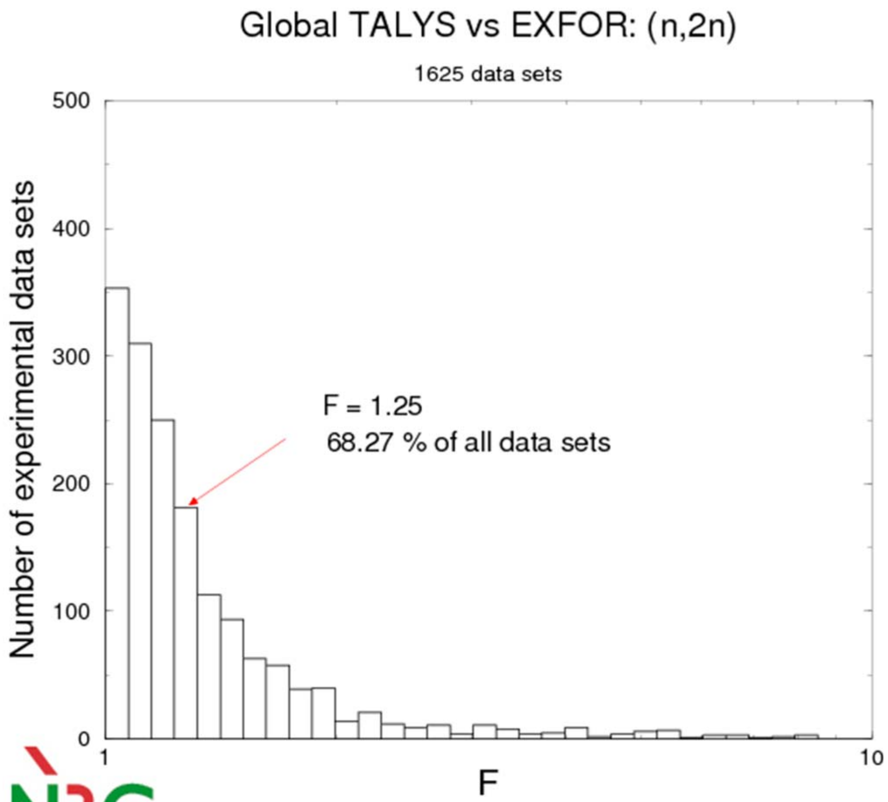
Table 1: Total number of neutron-induced *cross section* subentries available in XC4 format.

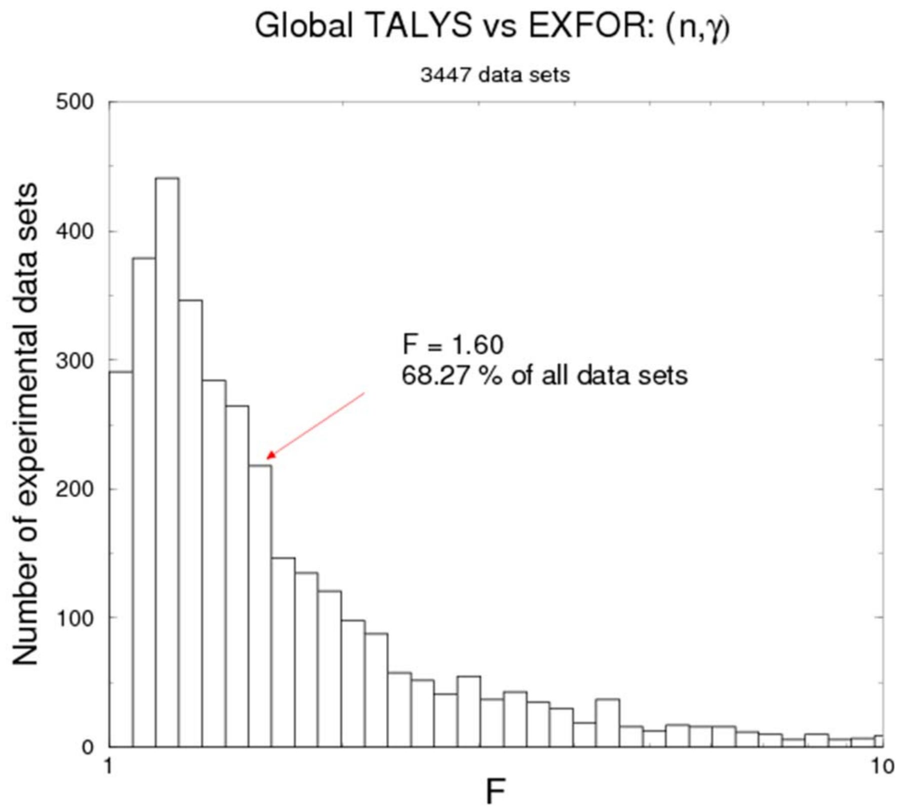
Initial probability distribution for cross sections

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

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

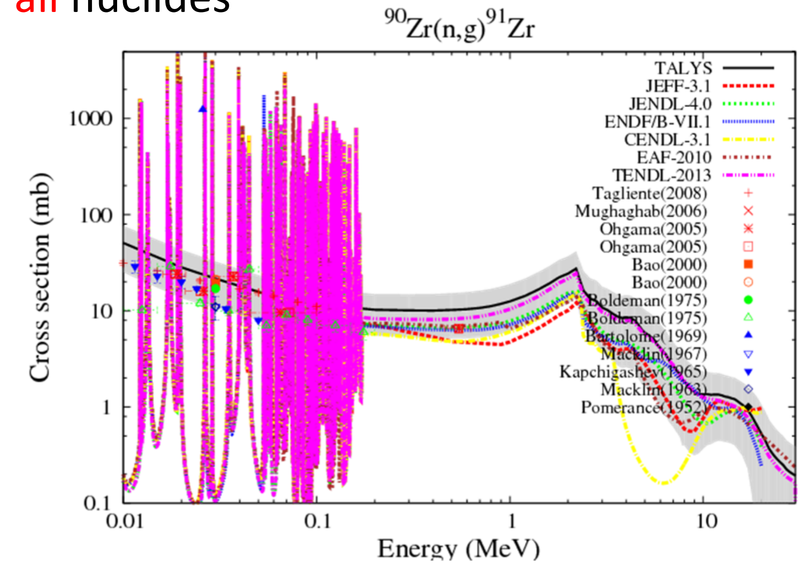
WPEC SG-30 on quality assessment of EXFOR

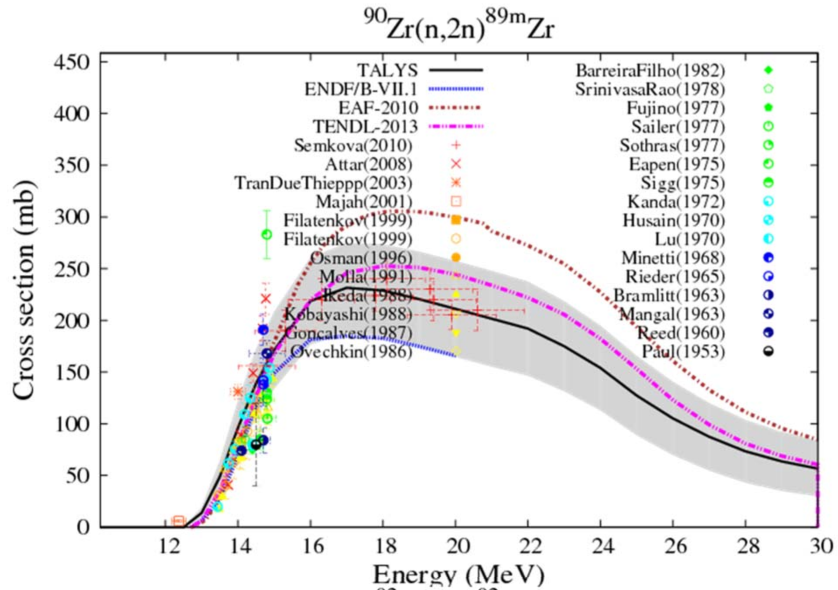


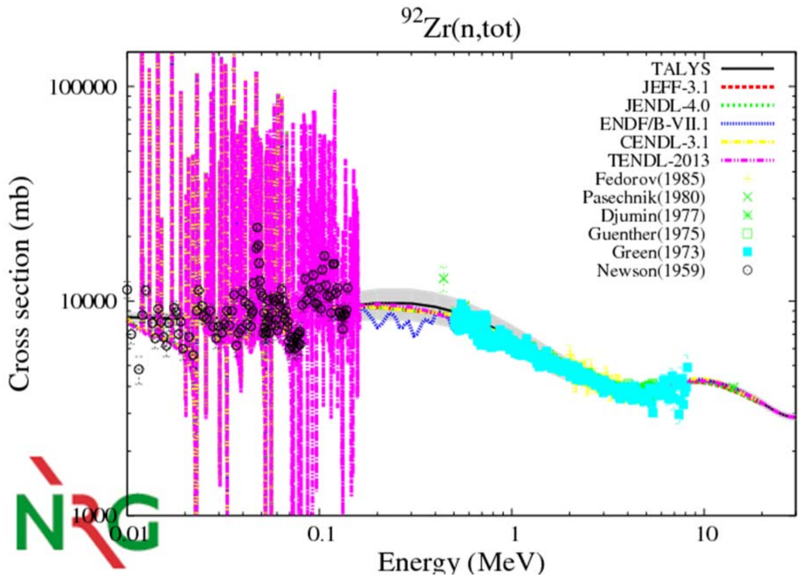


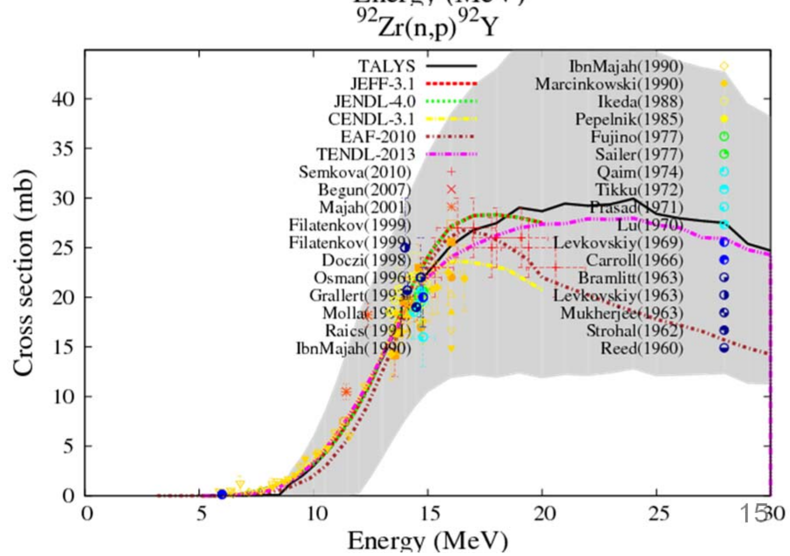
Prior probability distributions for cross sections

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
$\lambda_{V_{so}}$	5	$\lambda_{W_{so}}$	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

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**

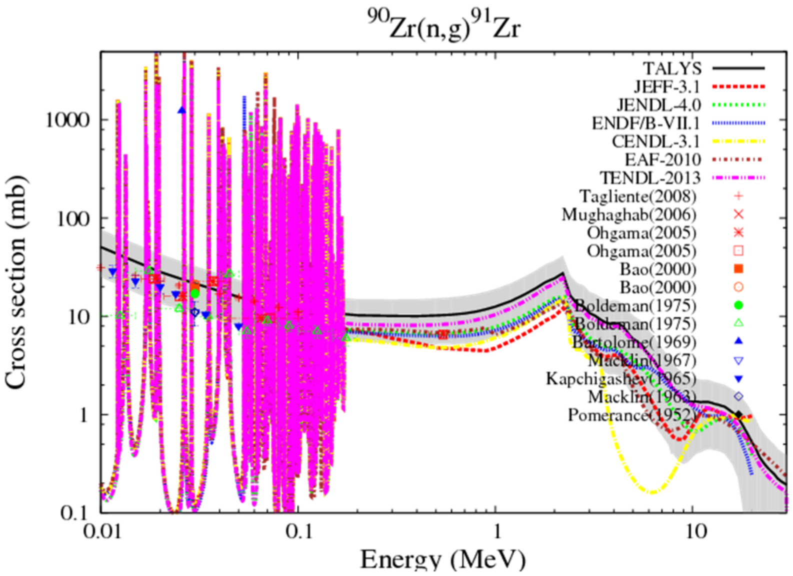
Zr-90

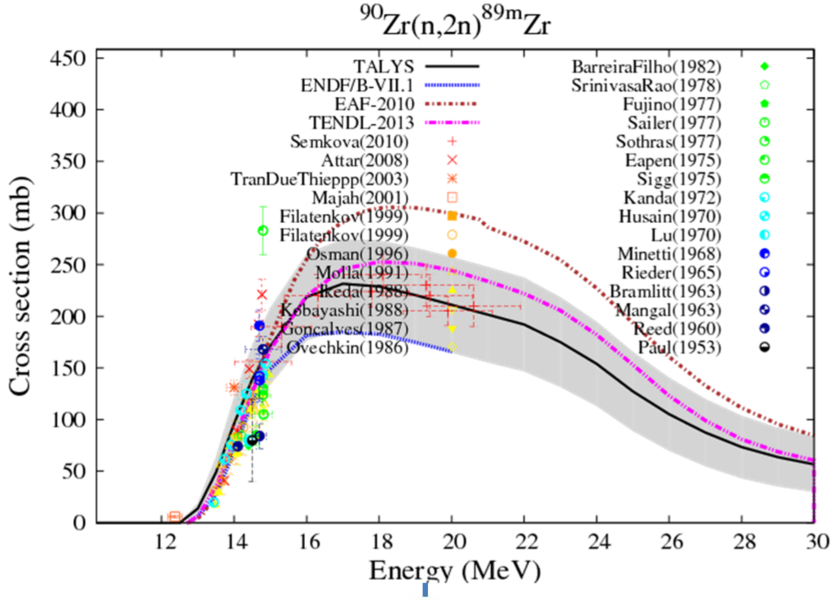
```
#
# General
#
ldmodel 2
#
# (n,tot), (n,el), (n,inl)
#
rvadjust n 1.0 4. 8. 6. 0.99
rvadjust n 1.0 12. 16. 14. 0.995
#
# (n,p), (n,2n), (n,np)
#
#
# (n,a)
#
#
# (n,g)
#
gamgamadjust 40  91 0.75 0.10 #t#
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
#
branch 40 89 17 1 4 1.0
branch 40 89 20 1 4 1.0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

Prior: Global TALYS – uncertainties from all EXFOR data

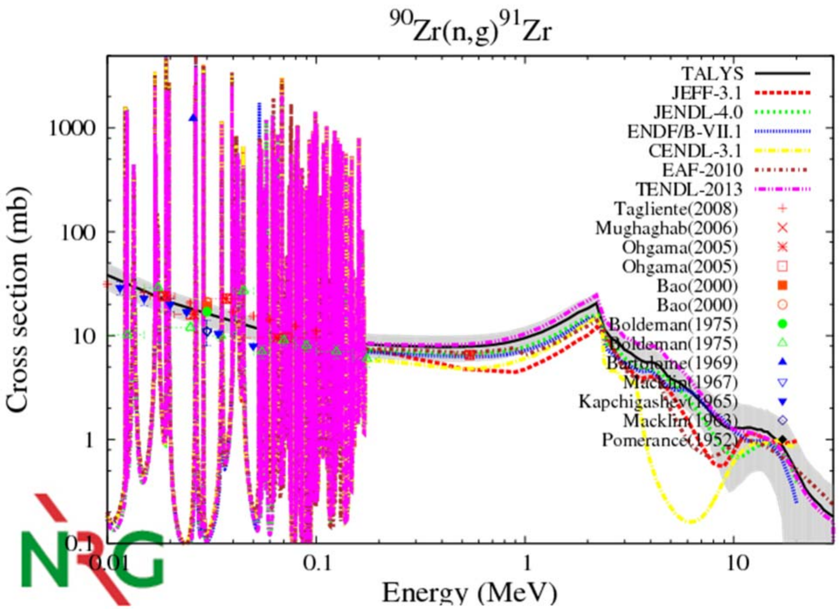


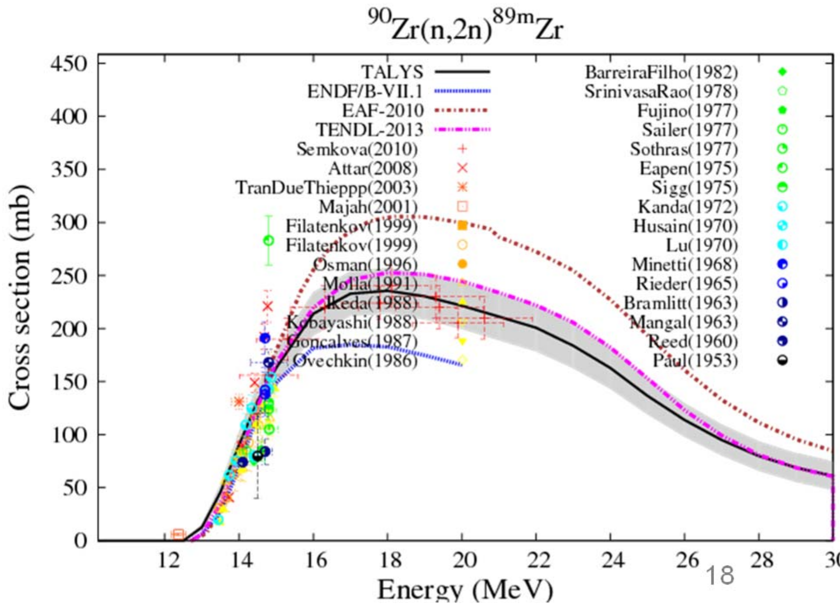


Use weights based on EXFOR for ^{90}Zr

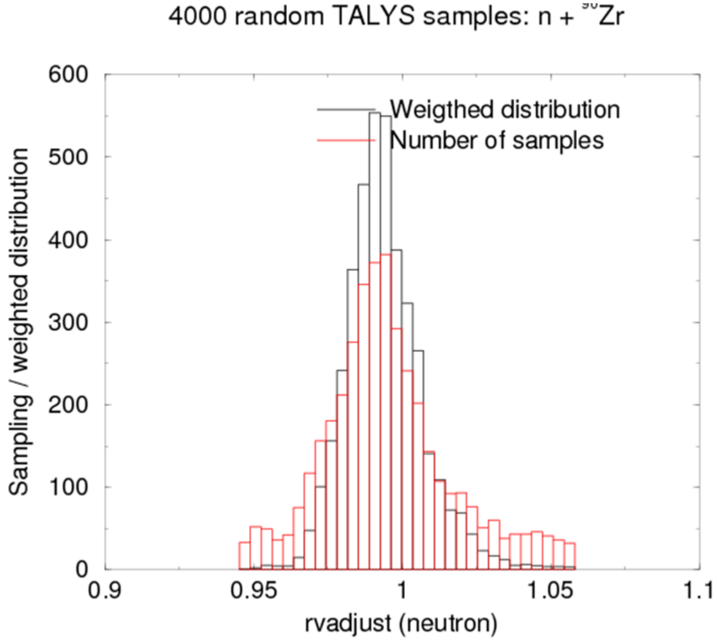
$$w^{(k)} = \exp(-\chi^{2(k)})/\exp(-\chi^{2(0)})$$

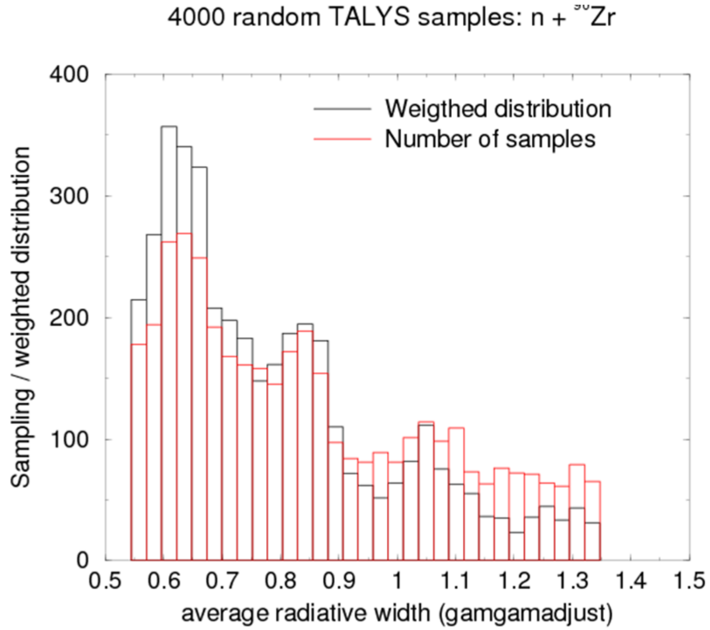
Final

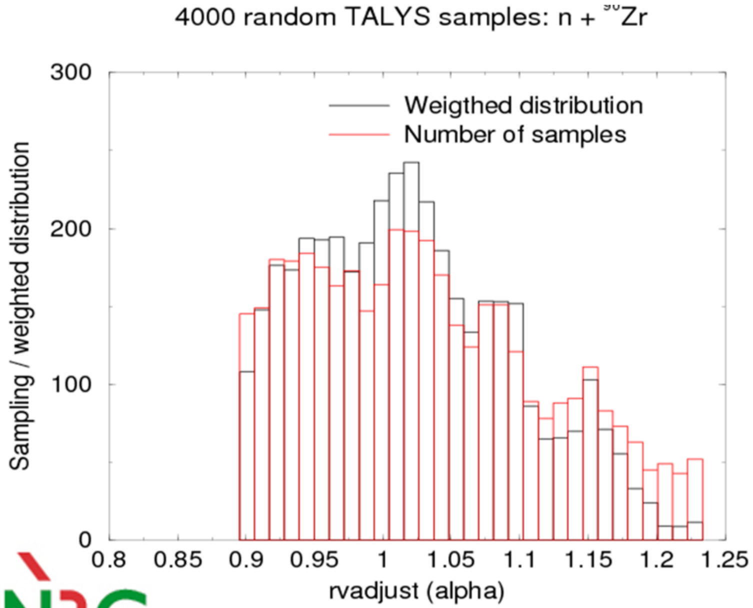


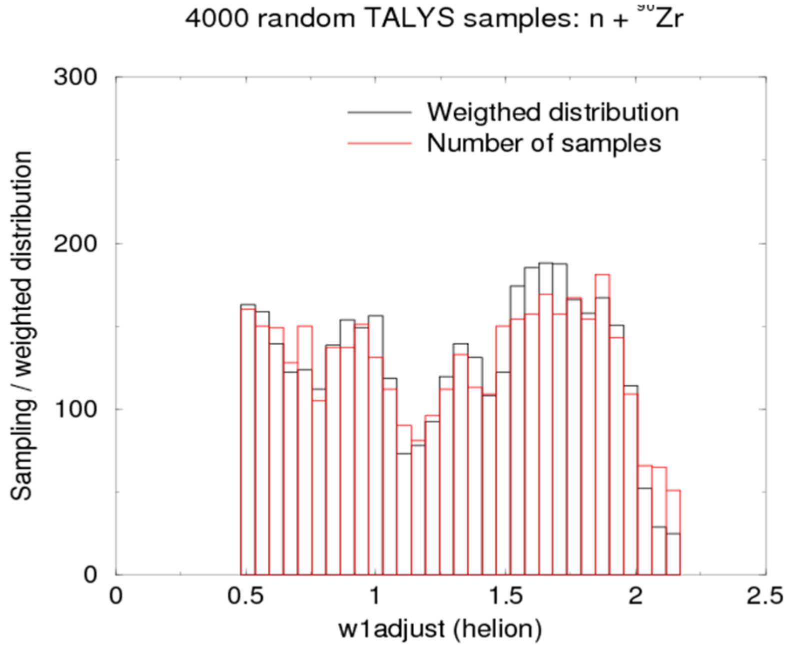


Finally, all sampling is done from the real weighted parameter distributions

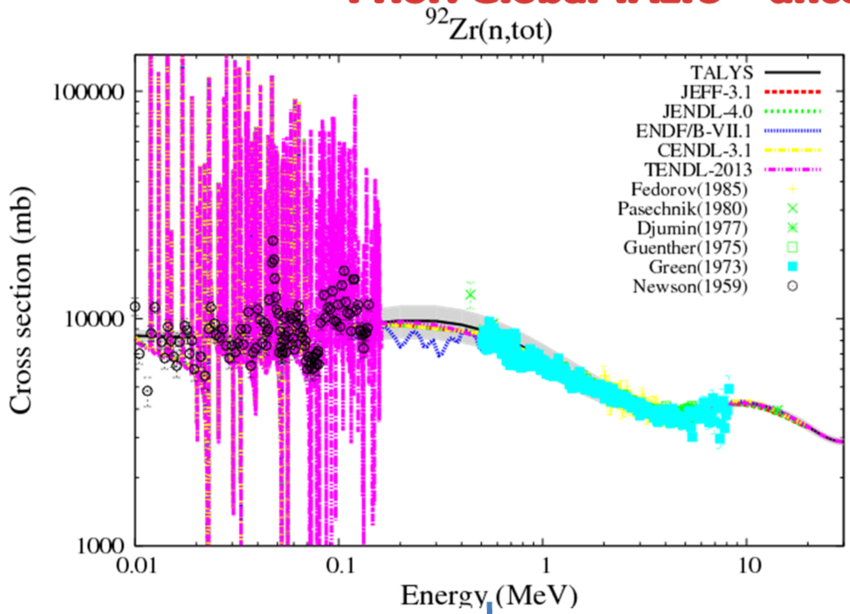


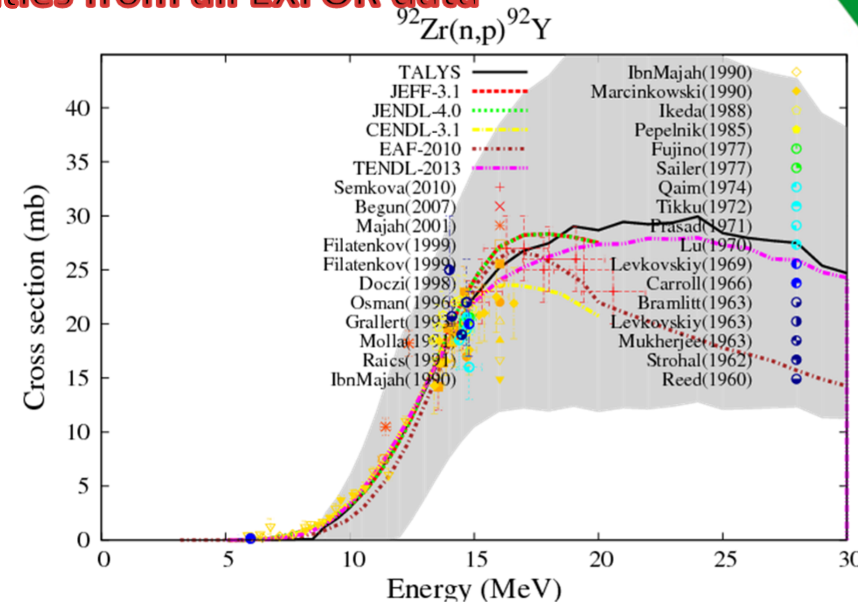






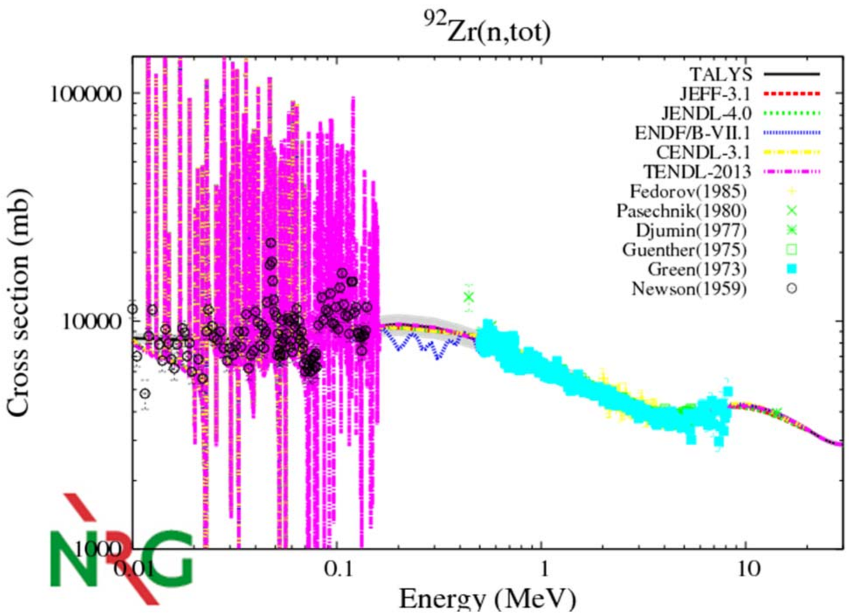
Prior: Global TALYS – uncertainties from all EXFOR data

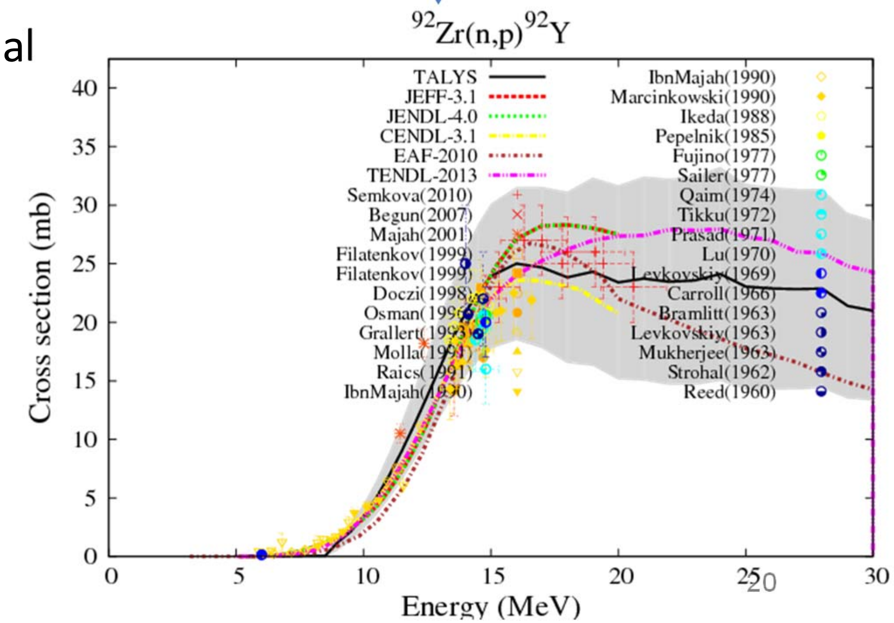




Use weights based on EXFOR for ^{90}Zr

Final



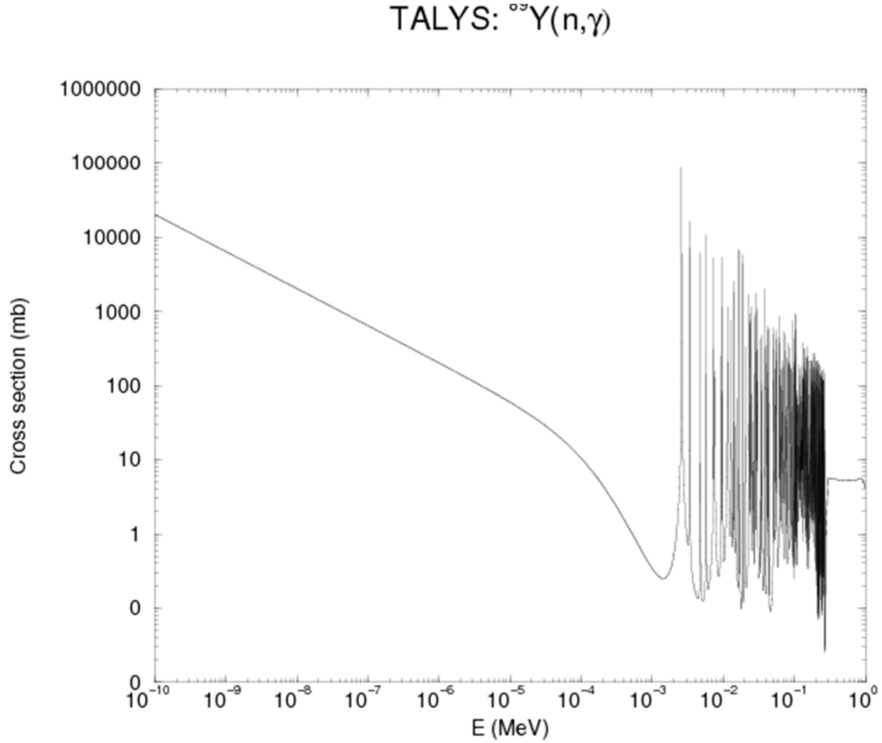


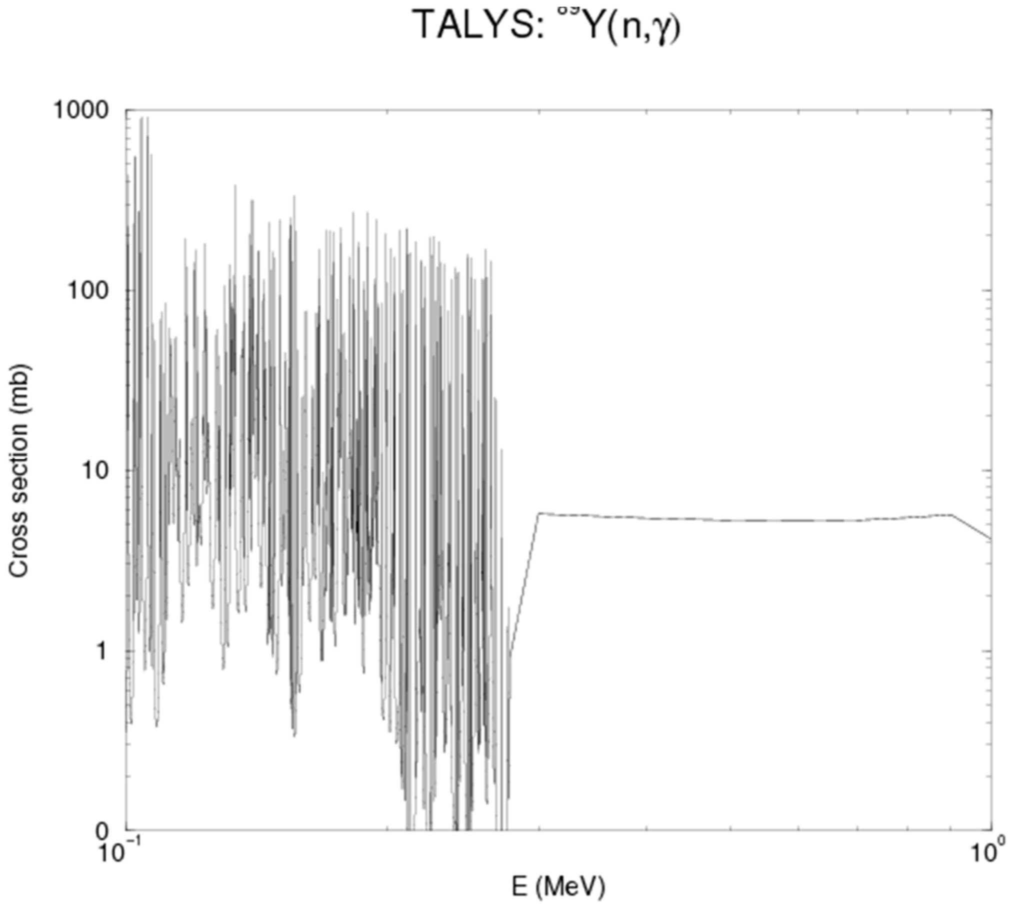
Towards TALYS-2.0

- 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
- First: 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.

NRG

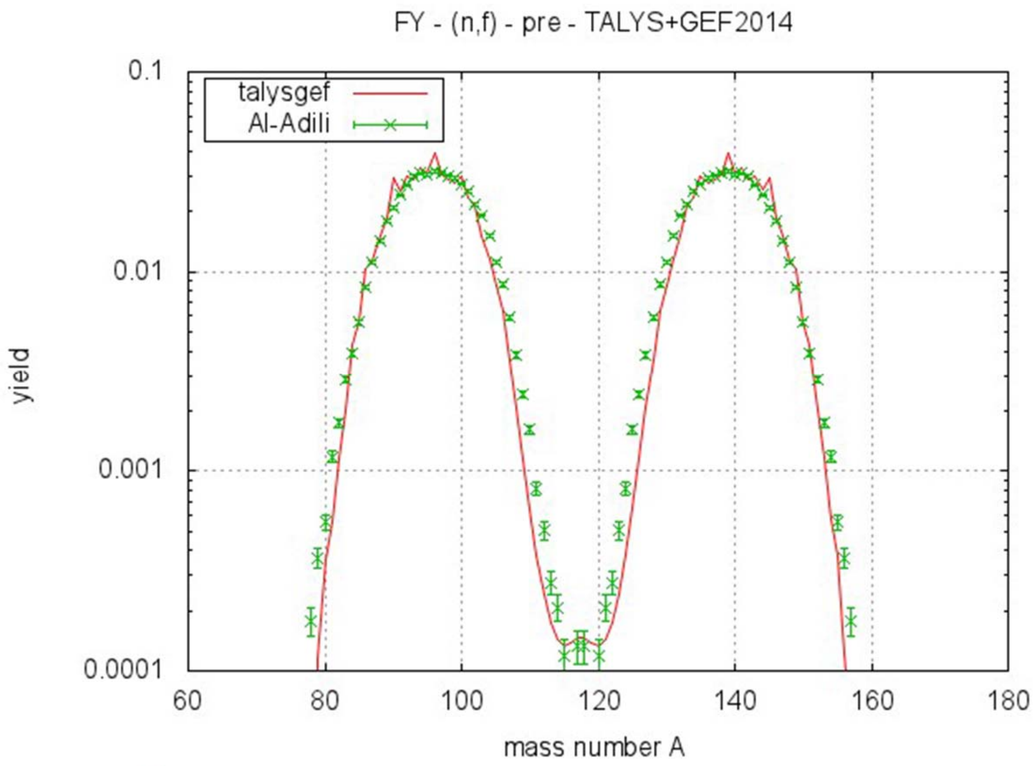
TALYS-1.8 reconstructs resonances (Thanks to Red Cullen and PREPRO)





Fission yields

- **TALYS is now coupled with GEF, a fission code by Karl-Heinz Schmidt (GSI), which calculates fission observables on a microscopic basis, starting from an excitation energy, spin and parity**
- **TALYS feeds GEF with that starting point**



$^{234}U(n,f)$

Experimental data from PhD thesis
of Ali Al-Adili,
Uppsala University 2013.

More examples: S. Pomp
Presentation at FIESTA 2014,
Santa Fe

“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 is at least as good as other libraries: again, after 2014 more nuclides fall in this category.**
- **Completeness (MF1-40) and processability (PREPRO, NJOY): no real competitor left.**
- **For "big 3": ICSBEP included in the Monte Carlo optimization (this has advanced most for Pu-239)**
- **TENDL team now scattered over more places, but aims to continue.**

NRG