TENDL-2009: Towards completeness and accuracy

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Contents

Motivations: A long term goal is to rule out nuclear data libraries

Short-term goal:

We need a consistent, complete and reproducible nuclear data library to be integrated in reactor calculations, including realistic covariance data.

(*None of the existing libraries fulfill these requirements.*)

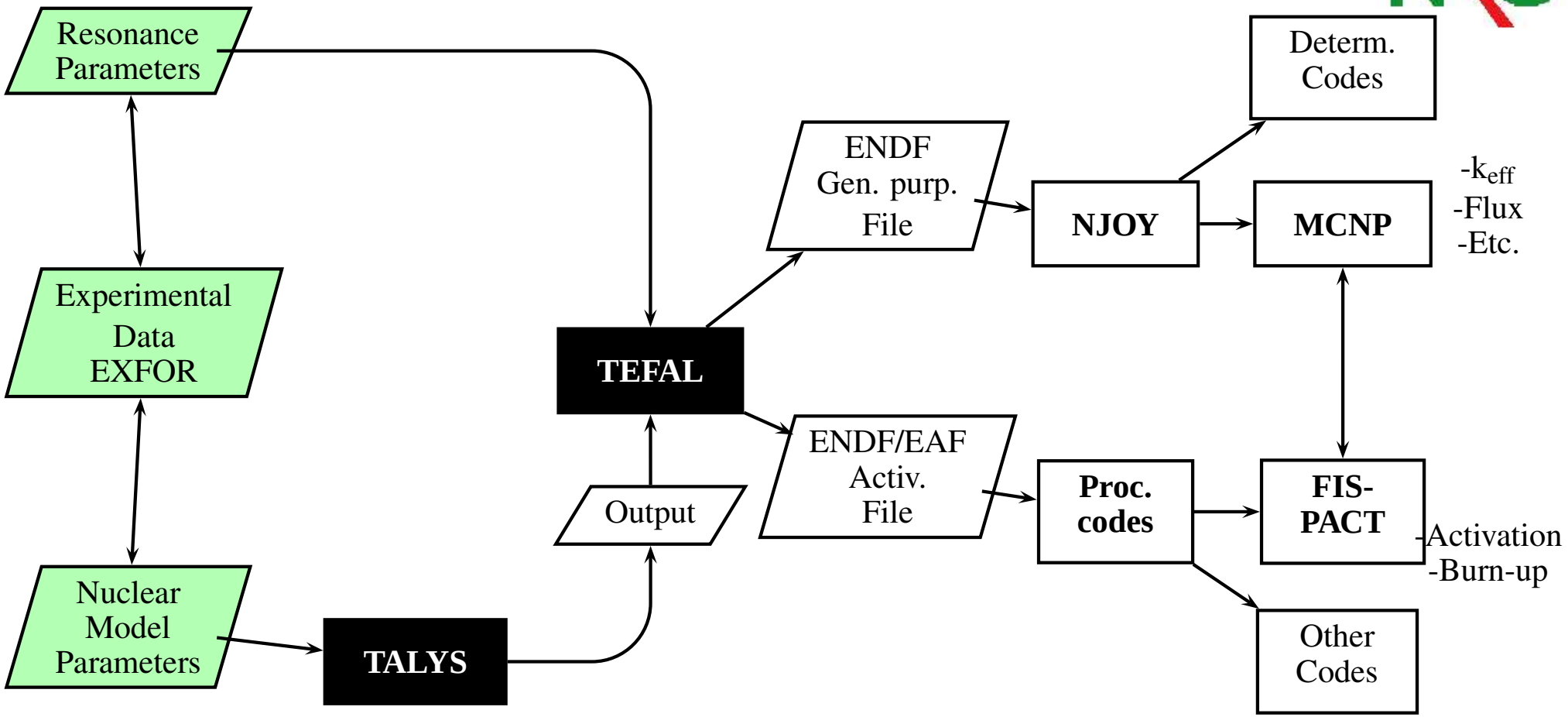
- Use global, robust TALYS method for a bulk of nuclides
- Use in-depth evaluation, adjustment... for important nuclides (e.g. ^{56}Fe, ^{239}Pu)

Long-term goal:

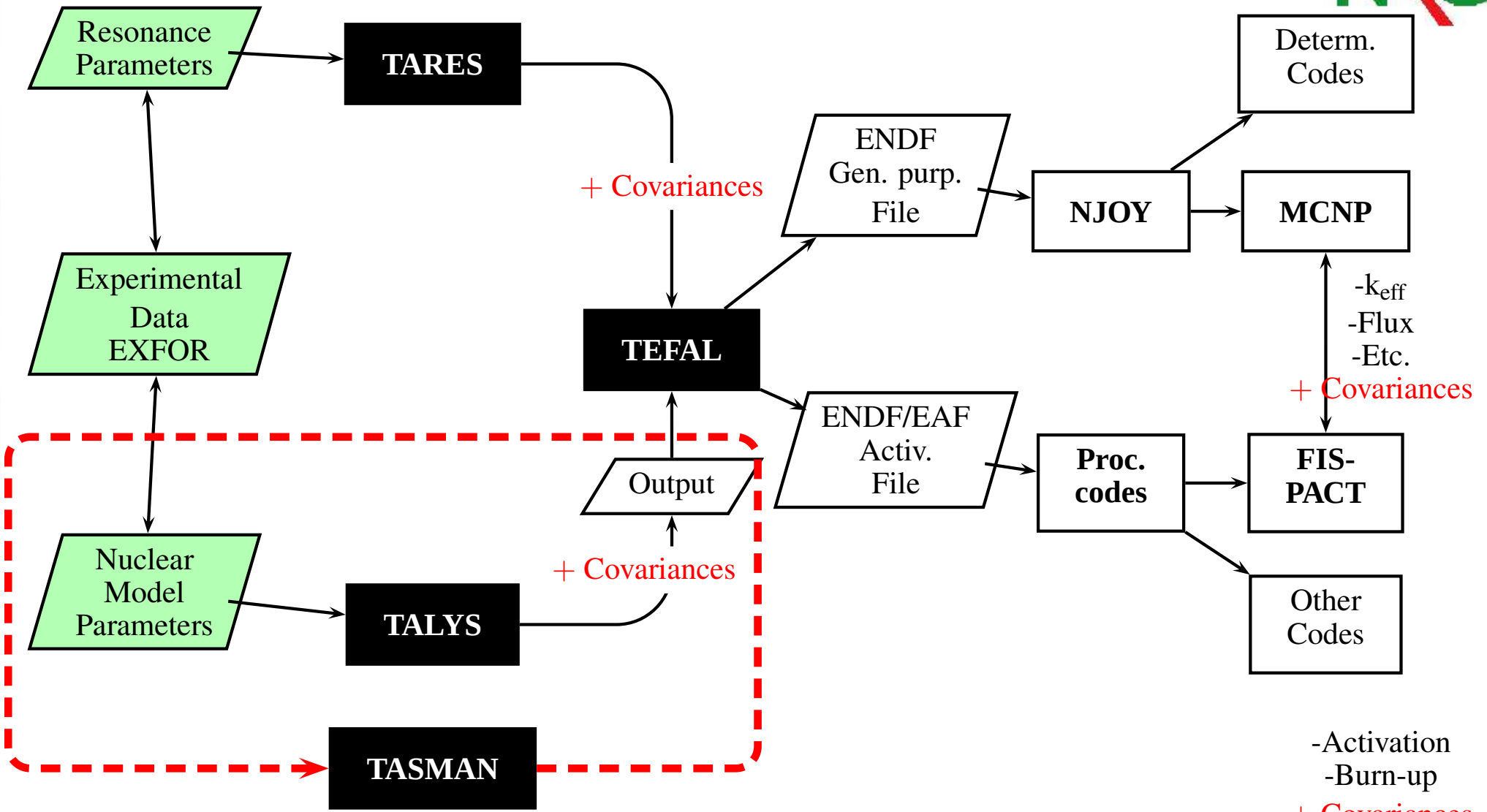
Generate nuclear data on the flight $\Longrightarrow$ no need of libraries anymore.
Until that time: TENDL-2009, TENDL-2010...

(*See last slide.*)

Concept: Standard nuclear data scheme



Concept: Nuclear Data Scheme with covariances



Monte Carlo: 1000 TALYS runs

Is that available ?

Yes !

Is that available ?

Yes !

Here

Here

Here

www.talys.eu/tendl-2009

Here

Here

Here

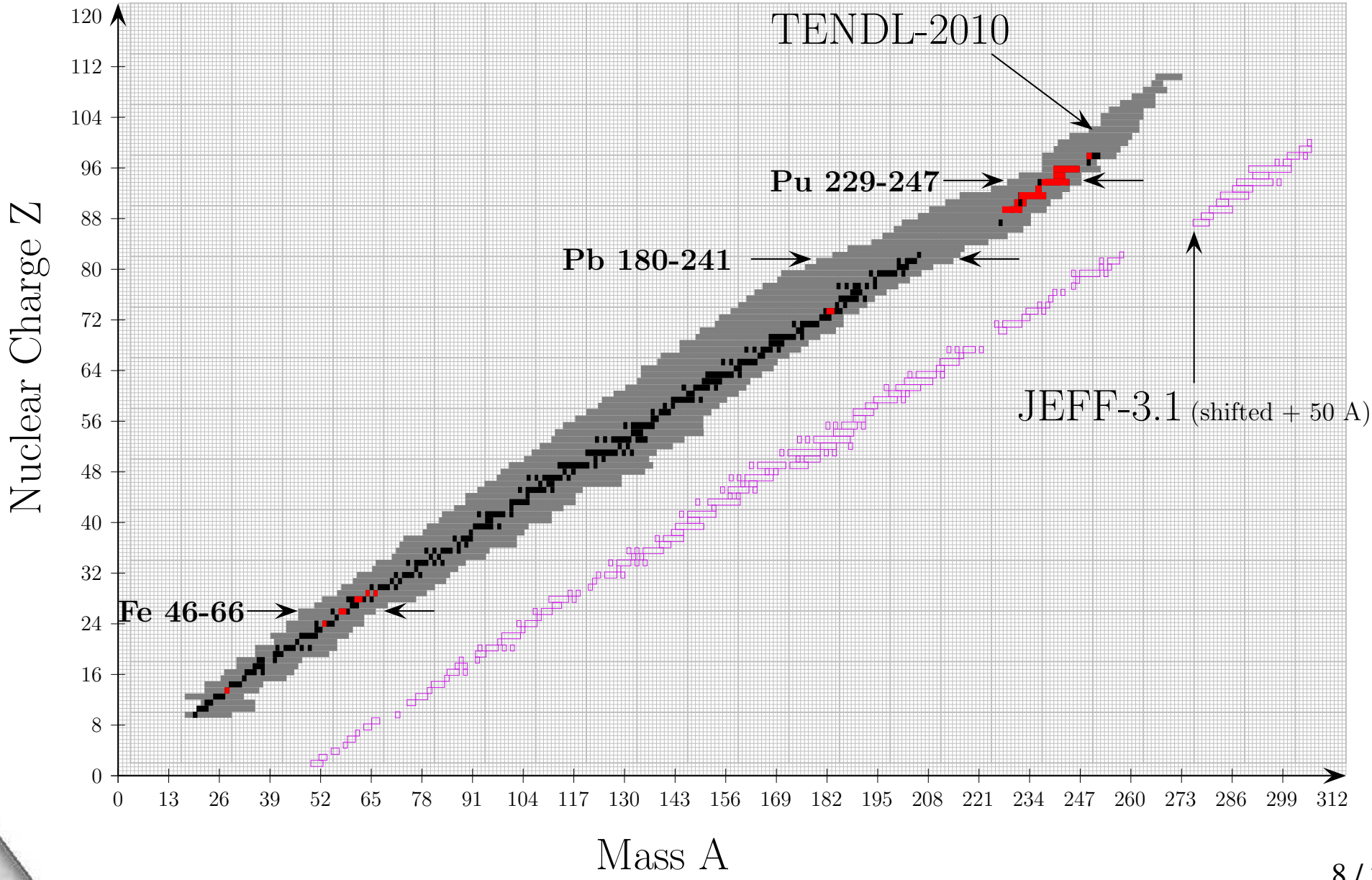
Content 1- TENDL-2009

- Neutrons: ENDF files, plots, ACE, EAF, processed files
- Protons, deuterons, tritons, alphas, gammas: ENDF files, ACE, EAF files
- Heavily based on TALYS, + other sourcesif TALYS is not yet good enough
- ...

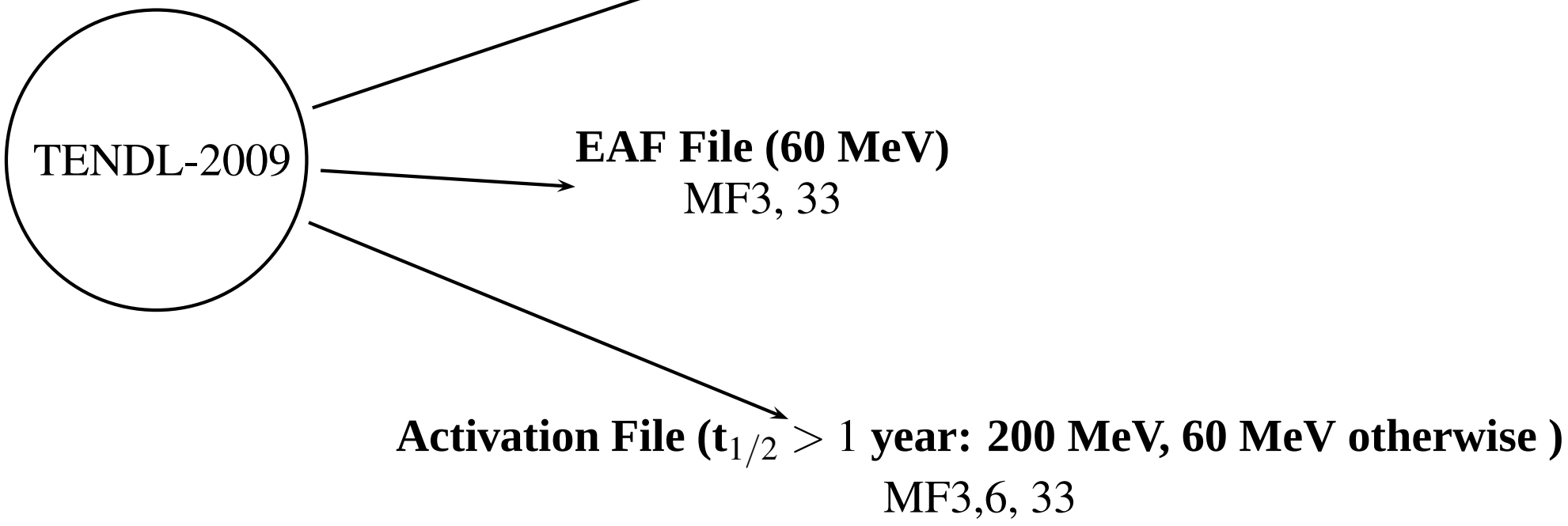
	Neutron	Proton	Deuteron	Triton	Alpha	Helium3	Photon	Fi. Yields
TENDL-2009	**2375**	**1163**	**1164**	**1116**	**1163**	**1127**	**1165**	**509**
TENDL-2008	348	344	336	339	342	338	327	
(JEFF-3.1)	*381*	*26*						*44*
(ENDF/B-VII.0)	*393*	*48*	*5*	*3*			*163*	*80*

Content 2- TENDL-2009 Neutron library: ^{19}F to ^{281}Ds ($t_{1/2} > 1$ sec)

Default Calculations | Medium Quality | Better Quality



Content 3- TENDL-2009 Transport, Activation and EAF files



Content 4- Available files

1. Tabular angular distributions
2. Tabular Gamma-ray intensities
3. Tabular partial cross sections to discrete levels
4. Tabular residual cross sections
5. Tabular cross sections
6. ENDF files including covariances
7. EAF cross section and variance files
8. Processed ACE files (with NJOY)
9. Processed AMPX files (with PUFF)
10. Processed covariances (tabular and plots)

Content 5- Fission yield sub-library

Independent and cumulative fission yields are provided for

- Isotopes: $^{223-226}$Ra, $^{225-227}$Ac, $^{227-234}$Th, $^{227-233}$Pa, $^{230-239}$U, $^{235-239}$Np, $^{236-244}$Pu, ^{240,241,243,244}Am, $^{240-249}$Cm, $^{245-249}$Bk, $^{248-253}$Cf, $^{252-255}$Es and ^{253,255,257}Fm
- Incident particles: spontaneous, neutron, proton, deuteron, triton, He3 and alpha
- Incident energies: (0.0253 eV, 1 eV, 100 eV, 500 keV, 1 MeV, 14 MeV) for neutrons and 20 MeV for others.

All independent and cumulative fission yields are calculated with the A. Wahl systematics.
But if evaluated in another library $\Longrightarrow$ imported if larger than 0.001 %.

Content 6- TENDL-2009 Neutron library: from MF-1 to MF-34

Content of a typical file up to 200 MeV:

- MF-1: Description + fission parameters
- MF-2: Resonance parameters (Reich-Moore or Multi-level Breit Wigner)
- MF-3: Cross sections (n,tot), (n,el), (n,non), (n,inl$_i$), ..., (n,γ), (n,p$_i$), (n,α_i)
- MF-4: Elastic angular distribution (Legendre Polynomials)
- MF-5: Fission neutron spectrum
- MF-6: Double differential distributions and spectra for (n,2n), ..., (n,α_i)
- MF- 8-10: Isomeric cross sections
- MF- 12-15: Gamma yields, angular distributions and spectra
- MF- 32-33-34: Resonance parameter covariances, cross section covariances, elastic angular distribution covariances

Content 7- TENDL-2009 Neutron library: Number of files

☞ Transport files	# Isotopes
❶ 200 MeV files:	376
❷ 60 MeV files:	1962
❸ 20 MeV files:	37
❹ MF-32 :	1123
❹ MF-33 & 34 :	1142
❺ ACE files:	1979
❻ AMPX files:	1100

☞ Fission Yields	
❶ Neutron induced:	78
❷ Spontaneous:	41

☞Activation files	# Isotopes
❶ 200 MeV files:	381
❷ 60 MeV files:	1993
❸ 20 MeV files:	34

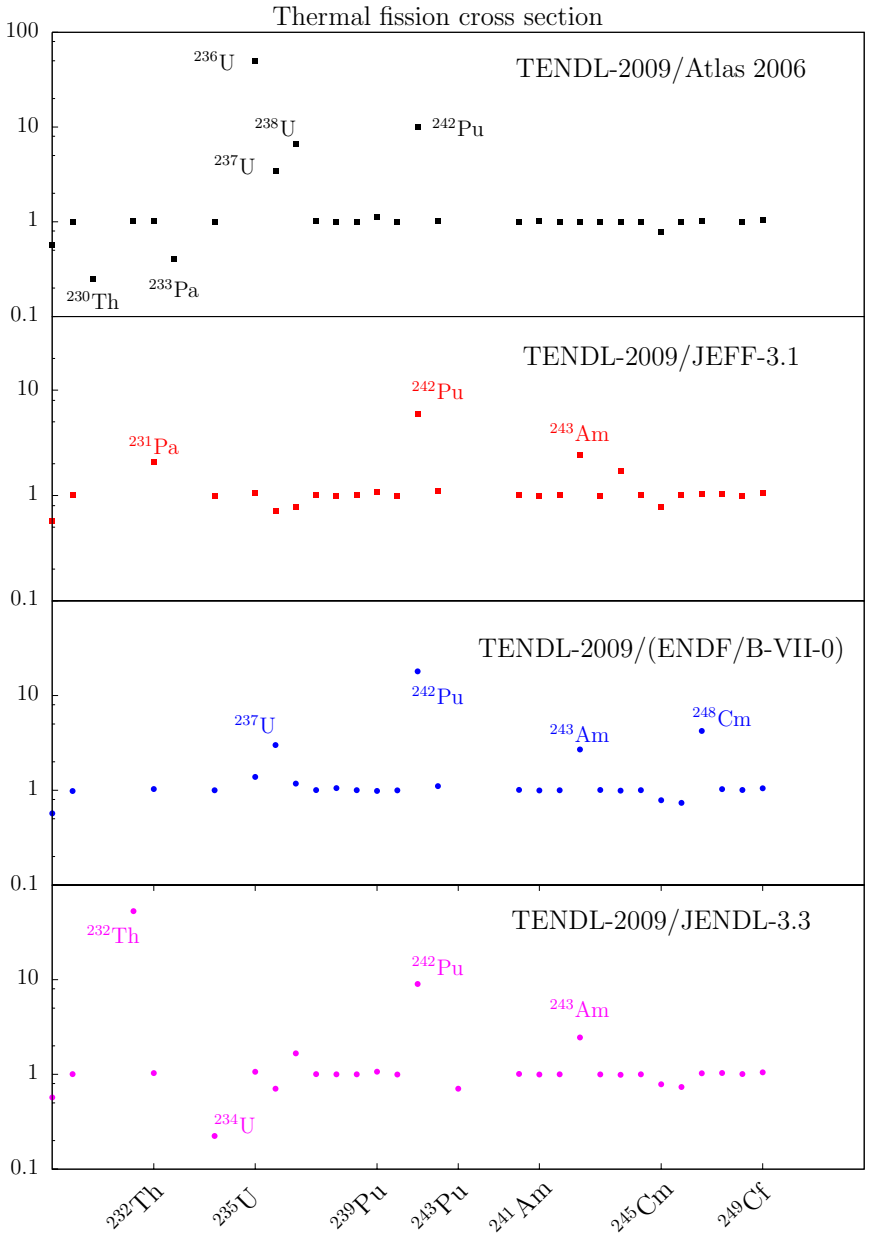
☞ EAF files	
❶ 60 MeV files:	2408
❷ Variance files:	1148

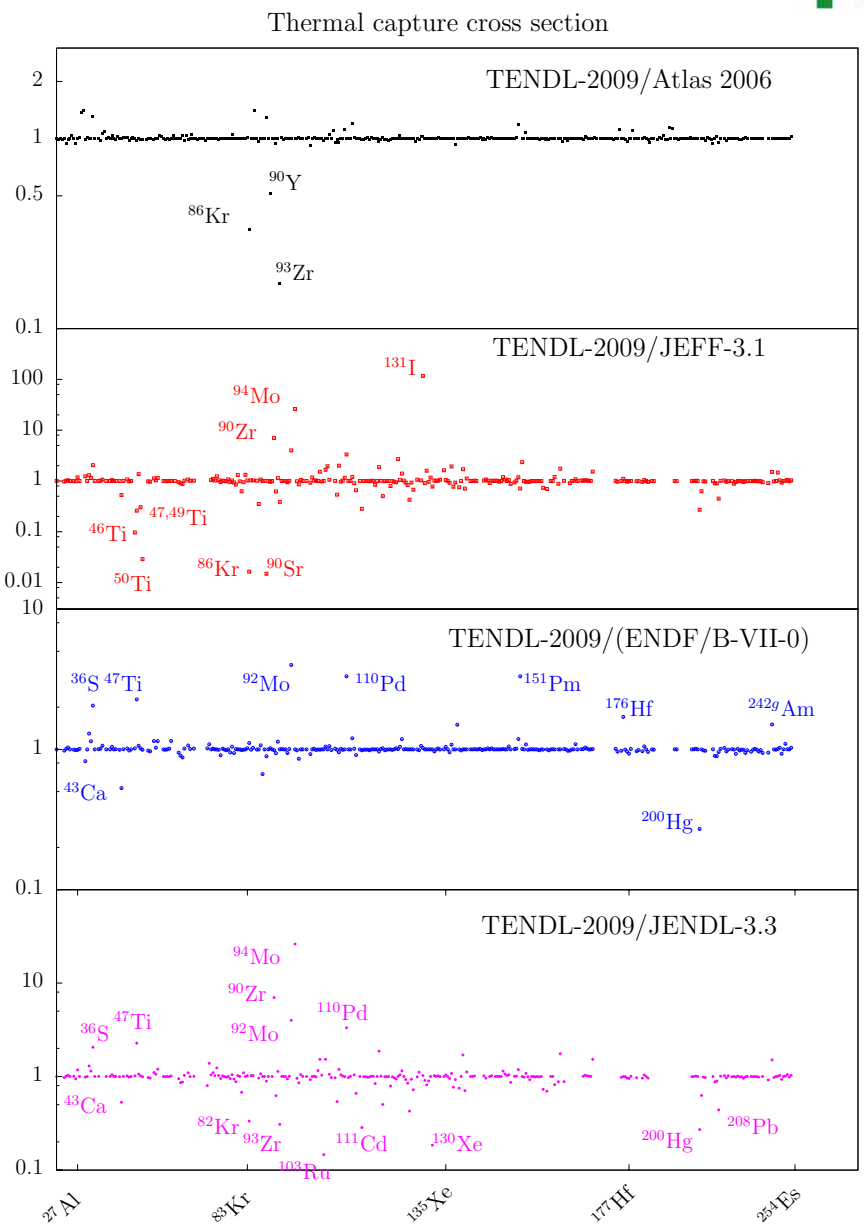
Content 8- TENDL-2009 Neutron library: Actinides

Element	Isotopes	Element	Isotopes
Th	208-227, 228-232, 233-239	Pa	213-230, 231,233, 234-239
U	222-232, 233-238, 239-242	Np	225-236, 237, 238-244
Pu	229-237, 238-244, 245-247	Am	232-238, 239-243, 245-247
Cm	238-242, 243-248, 249-252	Bk	238-248, 249, 250, 251
Cf	237-248, 249, 250-256	Es	241-253, 254, 255-257
Fm	242-257	Md	245-260
No...Ds			

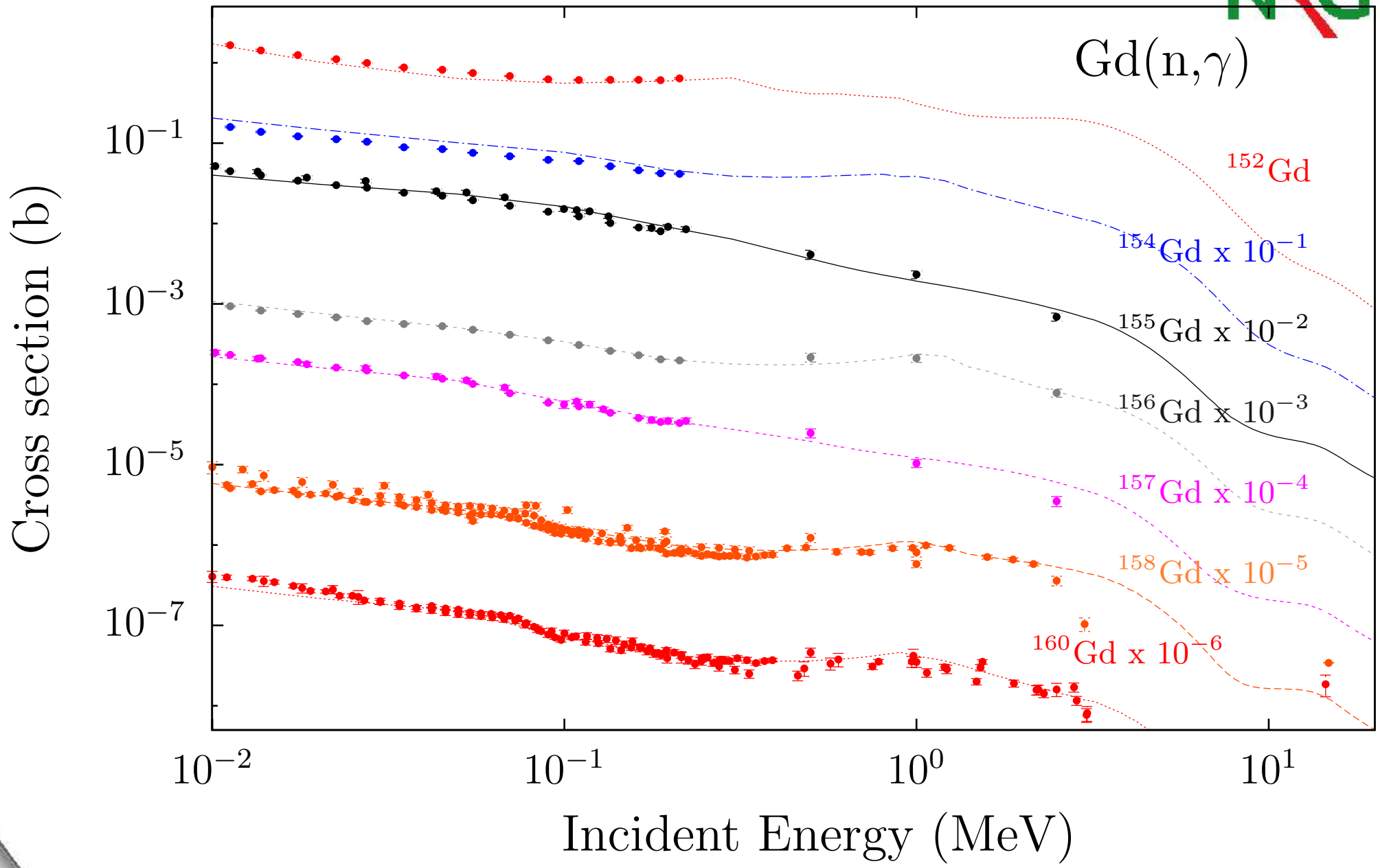
$\Longrightarrow$ 36 "medium" or "better" quality evaluations and 406 "default" quality evaluations (with isomers)

Examples 1: Ratio of capture thermal cross sections

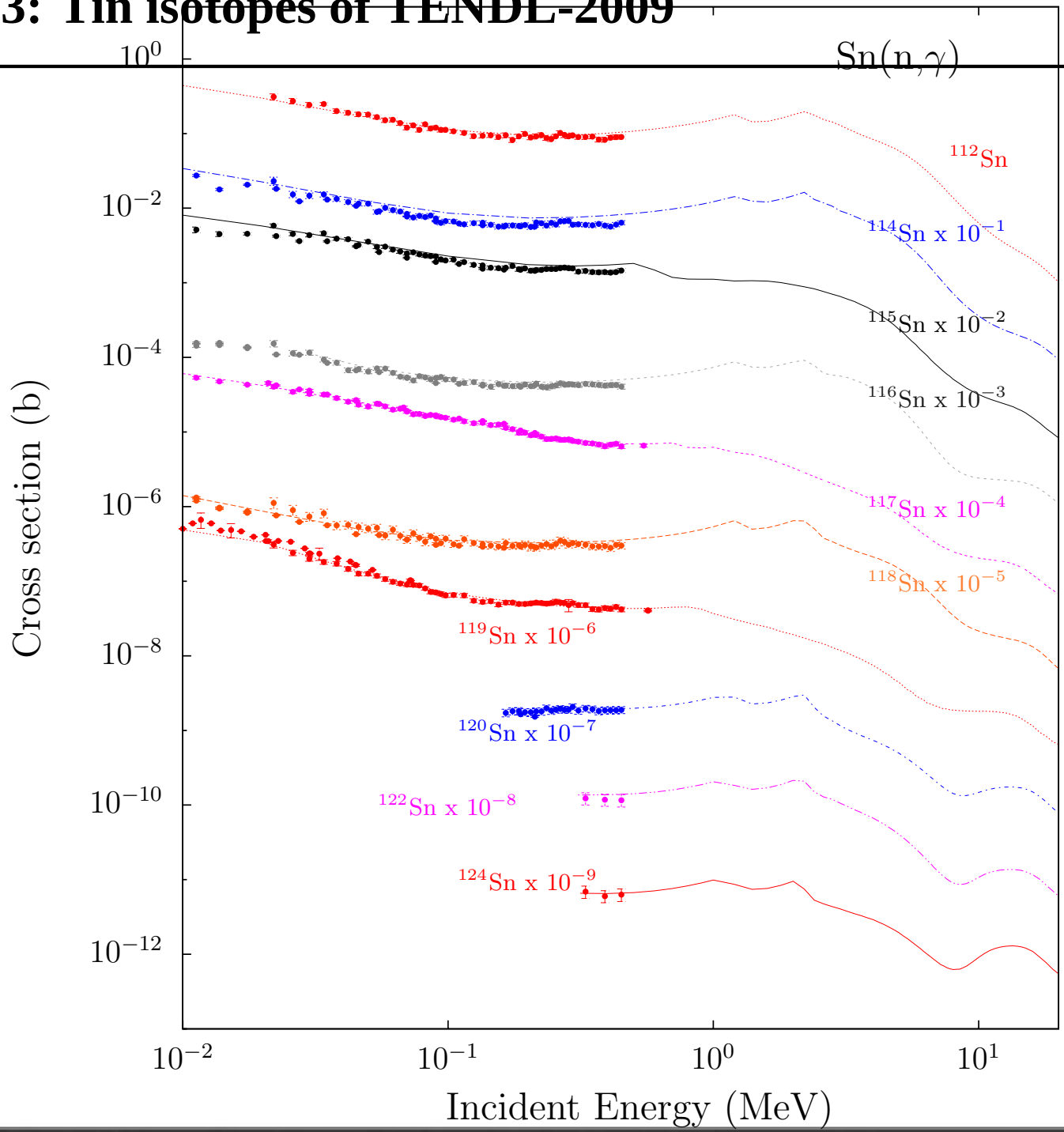




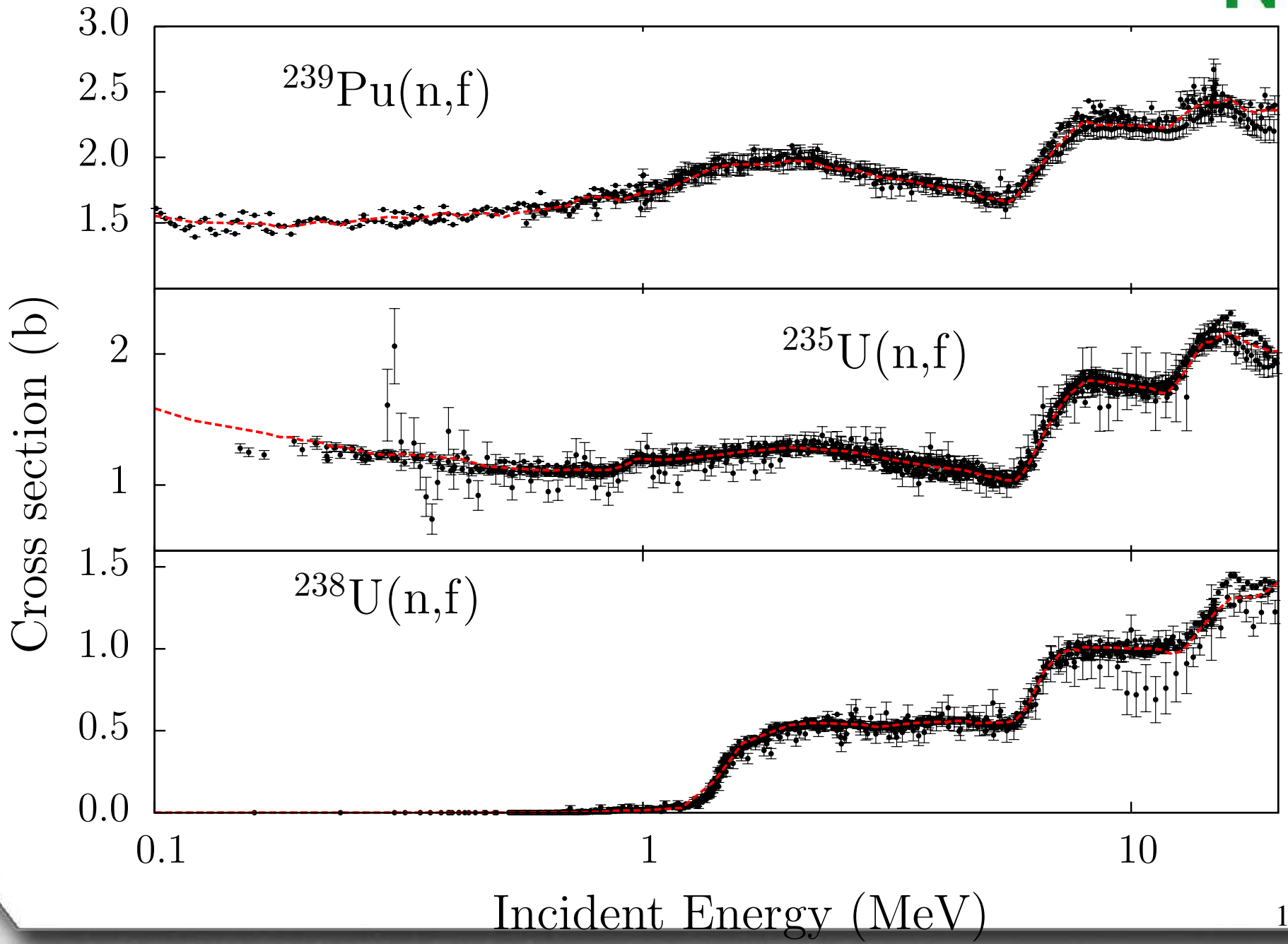
Examples 2: Gadolinium isotopes of TENDL-2009



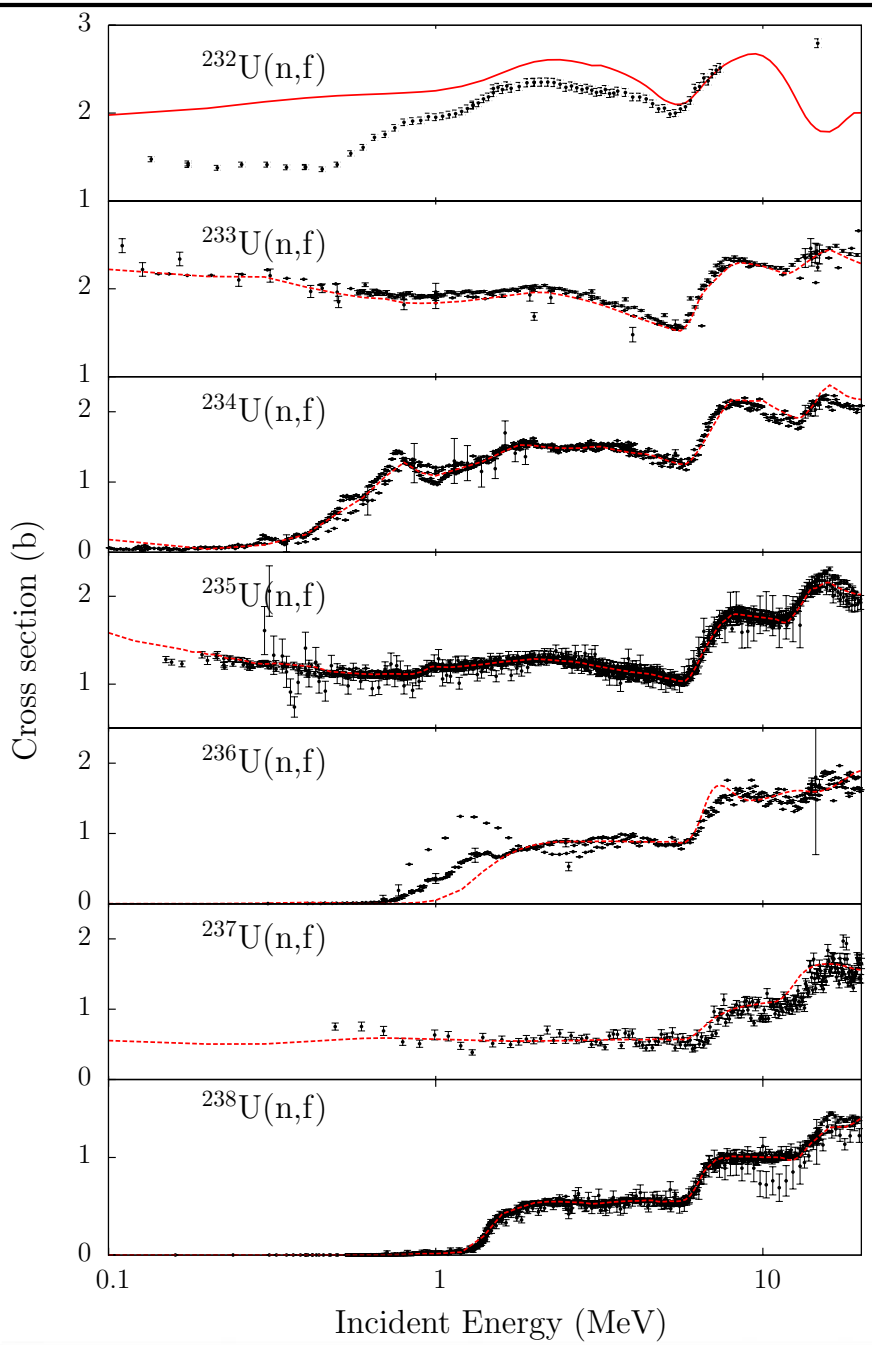
Examples 3: Tin isotopes of TENDL-2009

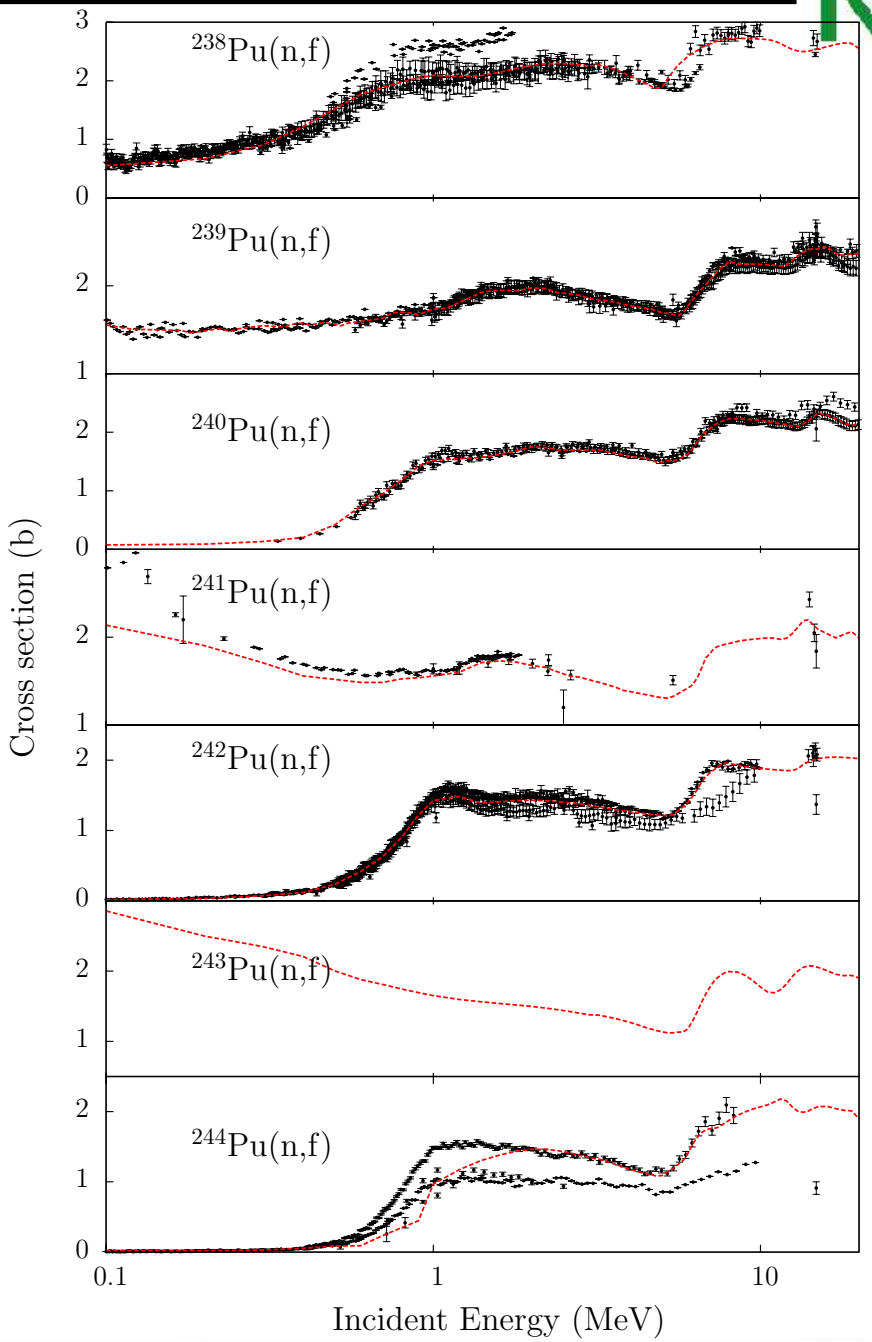


Examples 4: Some actinides of TENDL-2009



Examples 5: U and Pu isotopes of TENDL-2009





Covariance generation with TALYS via Monte Carlo

Let $\vec{\mathbf{p}}$ be the vector of the L adjustable nuclear model parameters that are relevant to the problem under consideration, *i.e.*

$$\vec{\mathbf{p}} = \{p_1, \ldots, p_l, \ldots, p_L\} \Longrightarrow p_l^{(k)} = p_l^{(0)} \pm \Delta p_l, \qquad l = 1, L$$

The basis of our method is to let TALYS perform many calculations:

$$\vec{\sigma}^{(k)} = T(\vec{\mathbf{p}}^{(k)})$$

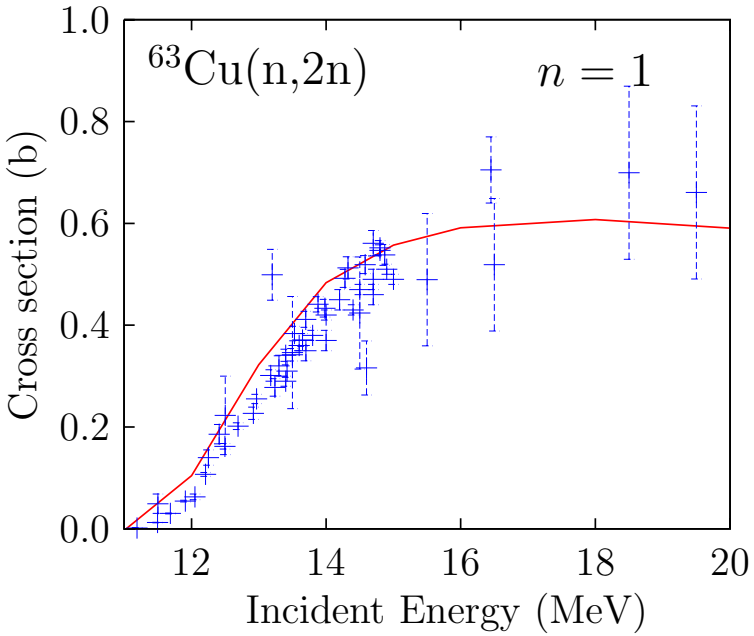
The average covariance matrix for cross sections is given by

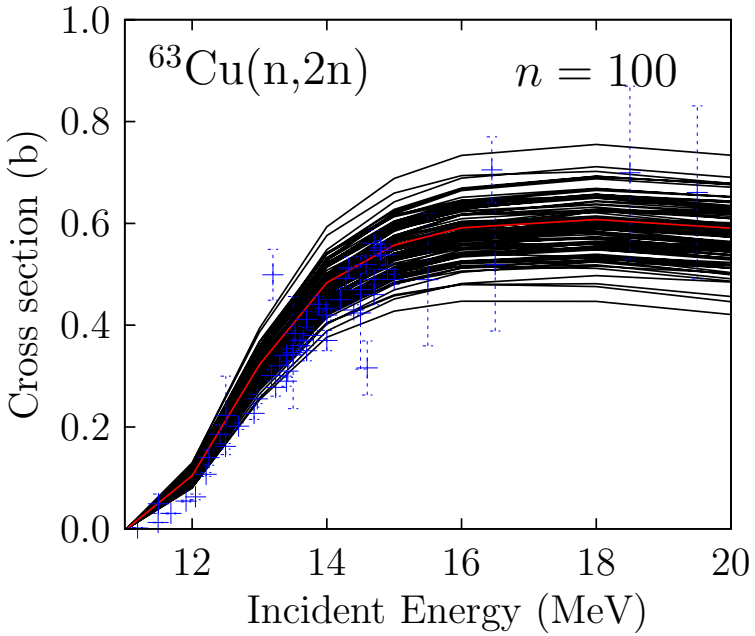
$$V_{ij} = \frac{1}{K} \sum_{k=1}^{K} (\sigma_i^{(k)} - \sigma_i^{(0)})(\sigma_j^{(k)} - \sigma_j^{(0)}), \qquad i, j = 1, N,$$

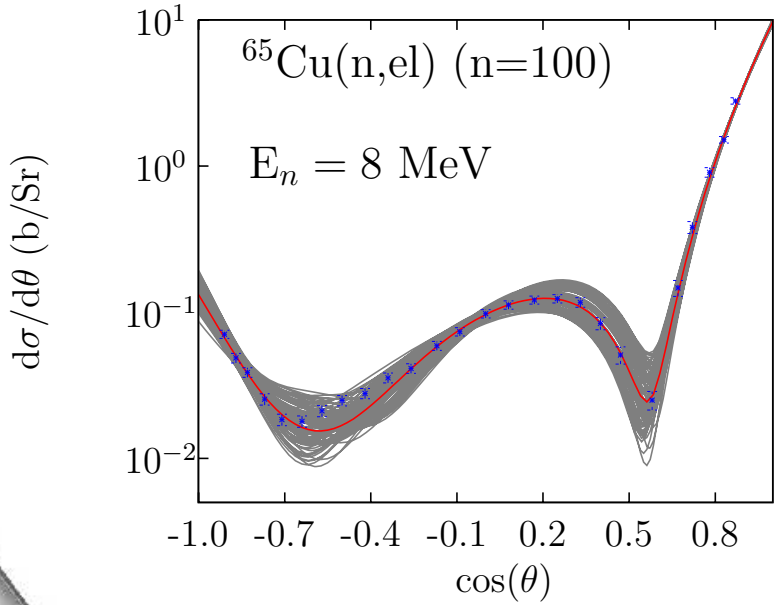
where K is the total number of TALYS runs needed for statistical convergence. The average calculated cross sections are

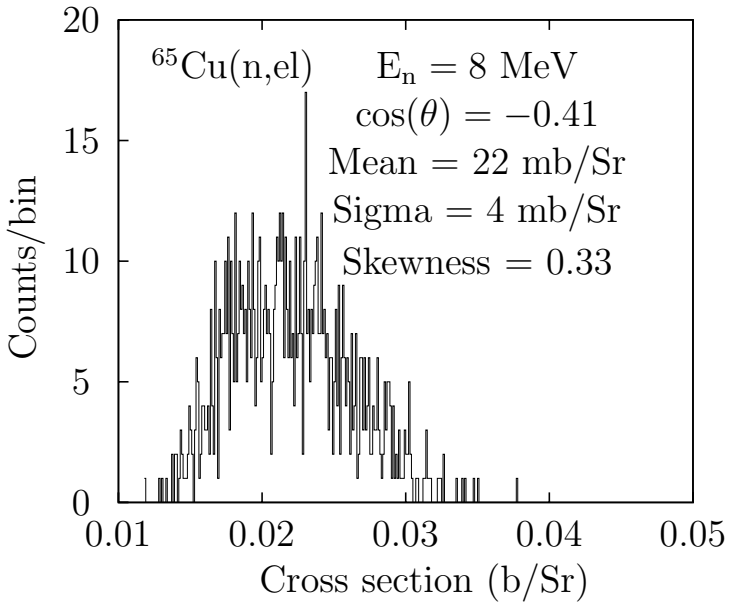
$$\bar{\sigma}_i = \frac{1}{K} \sum_{k=1}^{K} \sigma_i^{(k)}, \qquad i = 1, N,$$

Covariances: example









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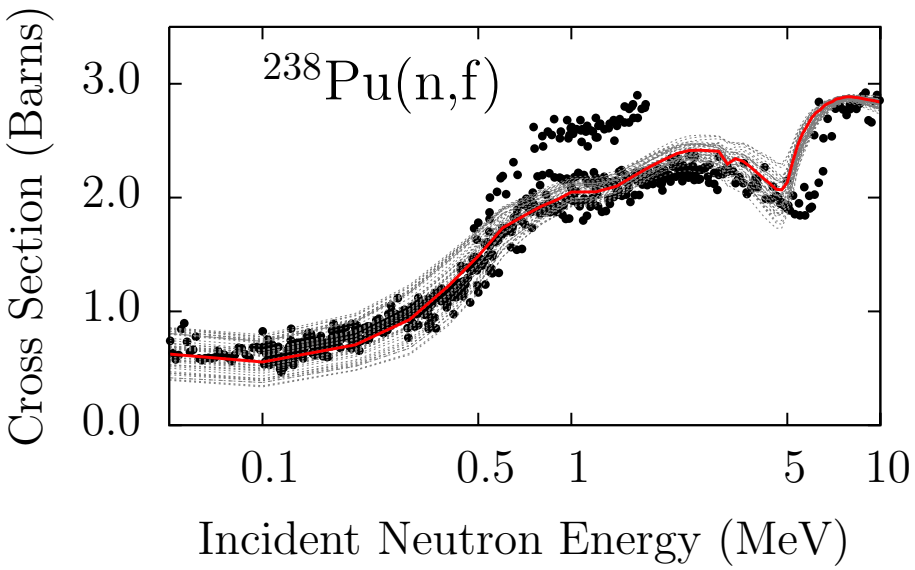

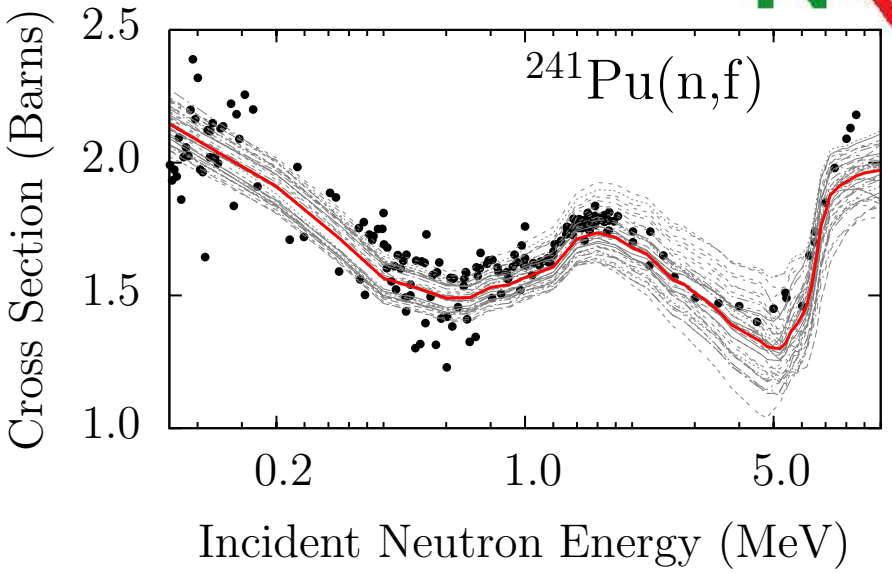

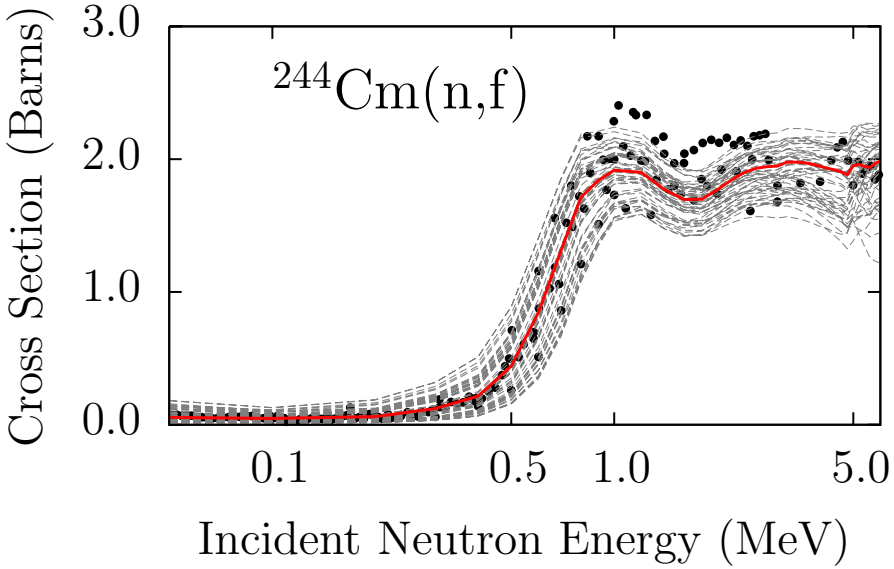

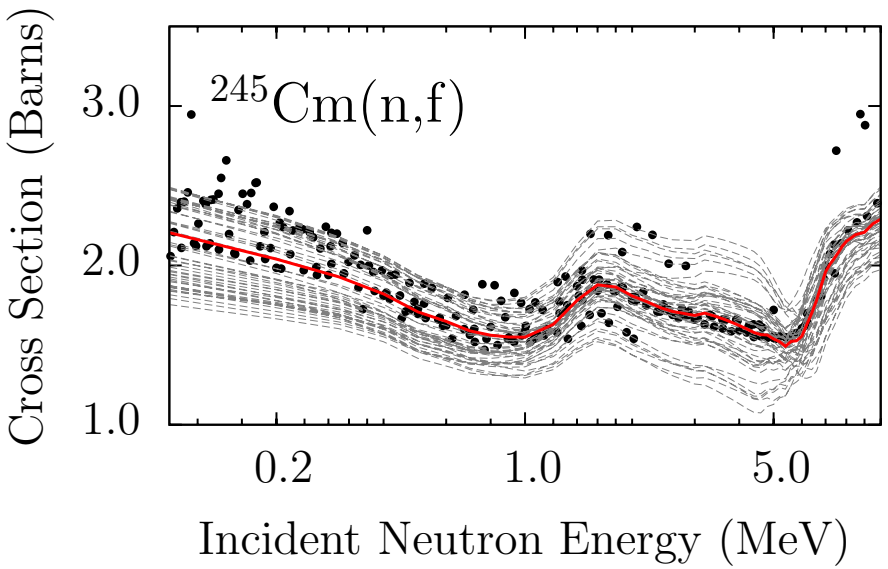

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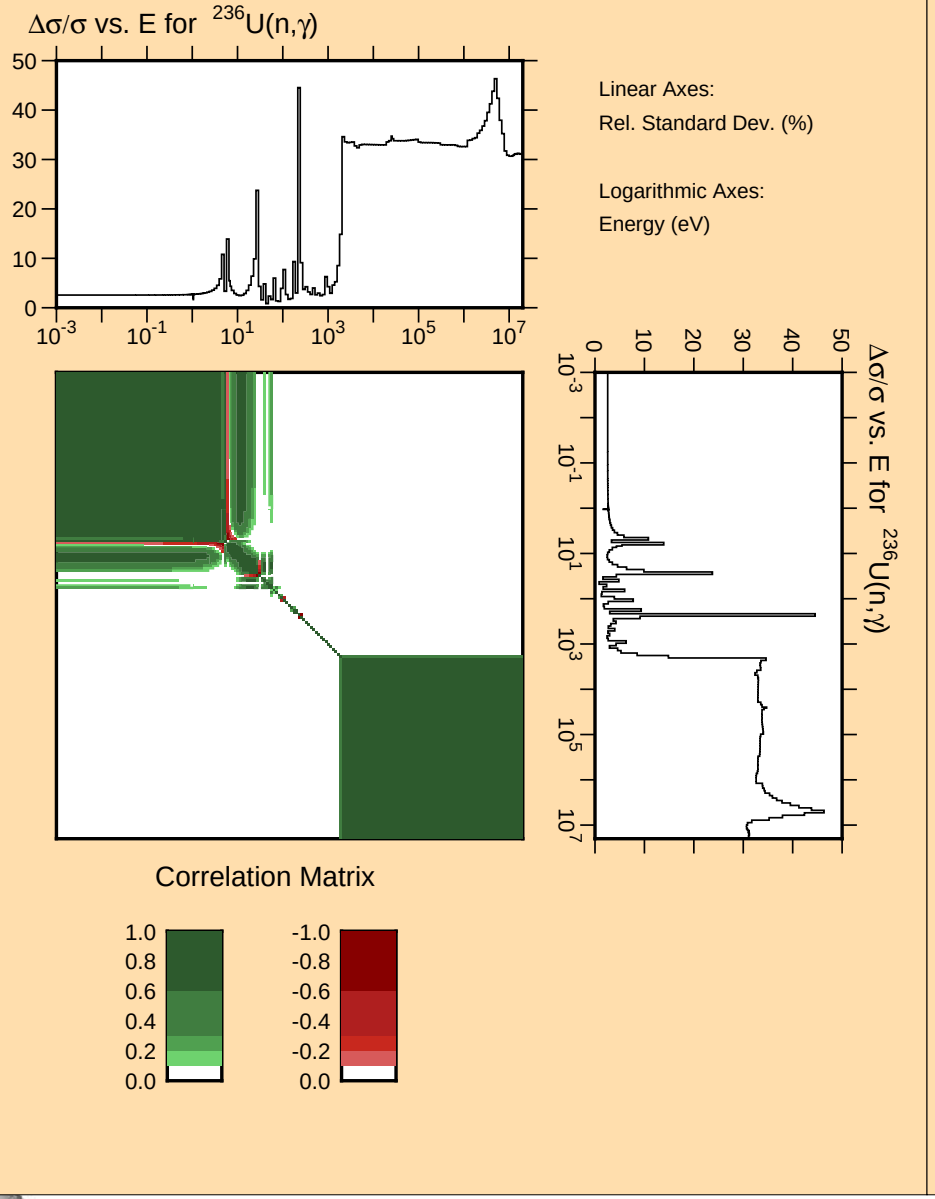
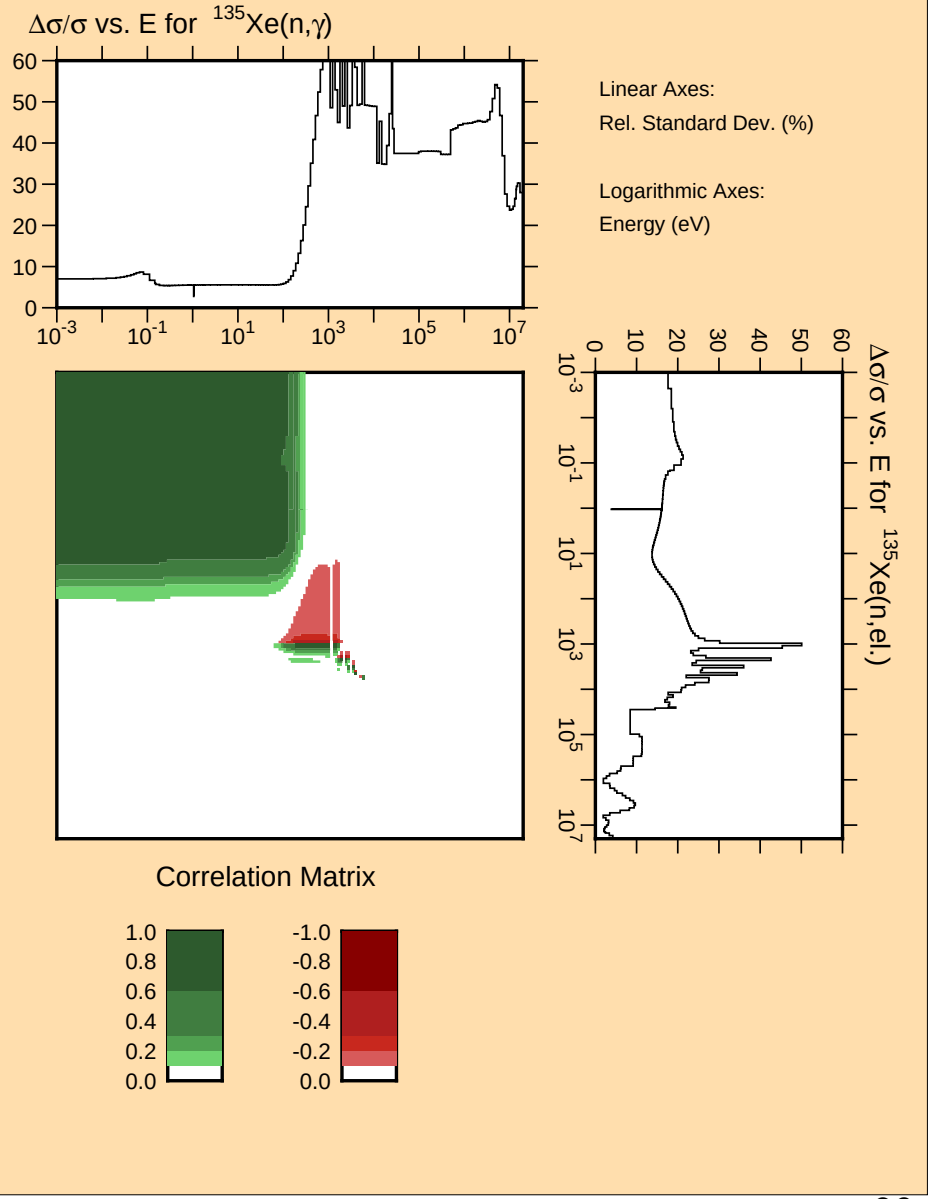




TENDL-2009: validation

Table 1: Number of benchmarks per main ICSBEP category used in the validation of TENDL-2009.

Category	Energy Range	Number	Category	Energy Range	Number
LEU	Thermal	219	^{239}Pu	Thermal	87
HEU	Thermal	92	^{239}Pu	Fast	5
HEU	Fast	64	^{239}Pu	Mixed	6
HEU	Inter	9	Other	Thermal	48
HEU	Mixed	5	Other	Fast	15
^{233}U	Thermal	13	^{233}U	Fast	4
Total		556			

Validation: global comparison of 556 crit-safety benchmarks

As a large number of results are available, a global normalised $\chi^2_{\mathrm{N,library}}$ is calculated over all k_{eff}s to facilitate comparison between libraries. The following formula is used for each library (C being the calculated value and E the value of the benchmark):

$$\chi^2_{\mathrm{library}} = \sum_{i}^{\mathrm{benchmarks}} \frac{(C_i^{\mathrm{library}} - E_i)^2}{E_i}$$

Then all $\chi^2_{\mathrm{library}}$ for the five libraries are normalized to $\chi^2_{\mathrm{ENDF/B-VII.0}}$:

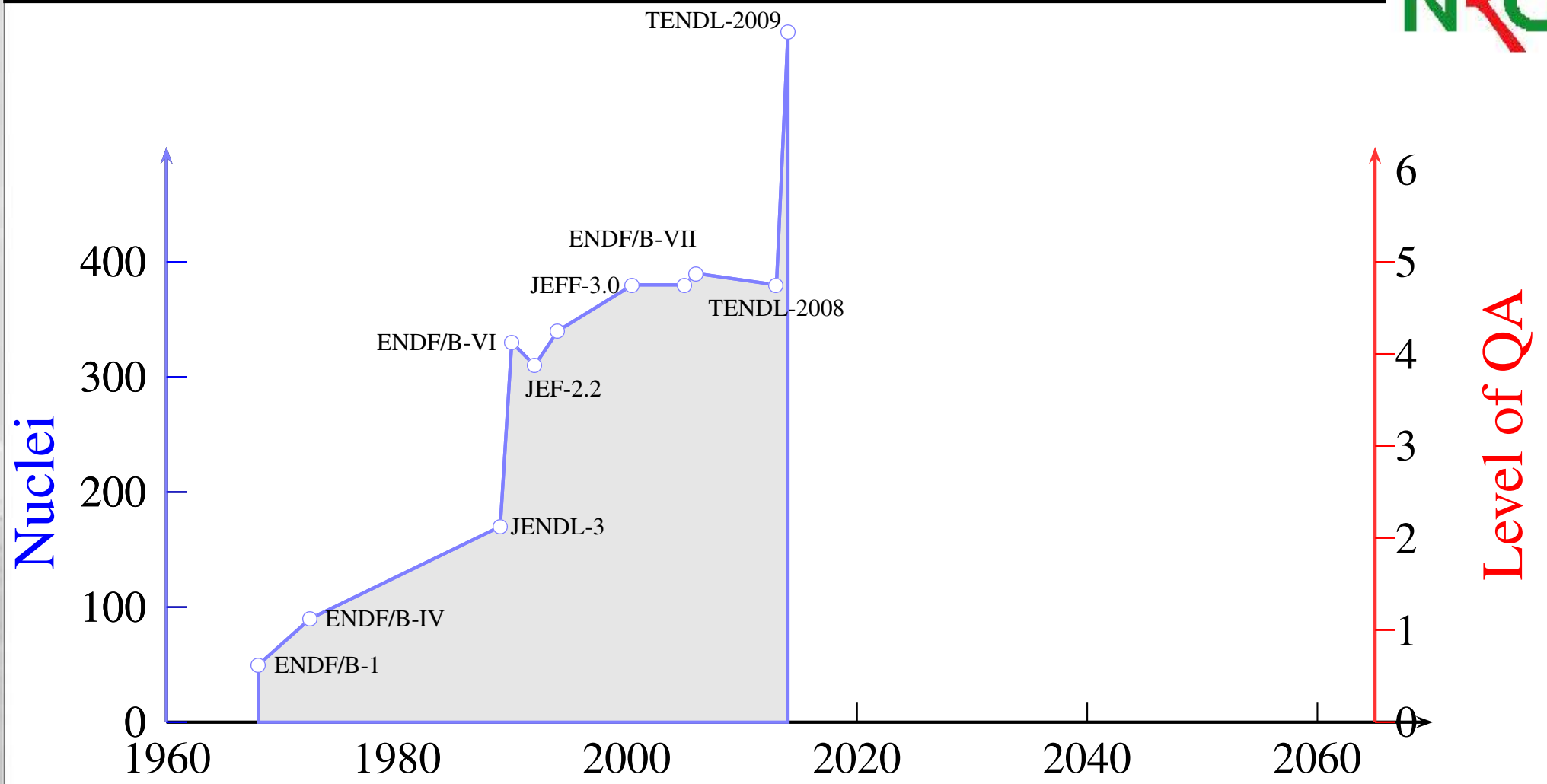
$$\chi^2_{\mathrm{Normalized,library}} = \frac{\chi^2_{\mathrm{library}}}{\chi^2_{\mathrm{ENDF/B-VII.0}}}$$

$$\mathrm{library} = \begin{pmatrix} \mathrm{ENDF/B-VII.0} \\ \mathrm{TENDL-2009} \\ \mathrm{JEFF-3.1} \\ \mathrm{JENDL-3.3} \\ \mathrm{ENDF/B-VI.8} \end{pmatrix} \quad (1)$$

Validation: global χ^2 comparison of 556 crit-safety benchmarks

Library	Normalized χ^2_N					
	Global	LEU	HEU	^{239}Pu	Other	^{233}U
	556	219	170	87	63	17
ENDF/B-VII.0	1.00	1.00	1.00	1.00	1.00	1.00
ENDF/B-VI.8	1.20	1.37	1.27	0.81	1.12	2.52
JEFF-3.1	1.18	0.80	1.43	0.77	1.04	1.68
JENDL-3.3	1.29	0.85	1.48	1.59	1.12	0.42
TENDL-2009	0.98	1.05	0.95	1.01	1.00	1.02

Back to the motivations: where are we ?



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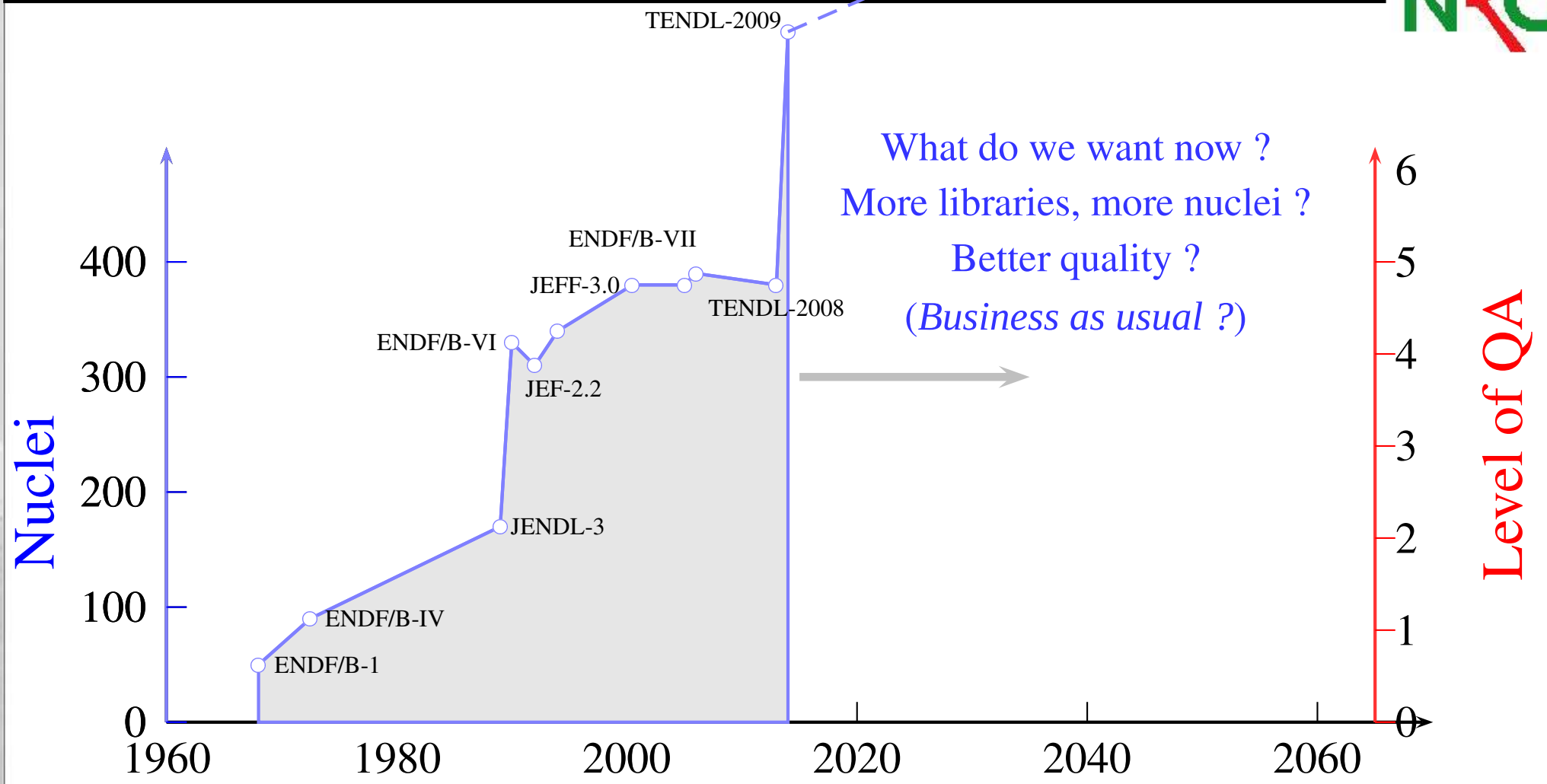

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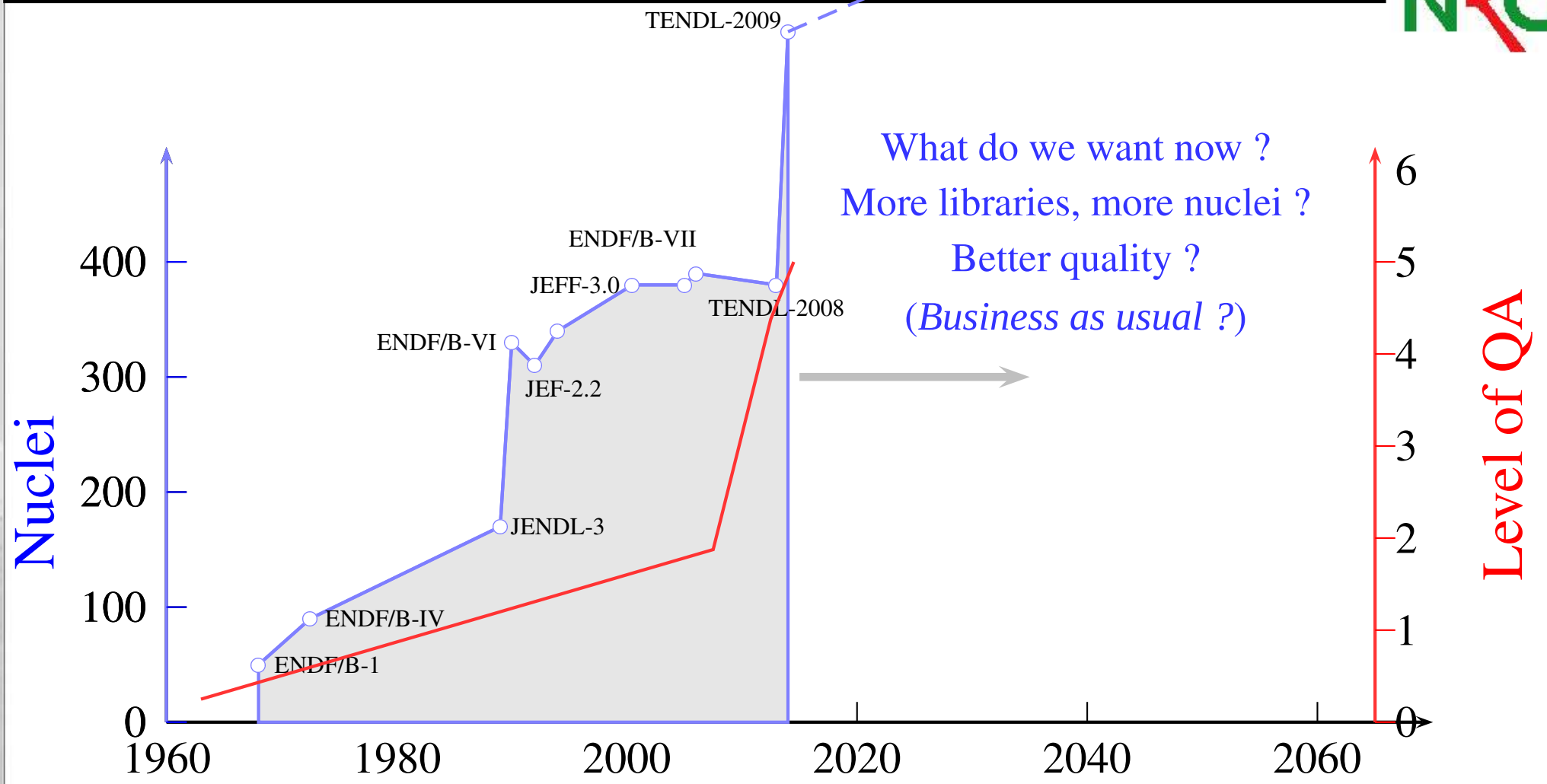

QA 0: All manual work

QA 1: Manual/auto + Checkr, Fizcon, Psyche

QA 2: QA 1 + Njoy, MCNP

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QA 5: QA 4 + full automation

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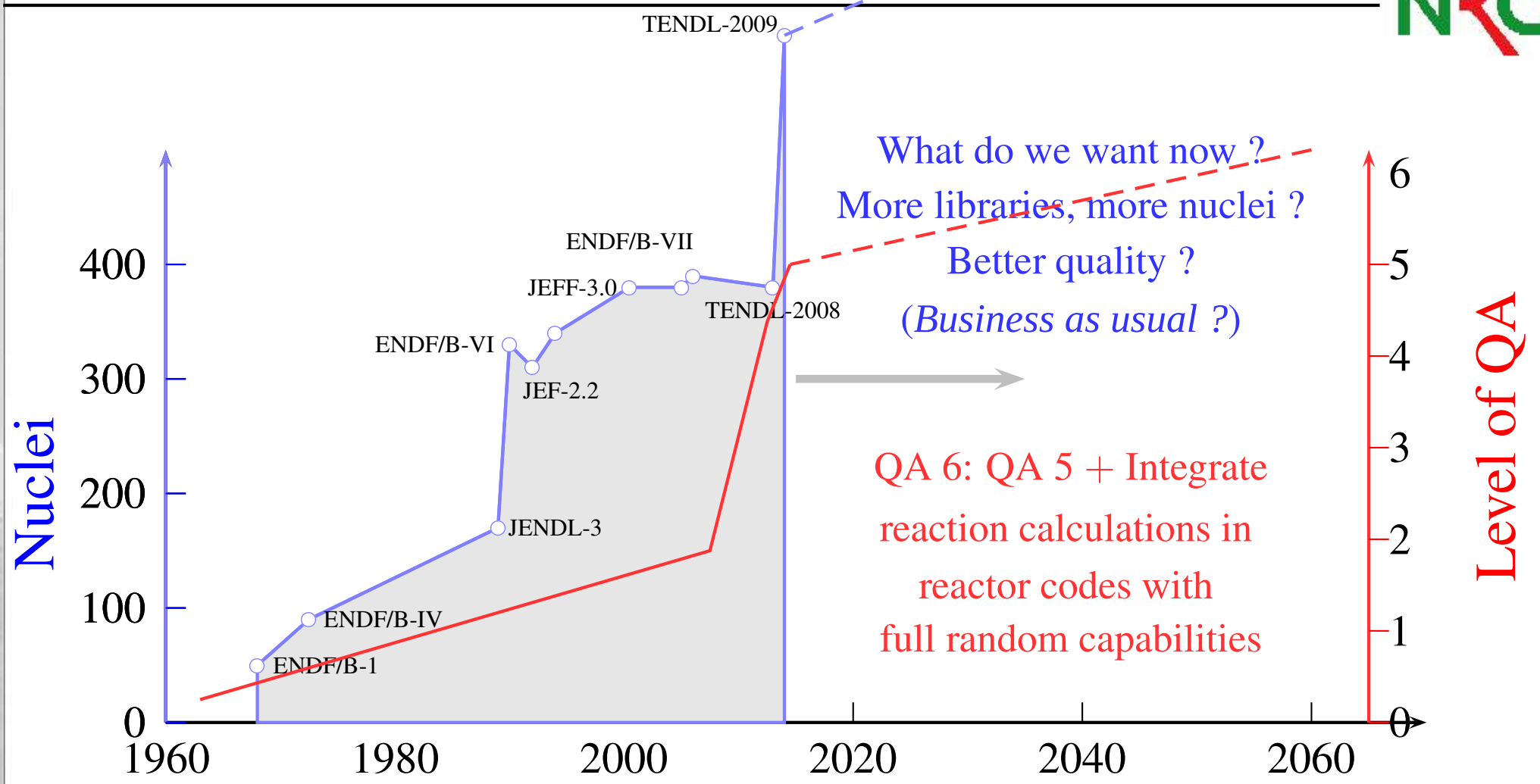

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Conclusions and Future improvements

- Consistent, complete data files with automatic updates for all actinides, projectiles, energies reaction channels and quantities,
- Extensive set of covariance files,
- Reproducible with TALYS-1.2 (released in December)
- Detailed TALYS and resonance parameter fitting per individual isotope
- Will be used to complete JEFF-3.2

Release date: November 23th, 2009

- Possibility to adopt an entire existing data library (e.g. JEFF-3.1.1)
- More extensive validation (shielding...)
- Improve global model and uncertainties, Addition of original URR, covariances for ν-bar and fission neutron spectrum