

TENDL-2009: Towards completeness and accuracy

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Contents



① Motivations:

\implies *a roadmap to consistent and state-of-the-art evaluations*

② Concept:

\implies *TALYS system + Monte Carlo = TENDL-2009*

③ Content 1:

\implies *Neutrons, protons, deuterons, tritons, alphas, photons*

④ Content 2:

\implies *Neutrons: ^{19}F to ^{281}Ds ($Z=110$), from MF-1 to MF-34*

⑤ Covariances

⑥ Validations

⑦ Conclusions and Future Improvements

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)

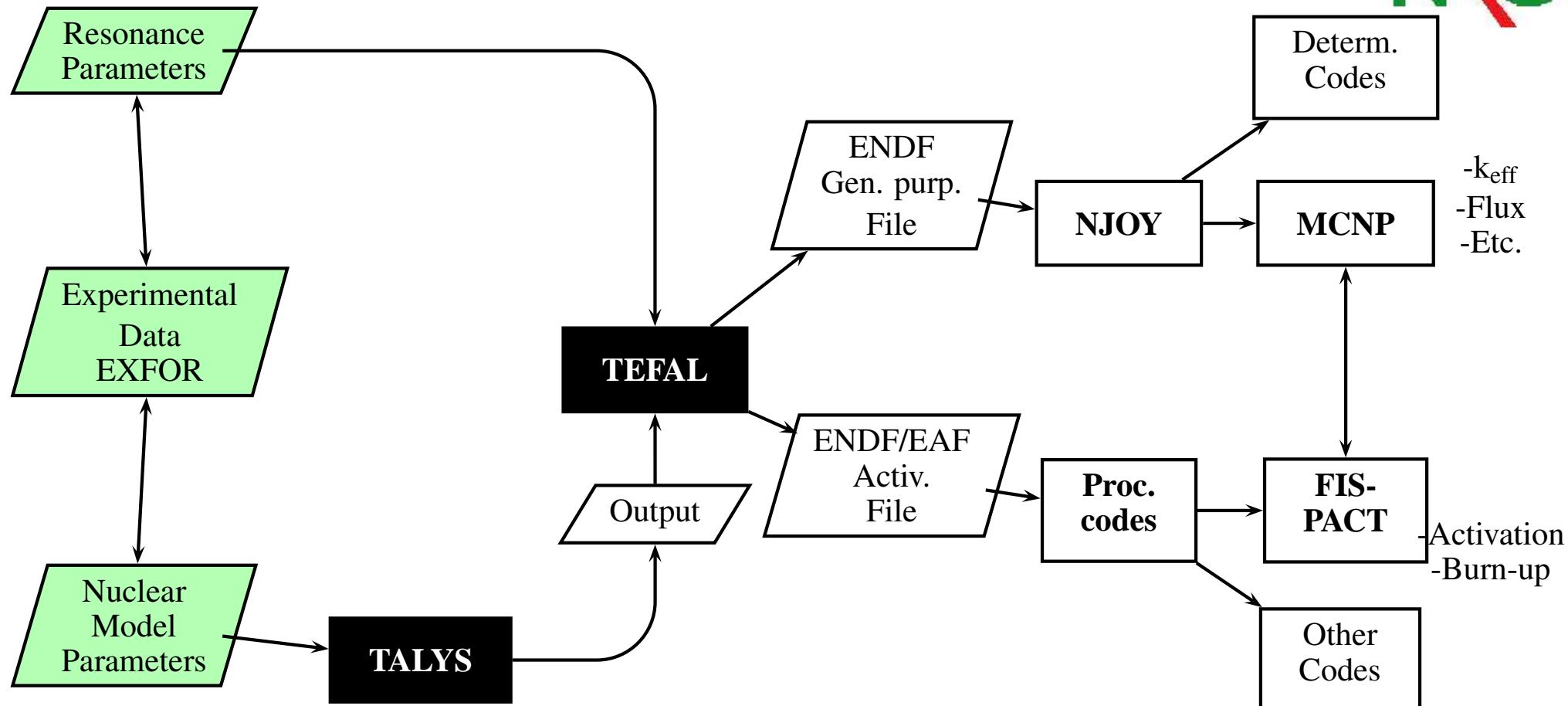
Long-term goal:

Generate nuclear data on the flight \implies no need of libraries anymore.

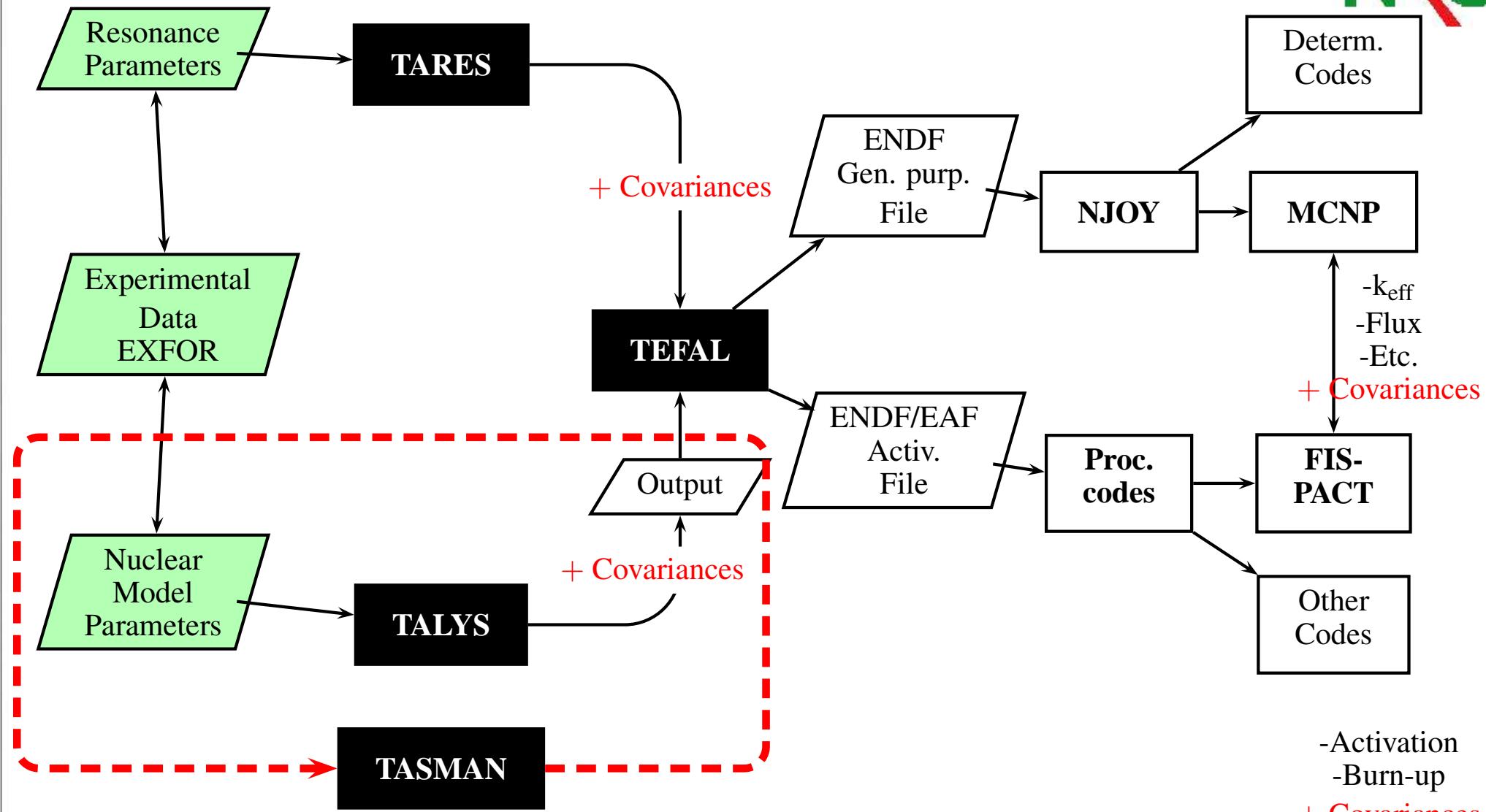
Until that time: TENDL-2009, TENDL-2010...

(See last slide.)

Concept: Standard nuclear data scheme



Concept: Nuclear Data Scheme with covariances



Monte Carlo: 1000 TALYS runs

-Activation
-Burn-up
+ Covariances

Is that available ?

Yes !



Is that available ?



Yes !

Here

Here

www.talys.eu/tendl-2009

Here

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 sources if TALYS is not yet good enough
- ...

	<i>Neutron</i>	<i>Proton</i>	<i>Deuteron</i>	<i>Triton</i>	<i>Alpha</i>	<i>Helium3</i>	<i>Photon</i>	<i>Fi. Yields</i>
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

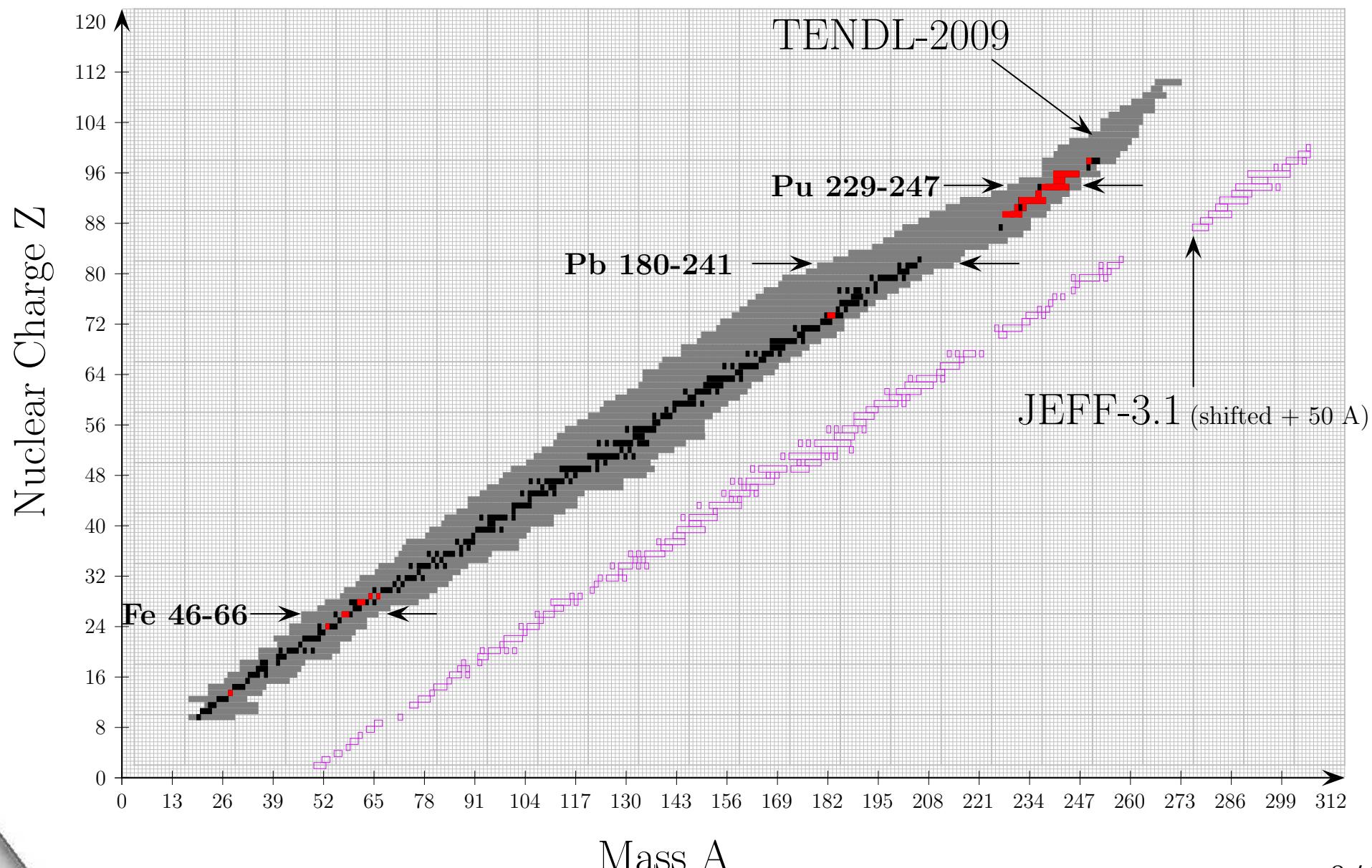
Content 2- TENDL-2009 Neutron library: ^{19}F to ^{281}Ds ($t_{1/2} > 1$ sec)

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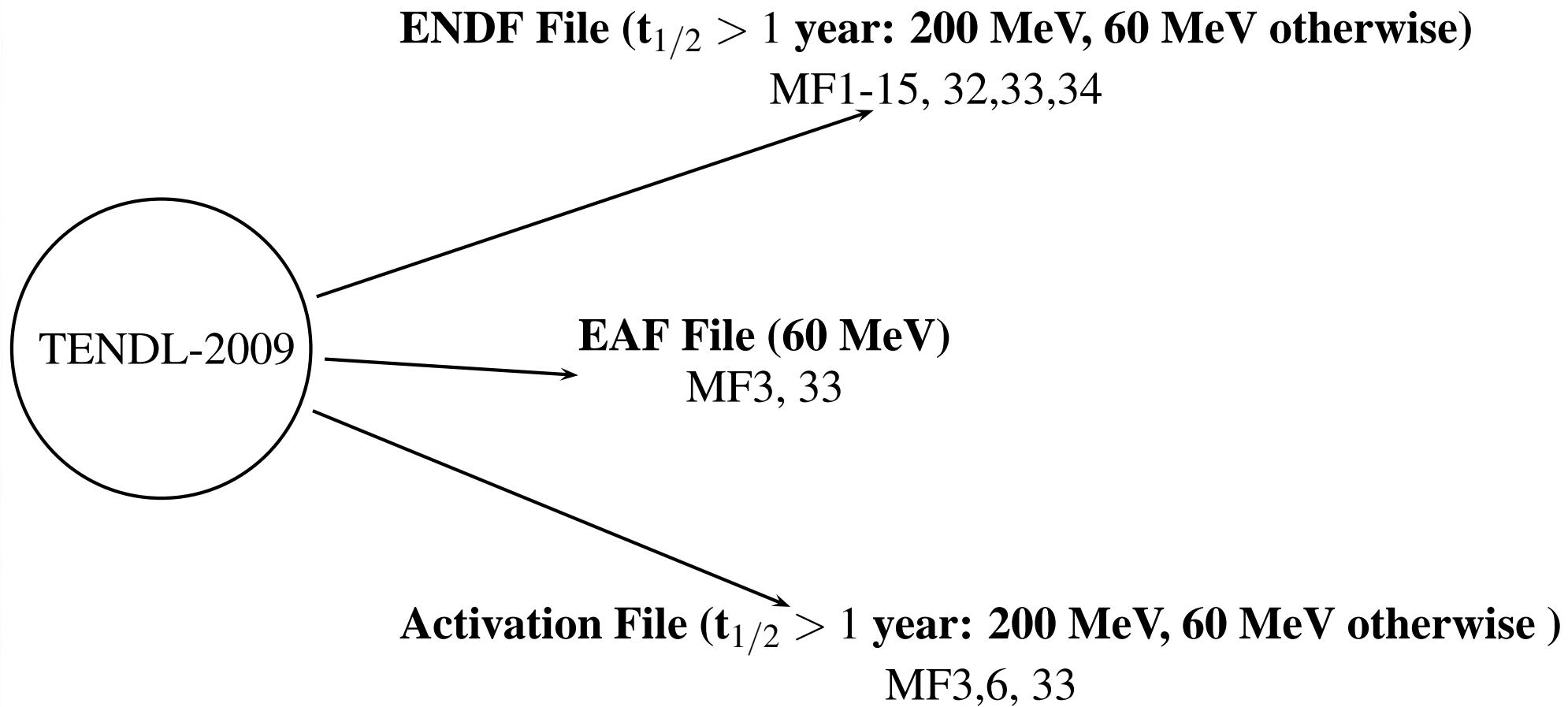
Default Calculations

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: $^{223-226}\text{Ra}$, $^{225-227}\text{Ac}$, $^{227-234}\text{Th}$, $^{227-233}\text{Pa}$, $^{230-239}\text{U}$, $^{235-239}\text{Np}$,
 $^{236-244}\text{Pu}$, $^{240,241,243,244}\text{Am}$, $^{240-249}\text{Cm}$, $^{245-249}\text{Bk}$, $^{248-253}\text{Cf}$, $^{252-255}\text{Es}$ and
 $^{253,255,257}\text{Fm}$
- ☞ 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 \Rightarrow 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	☞ Fission Yields	
① 200 MeV files:	376	① Neutron induced:	78
② 60 MeV files:	1962	② Spontaneous:	41
③ 20 MeV files:	37		
④ MF-32 :	1123		
④ MF-33 & 34 :	1142		
⑤ ACE files:	1979		
⑥ AMPX files:	1100		
☞ Activation files	# Isotopes	☞ EAF files	
① 200 MeV files:	381	① 60 MeV files:	2408
② 60 MeV files:	1993	② Variance files:	1148
③ 20 MeV files:	34		

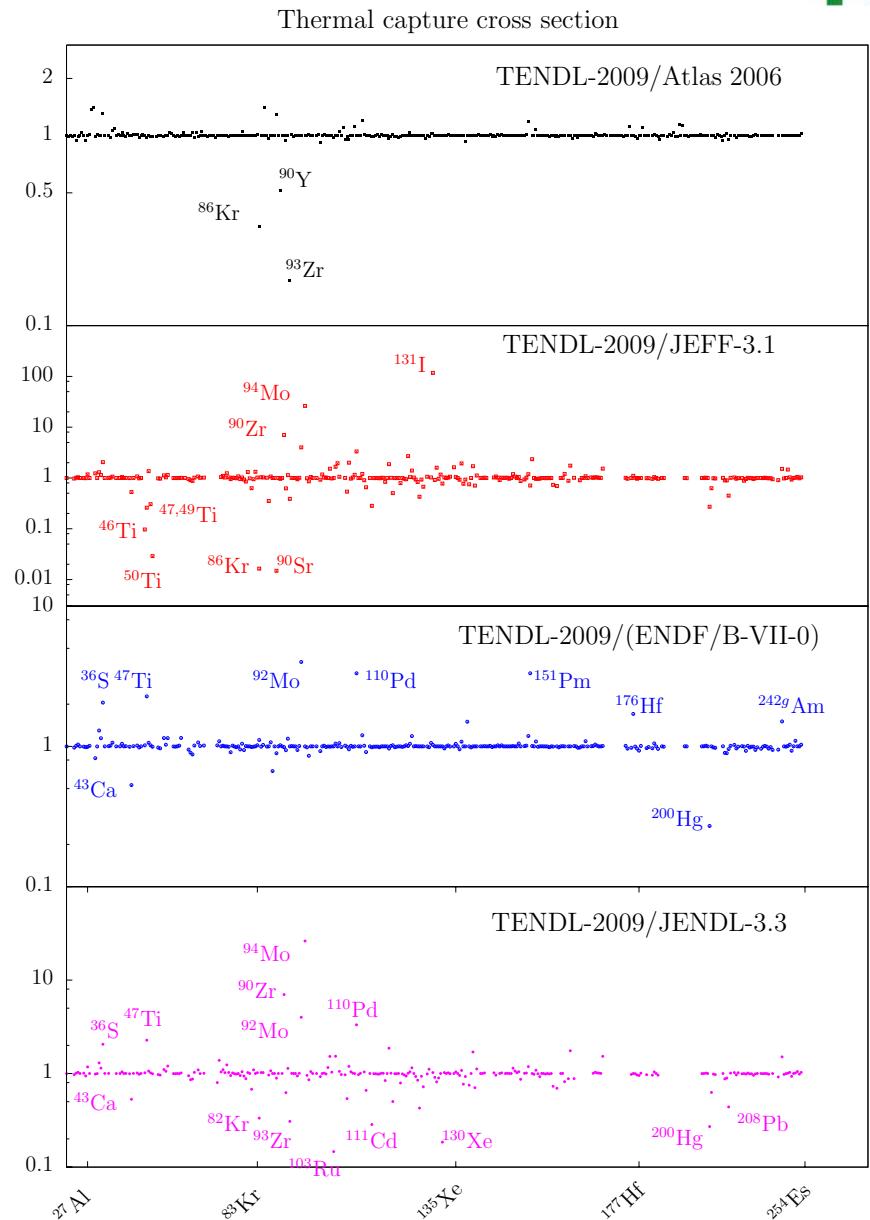
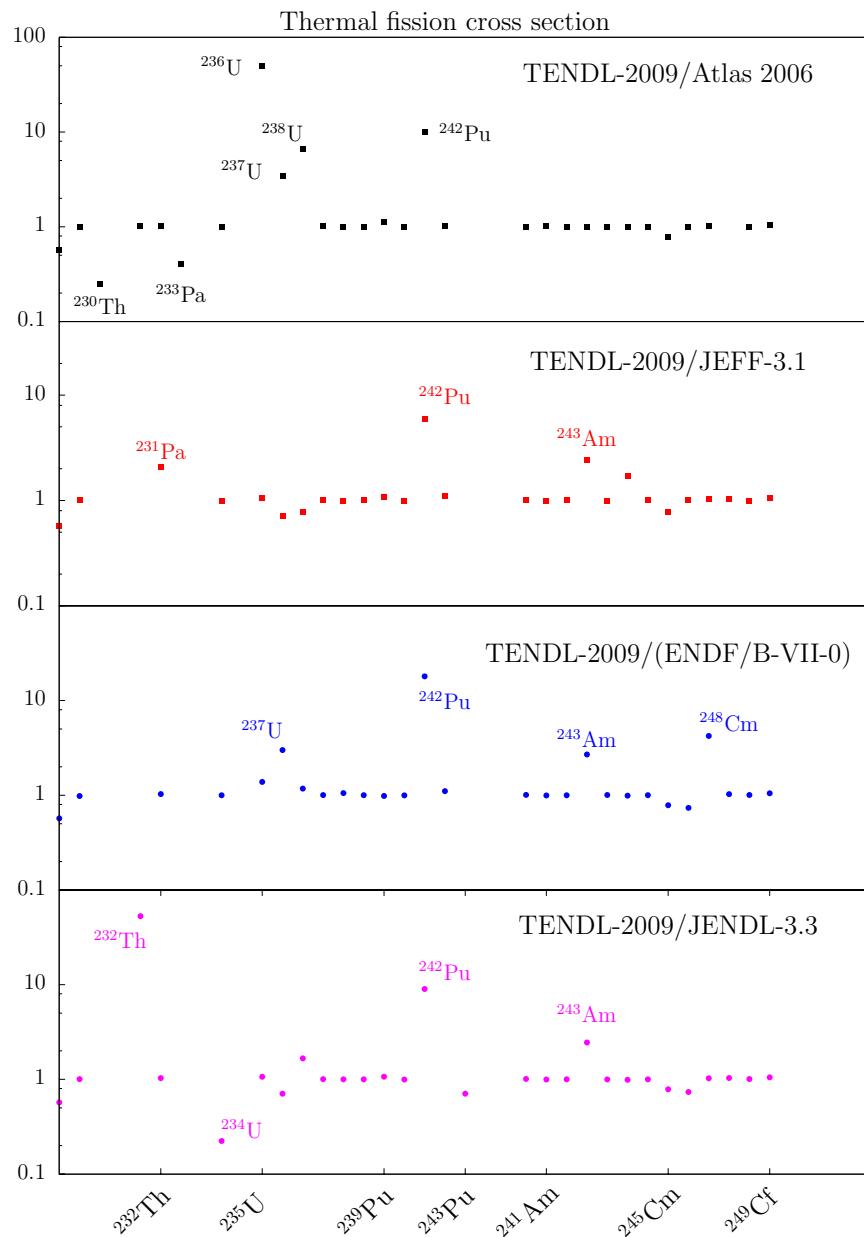
Content 8- TENDL-2009 Neutron library: Actinides



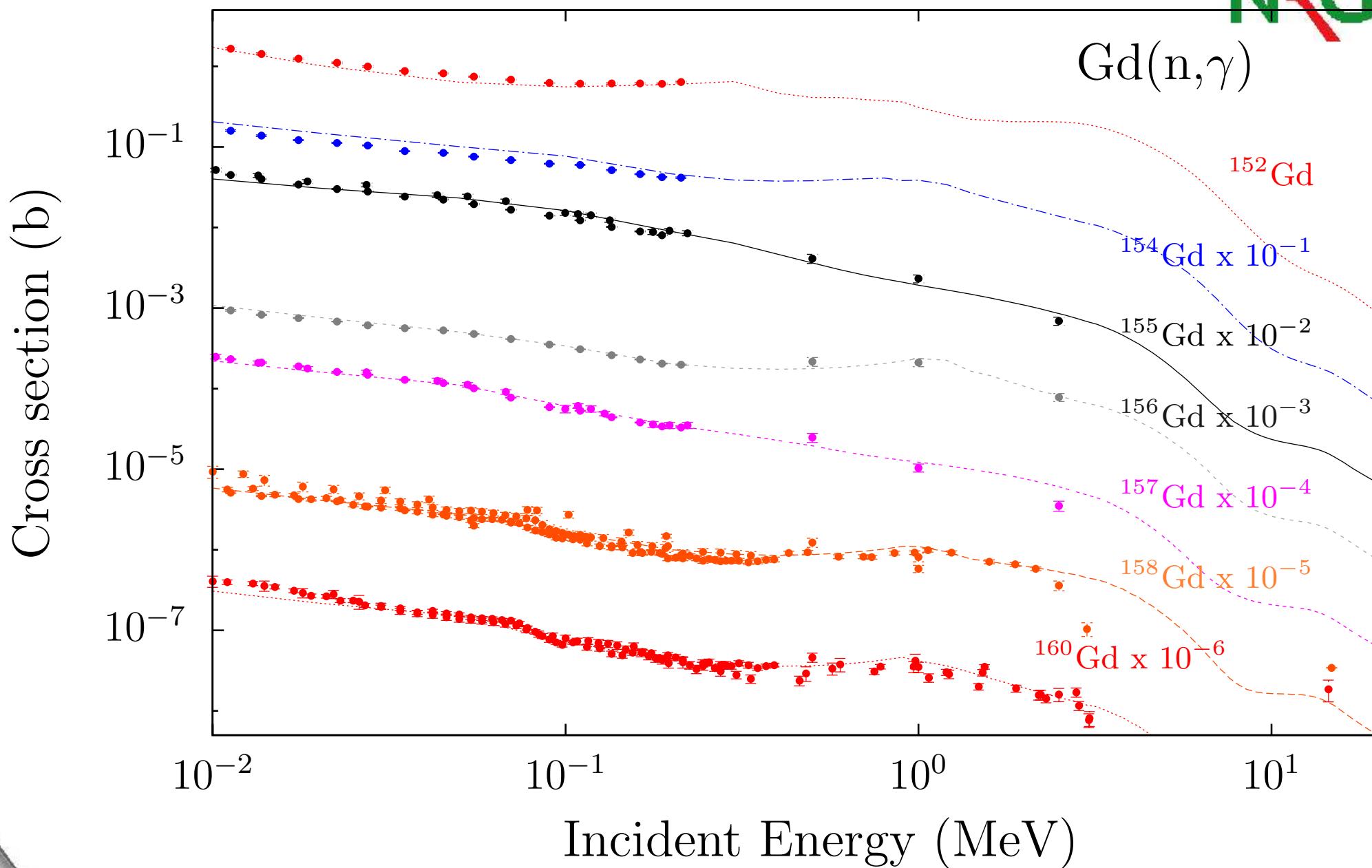
Element	Isotopes	Element	Isotopes
Th	208-227, 228-232 , 233-239	Pa	213-230, 231,233 , 234-239
U	222-232, 233-238 , 239-242	Np	225-236, 237 , 238-244
Pu	229-237, 238-244 , 245-247	Am	232-238, 239-243 , 245-247
Cm	238-242, 243-248 , 249-252	Bk	238-248, 249 , 250, 251
Cf	237-248, 249 , 250-256	Es	241-253,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

⇒ 36 "medium" or "**better**" quality evaluations and 406 "default" quality evaluations (with isomers)

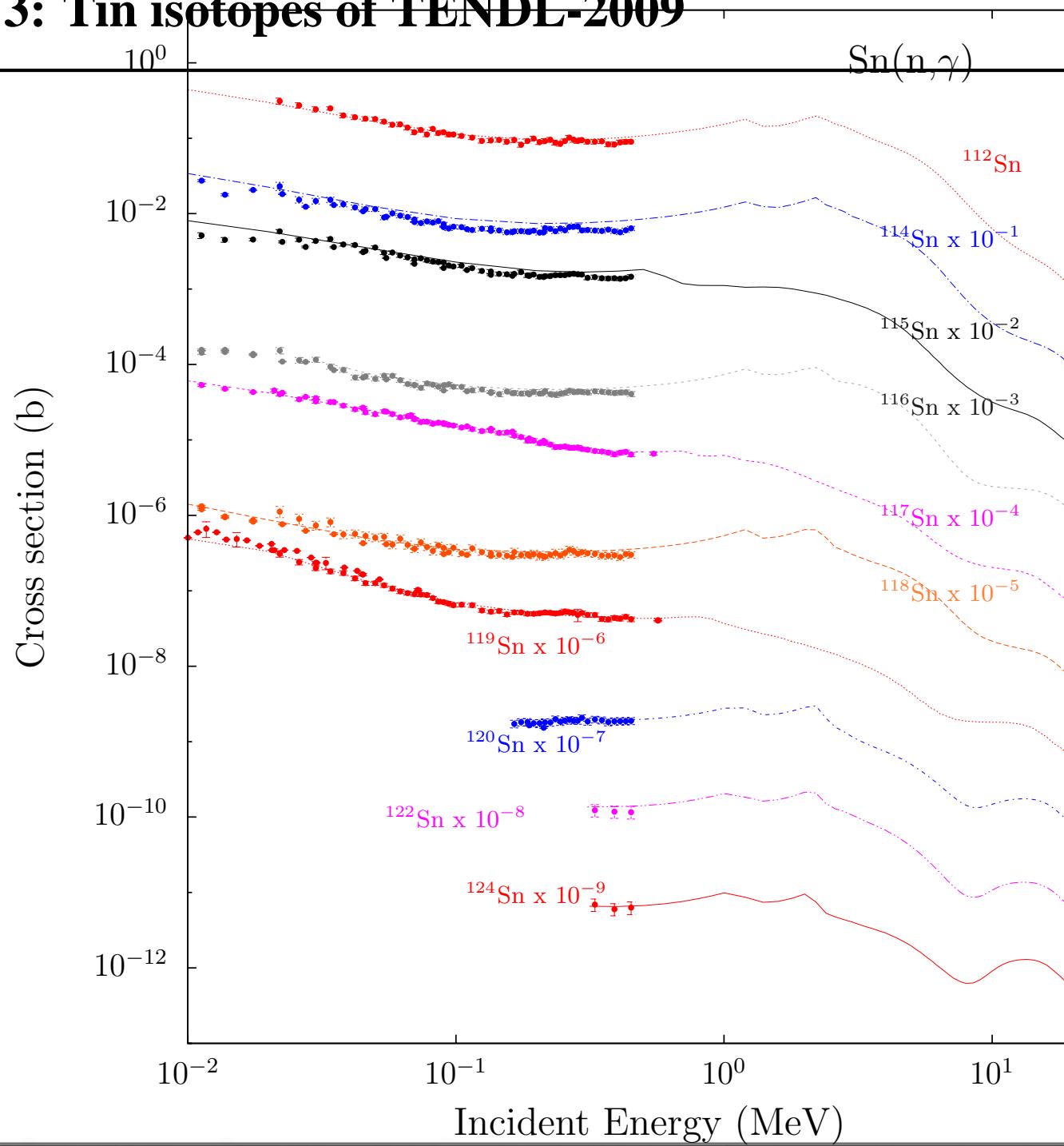
Examples 1: Ratio of capture thermal cross sections



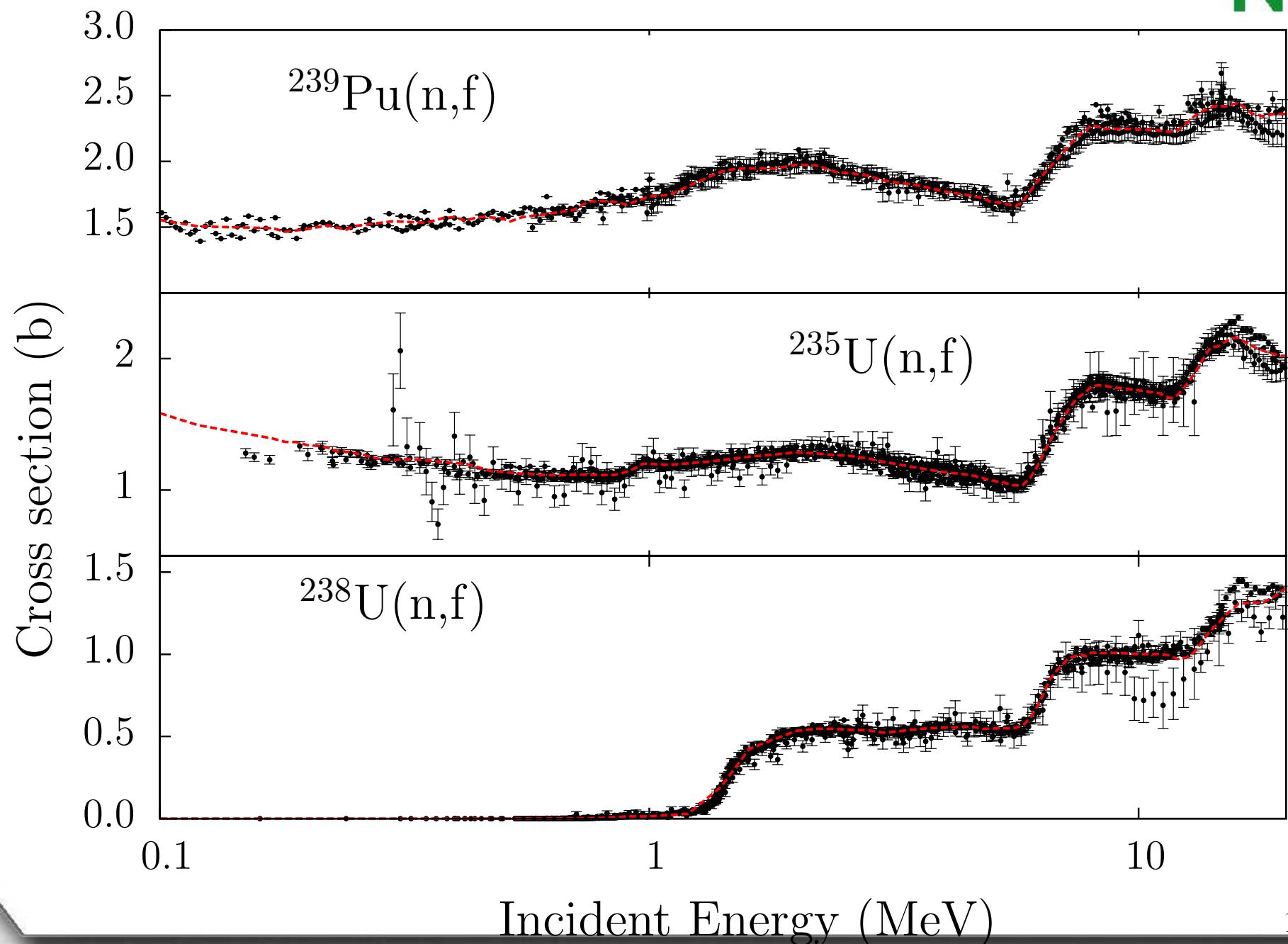
Examples 2: Gadolinium isotopes of TENDL-2009



Examples 3: Tin isotopes of TENDL-2009

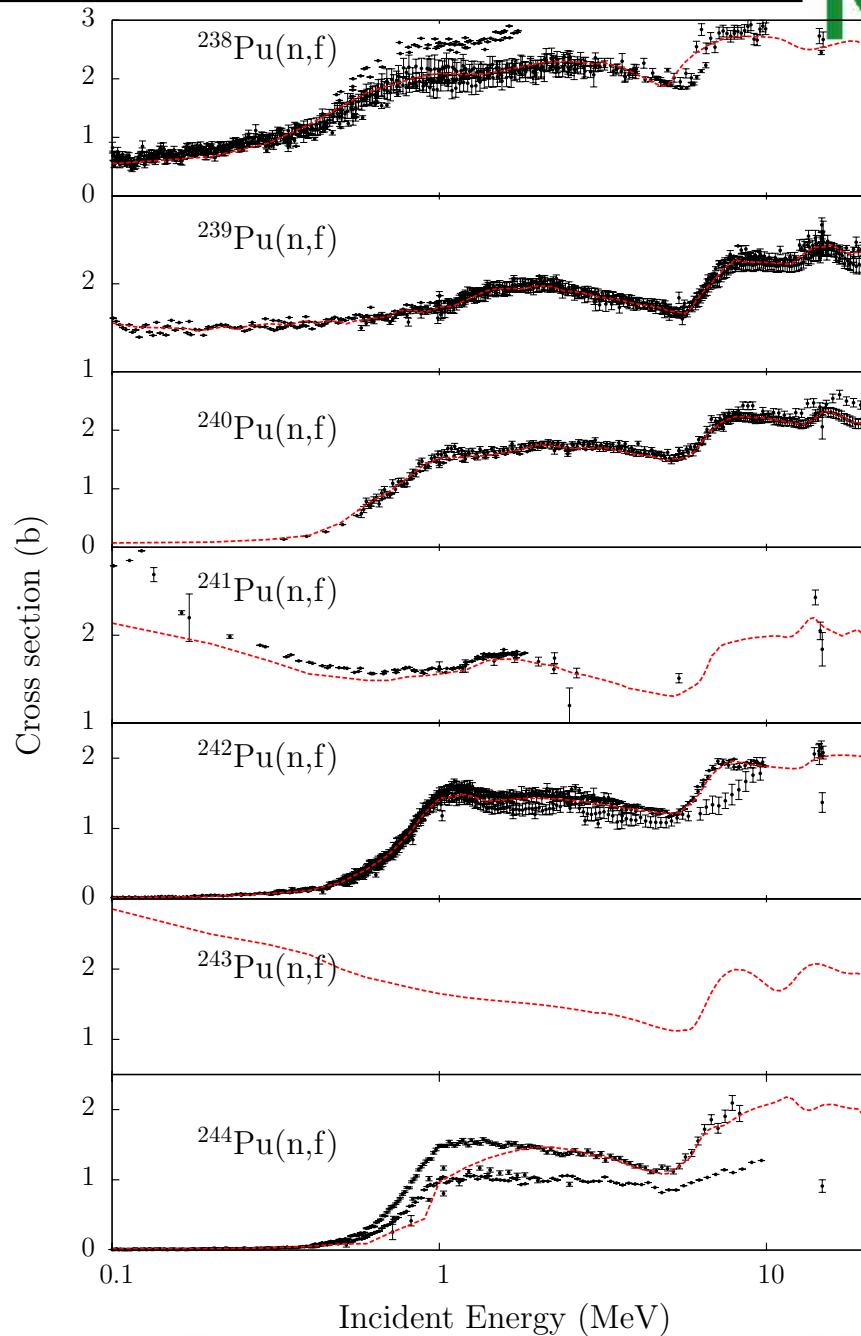
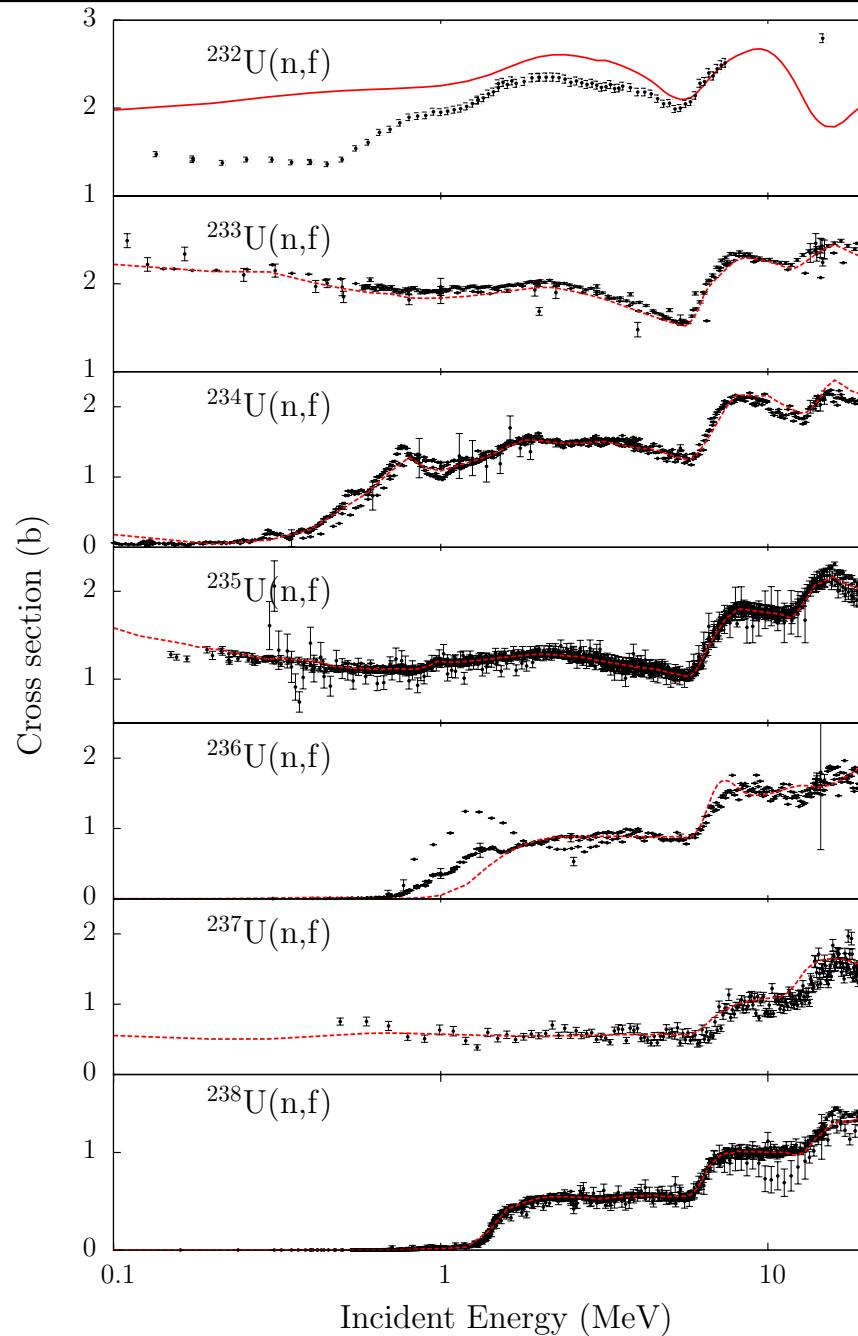


Examples 4: Some actinides of TENDL-2009



Examples 5: U and Pu isotopes of TENDL-2009

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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.*

$$\vec{\mathbf{p}} = \{p_1, \dots, p_l, \dots, p_L\} \implies p_l^{(k)} = p_l^{(0)} \pm \Delta p_l, \quad l = 1, L$$

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

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

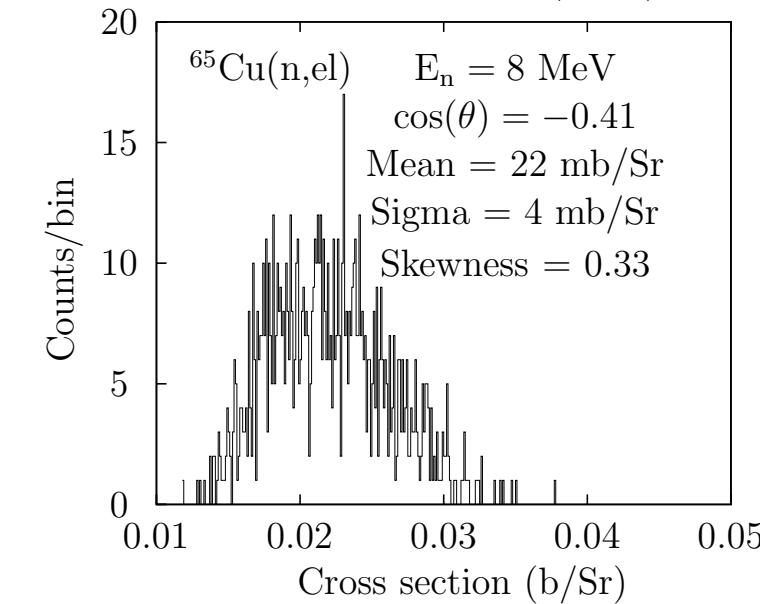
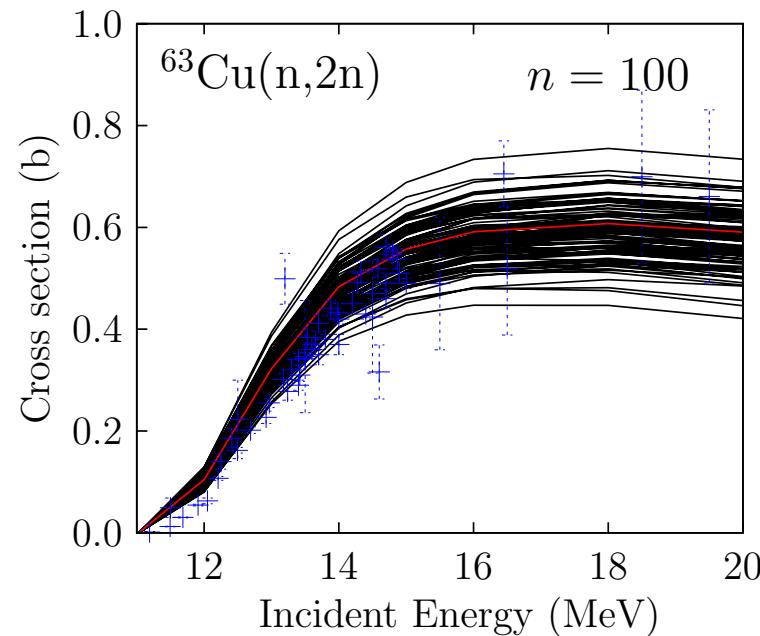
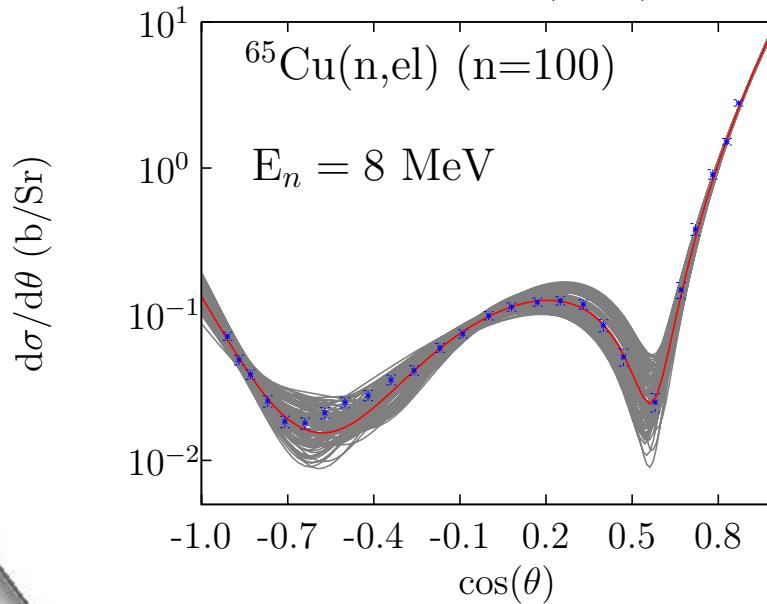
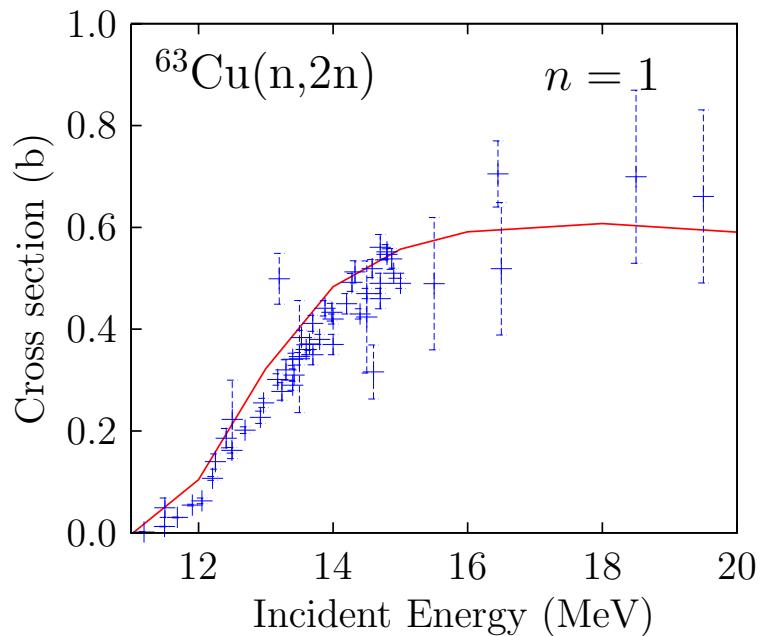
The average covariance matrix for cross sections is given by

$$V_{ij} = \frac{1}{K} \sum_{k=1}^K (\sigma_i^{(k)} - \bar{\sigma}_i)(\sigma_j^{(k)} - \bar{\sigma}_j), \quad i, j = 1, N,$$

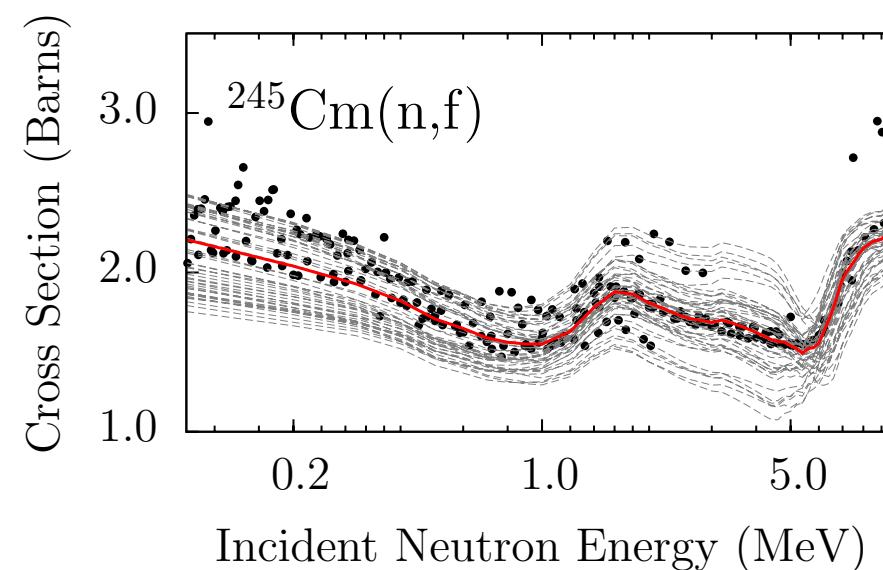
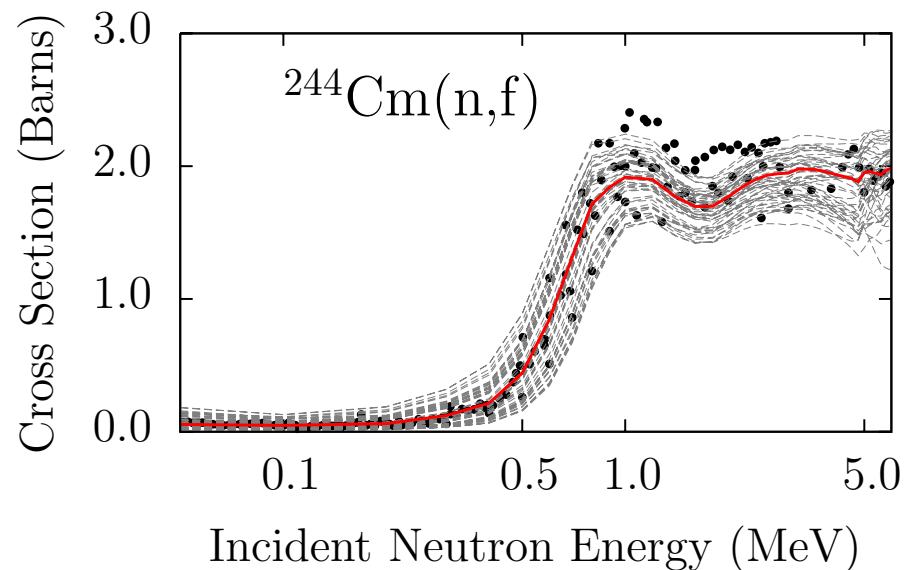
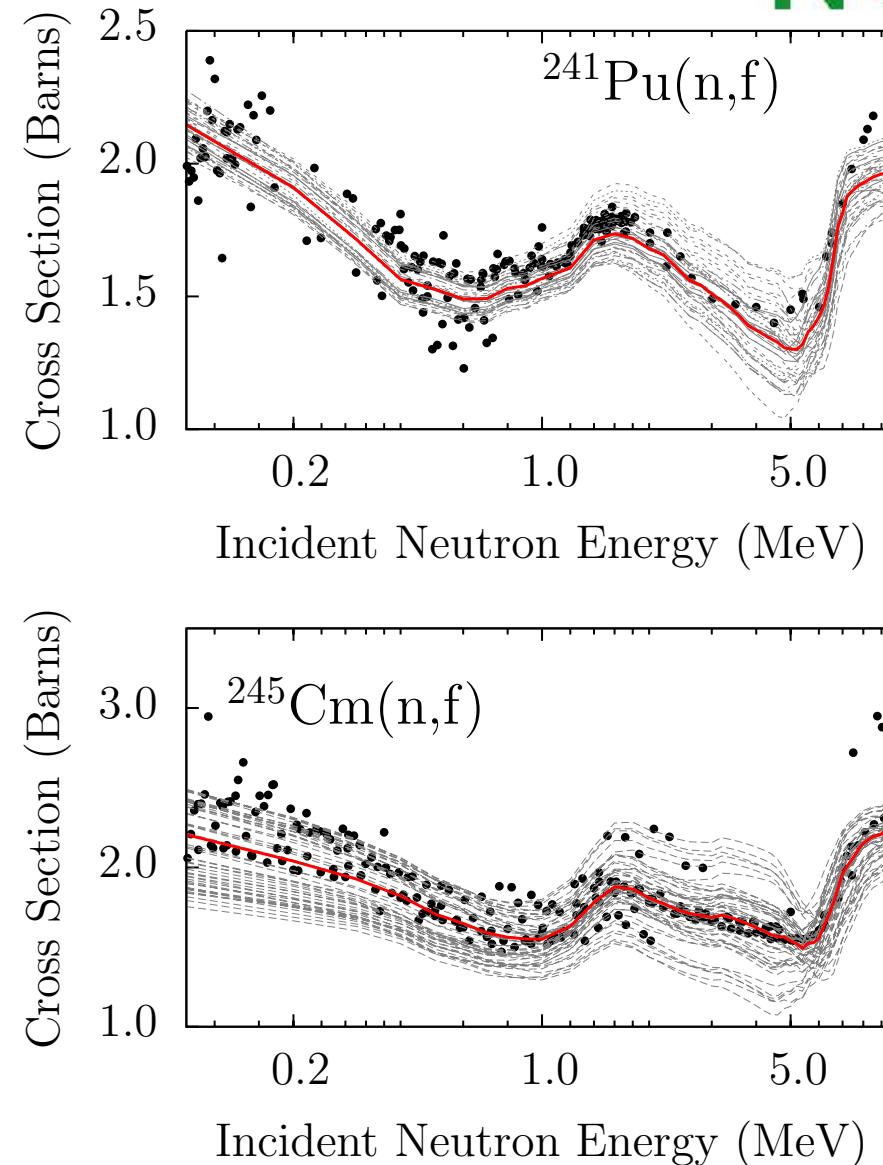
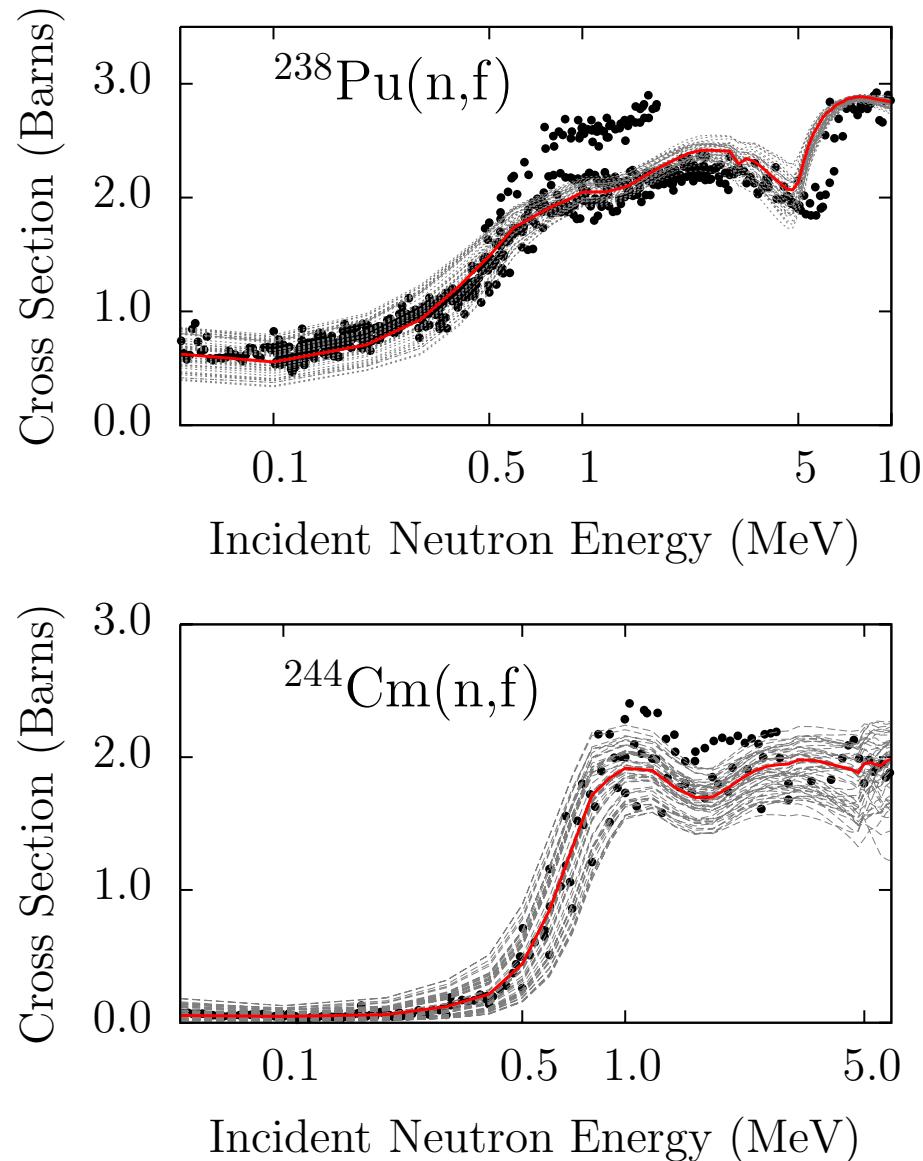
where K is the total number of TALYS runs needed for statistical convergence.
The average calculated cross sections are

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

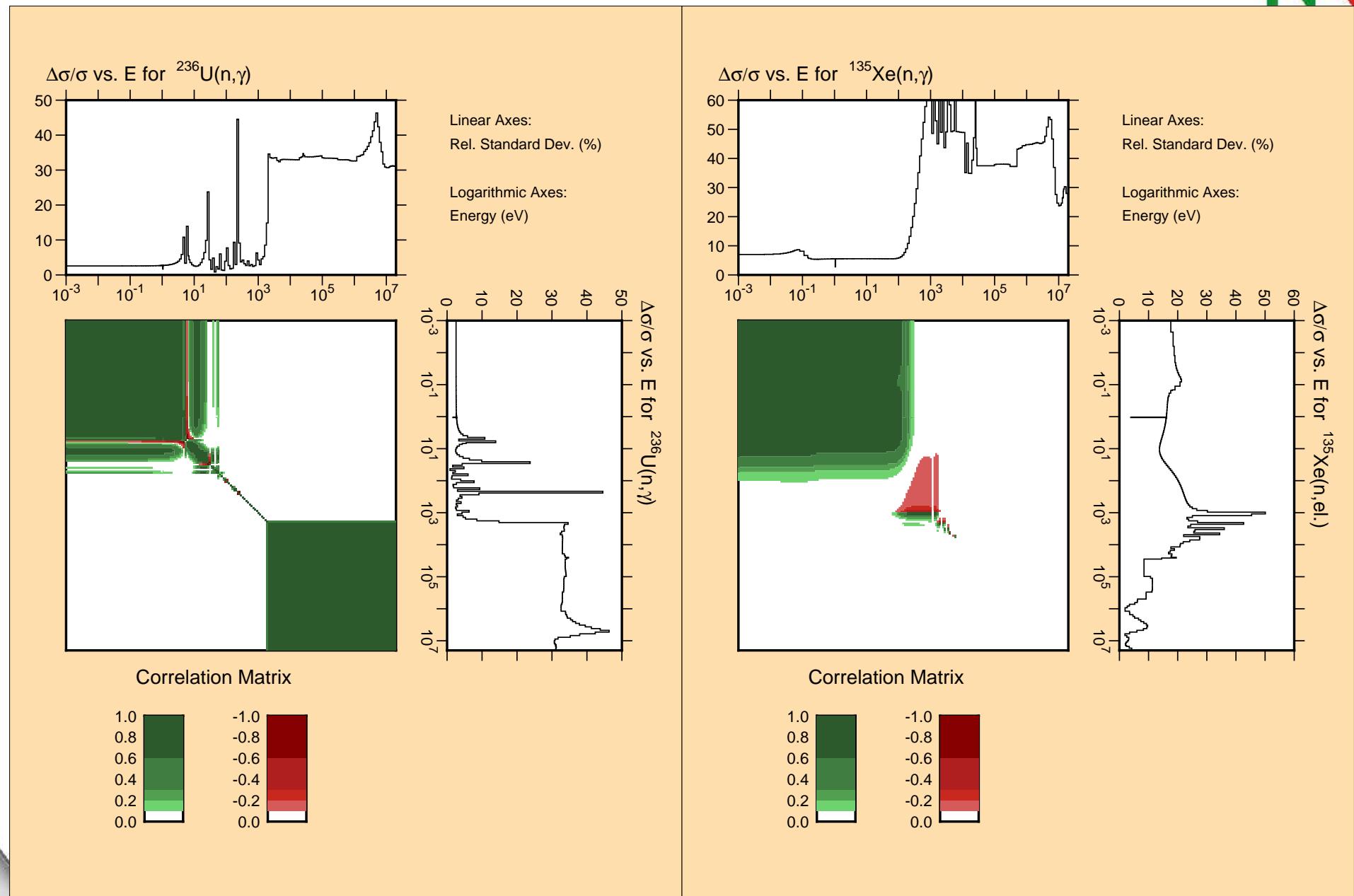
Covariances: example



Covariances: example



Covariances: example



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 $\chi^2_{\text{N,library}}$ 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):

$$\chi^2_{\text{library}} = \sum_i^{\text{benchmarks}} \frac{(C_i^{\text{library}} - E_i)^2}{E_i}$$

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

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

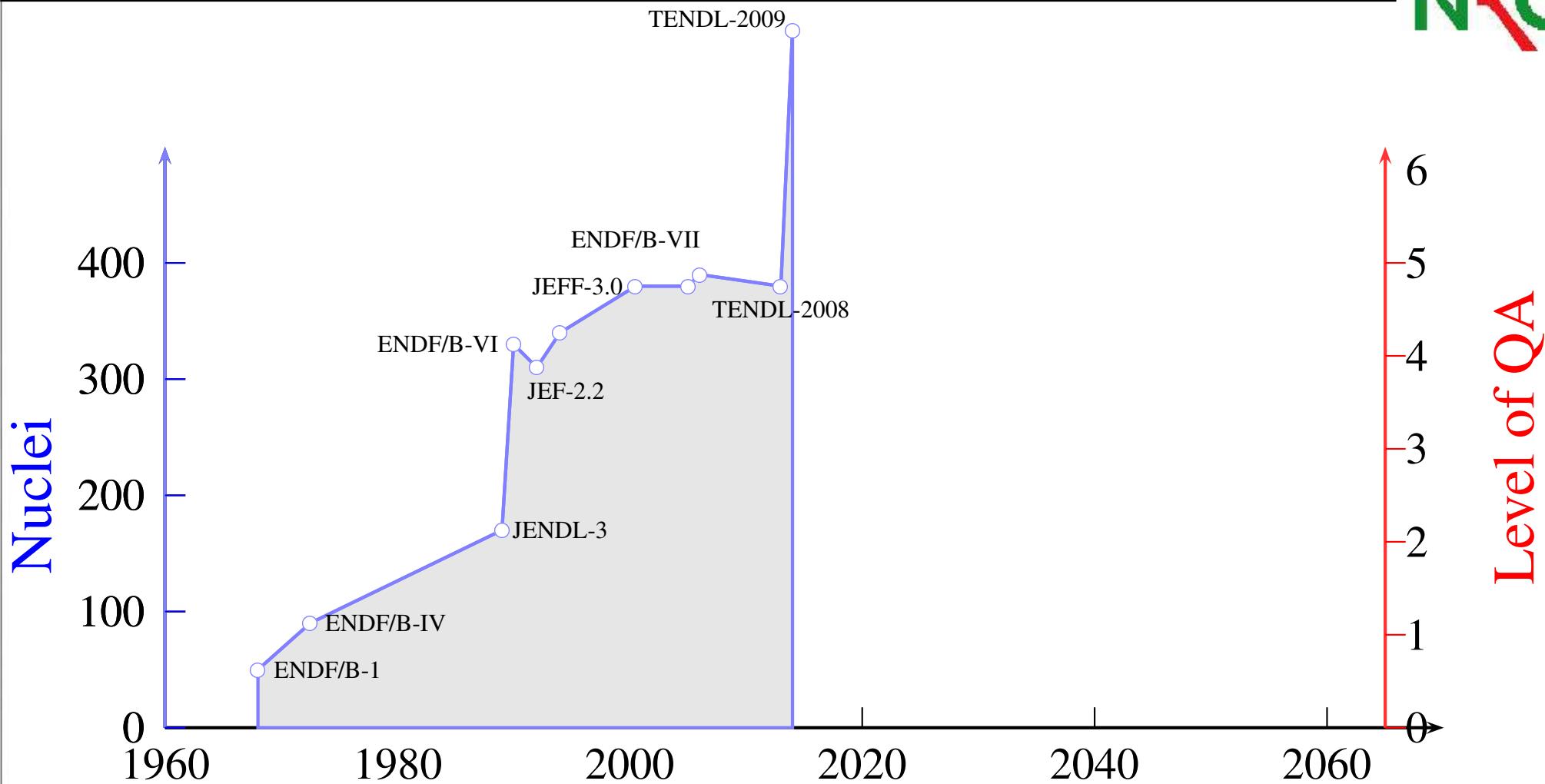
$$\text{library} = \begin{pmatrix} \text{ENDF/B - VII.0} \\ \text{TENDL - 2009} \\ \text{JEFF - 3.1} \\ \text{JENDL - 3.3} \\ \text{ENDF/B - VI.8} \end{pmatrix} \quad (1)$$

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

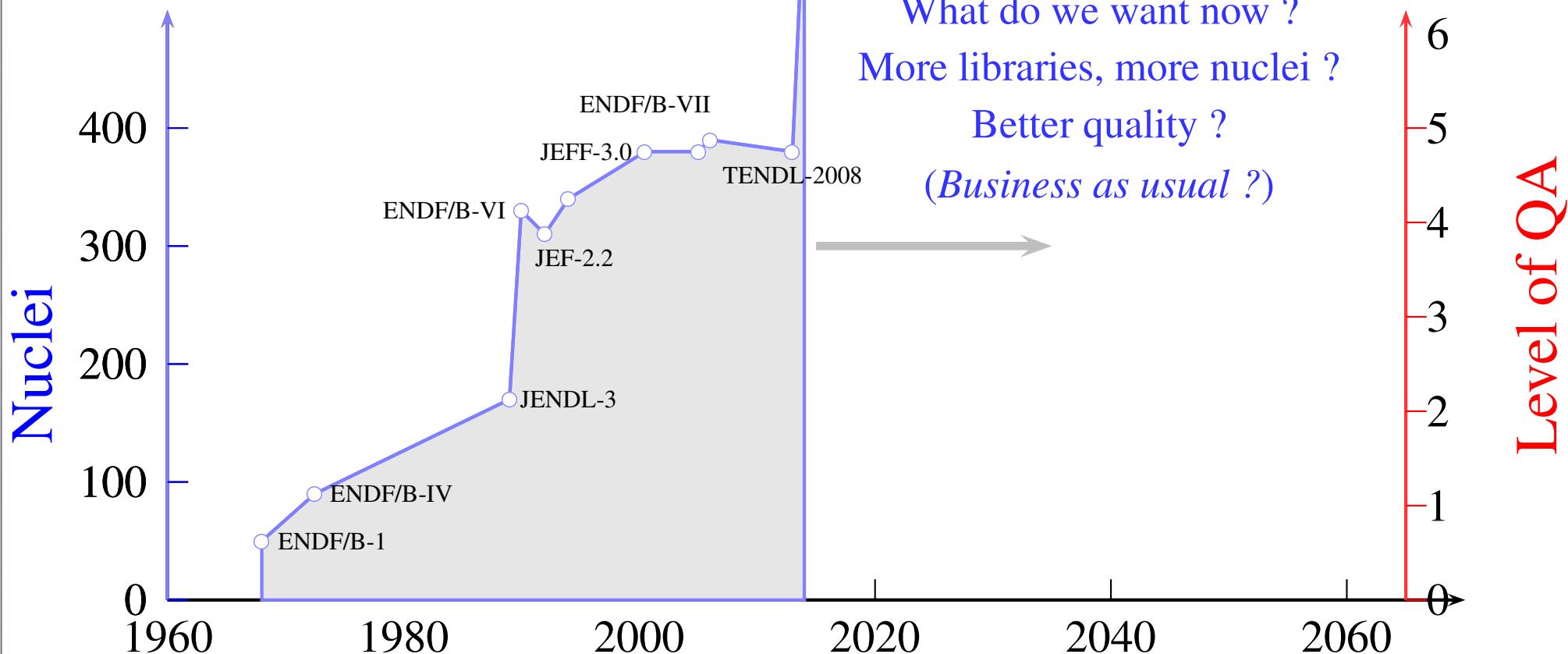


Library	Global 556	Normalized χ^2_N				
		LEU 219	HEU 170	^{239}Pu 87	Other 63	^{233}U 17
ENDF/B-VII.0	1.00	1.00	1.00	1.00	1.00	1.00
ENDF/B-VI.8	1.20	1.37	1.27	0.81	1.12	2.52
JEFF-3.1	1.18	0.80	1.43	0.77	1.04	1.68
JENDL-3.3	1.29	0.85	1.48	1.59	1.12	0.42
TENDL-2009	0.98	1.05	0.95	1.01	1.00	1.02

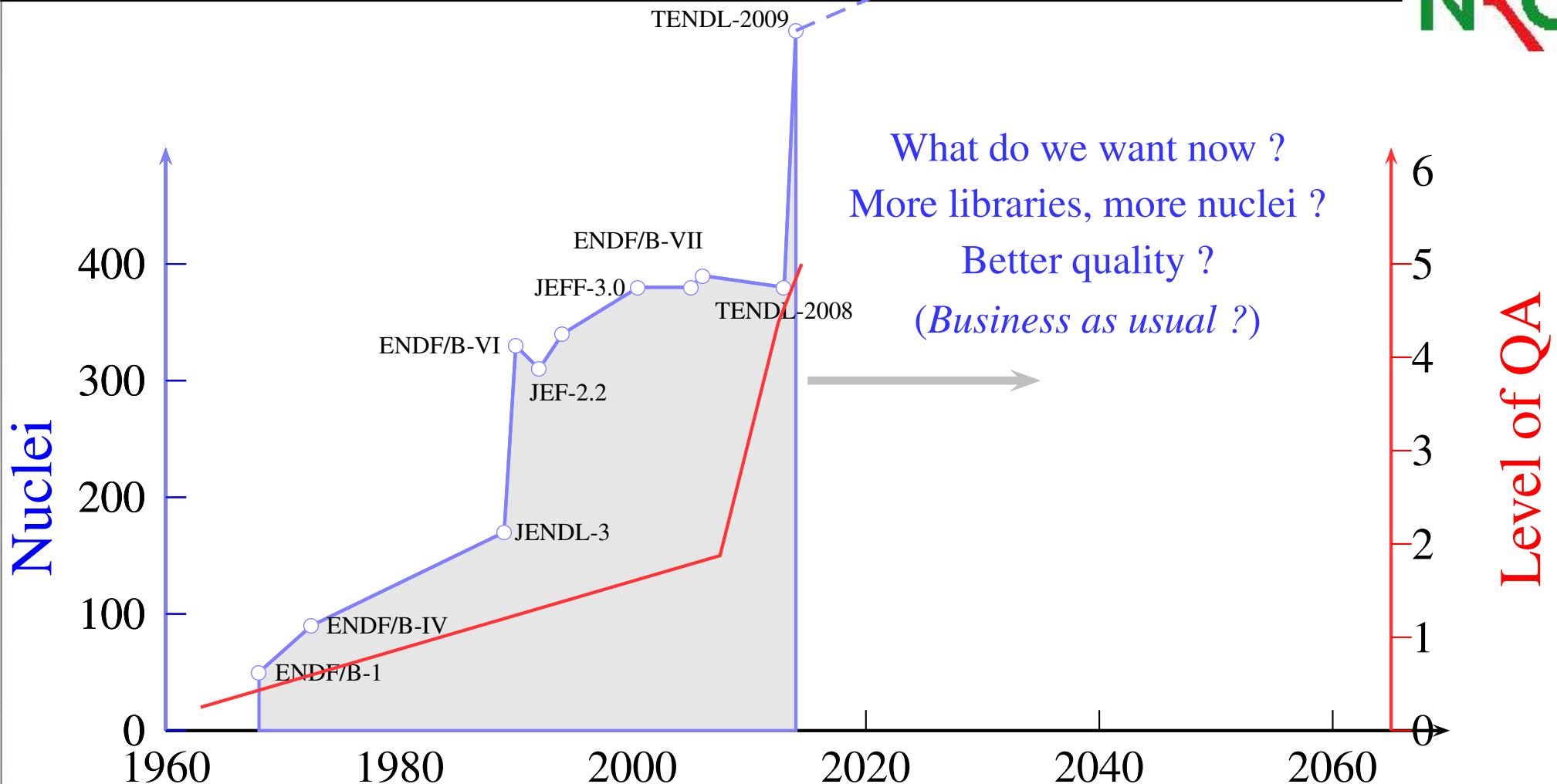
Back to the motivations: where are we ?



Back to the motivations: where are we ?



Back to the motivations: where are we ?



QA 0: All manual work

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

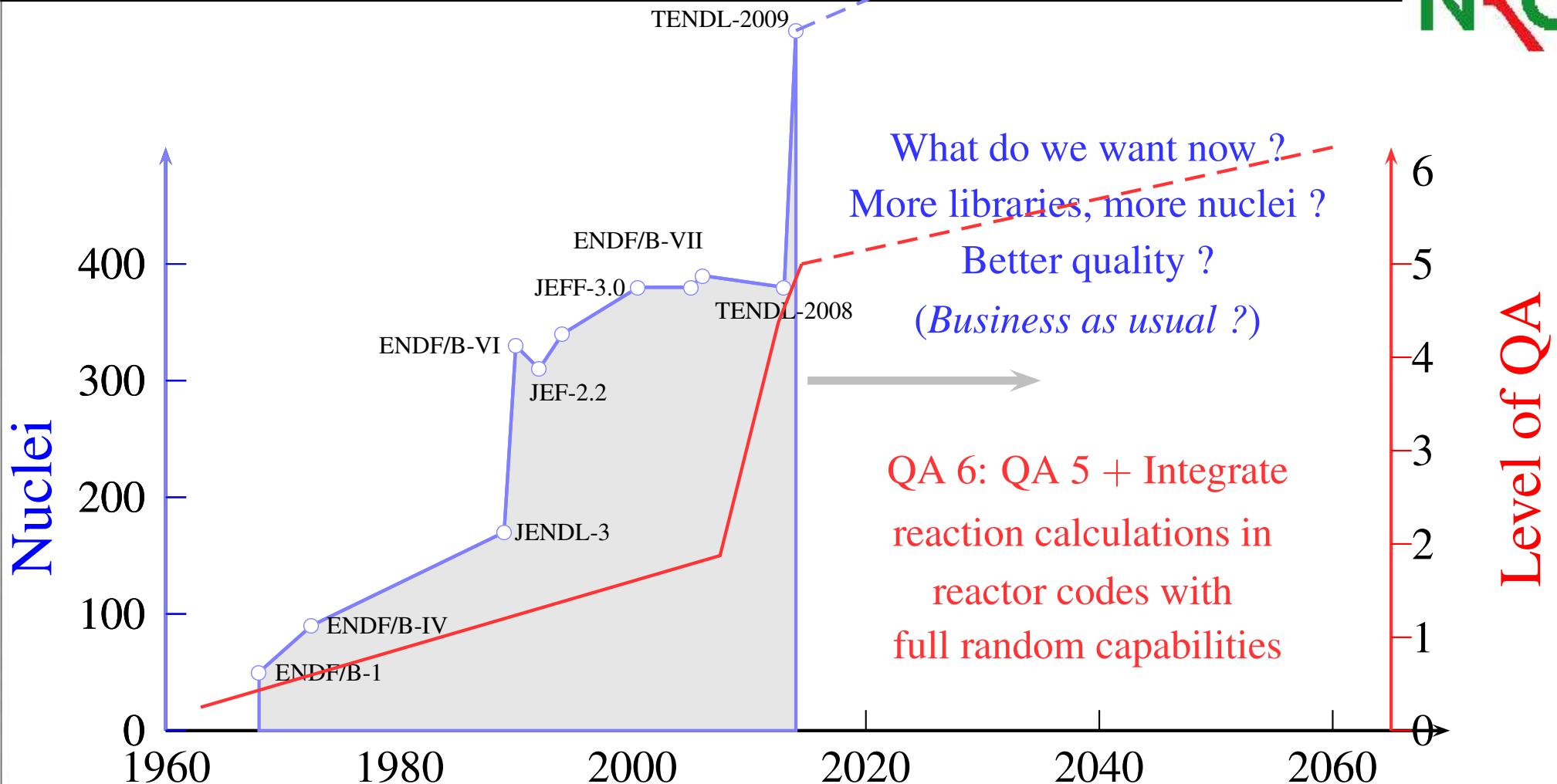
QA 2: QA 1 + Njoy, MCNP

QA 3: QA 2 + other codes (Puff, Eranos...)

QA 4: QA 3 + completeness, reproducibility

QA 5: QA 4 + full automation

Back to the motivations: where are we ?



QA 0: All manual work

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

QA 2: QA 1 + Njoy, MCNP

QA 3: QA 2 + other codes (Puff, Eranos...)

QA 4: QA 3 + completeness, reproducibility

QA 5: QA 4 + full automation

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 isotop
- 👉 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