TENDL-2009: on Evaluations and Monte Carlo Covariances

D. Rochman and A.J. Koning

Nuclear Research and Consultancy Group,

NRG, Petten, The Netherlands

October 1, 2009

Contents

① Motivations:

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

② Concept:

$\Longrightarrow$ *TALYS system + Monte Carlo = TENDL-2009*

③ Content 1:

$\Longrightarrow$ *Neutrons, protons, deuterons, tritons, alphas, photons*

④ Content 2:

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

⑤ Covariances

⑥ Validations

⑦ Conclusions and Future Improvements

Motivations: Our 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.

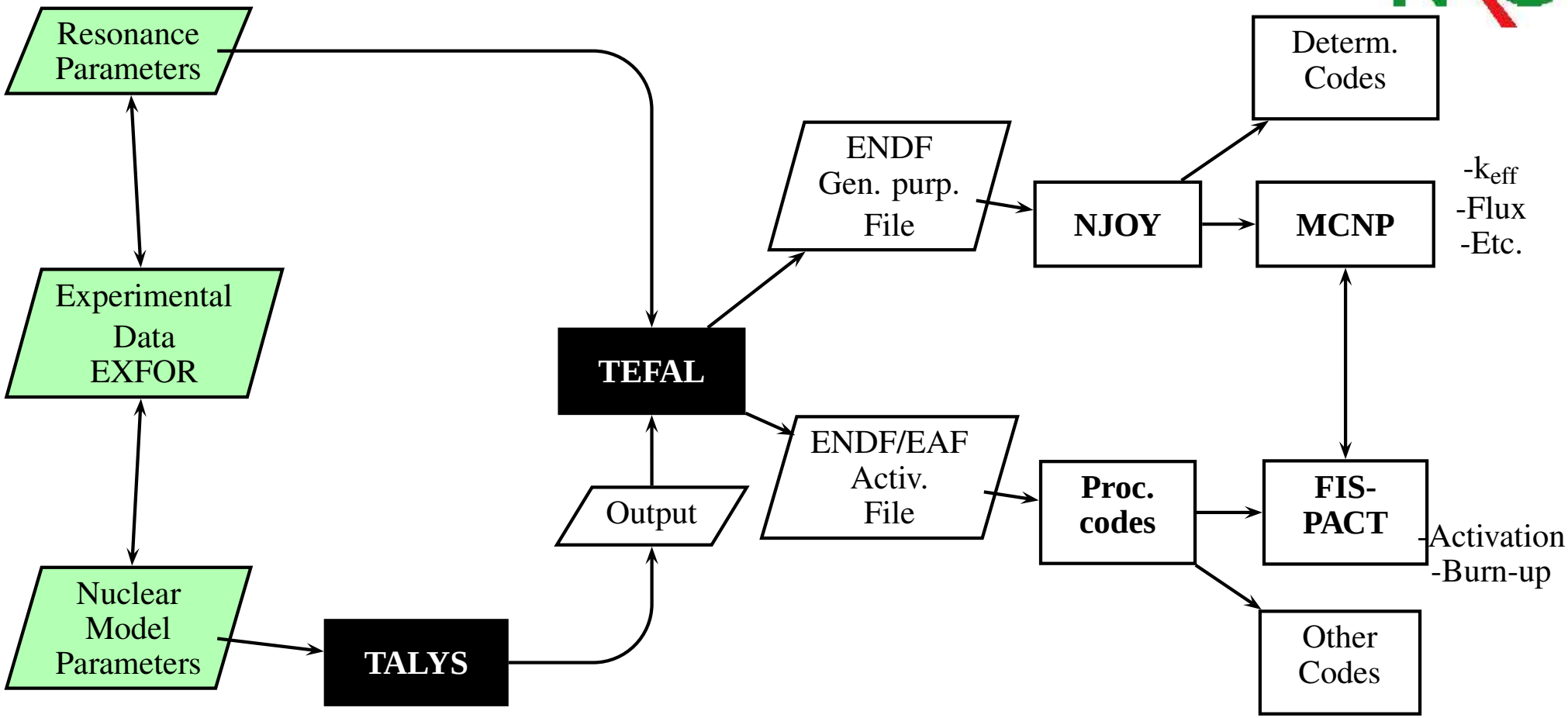
(*None of the existing libraries fulfill these requirements.*)

Long-term goal:

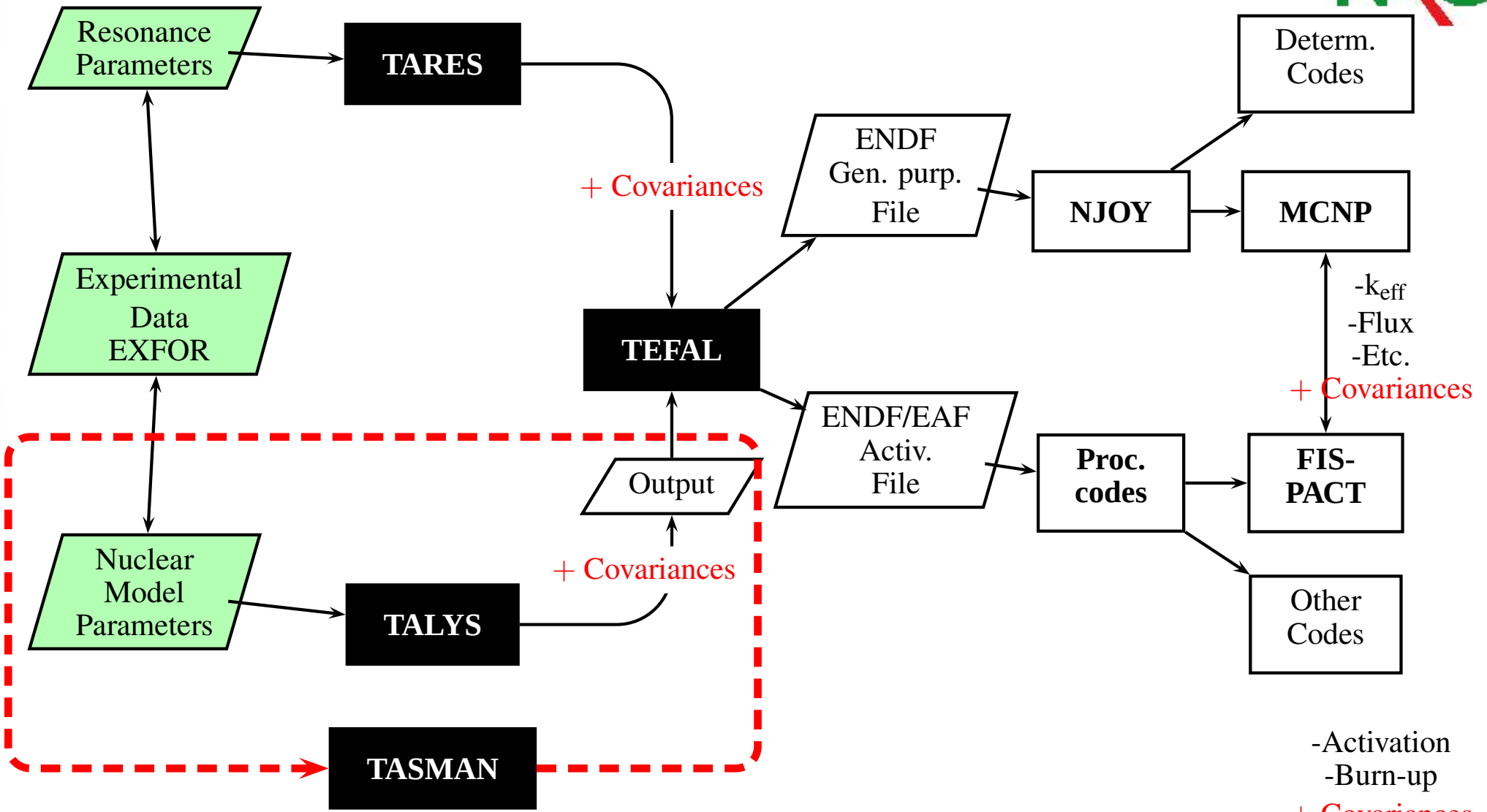
Generate nuclear data on the flight $\Longrightarrow$ no need of libraries anymore.

(*See last slide.*)

Concept: Standard nuclear data scheme



Concept: Nuclear Data Scheme with covariances



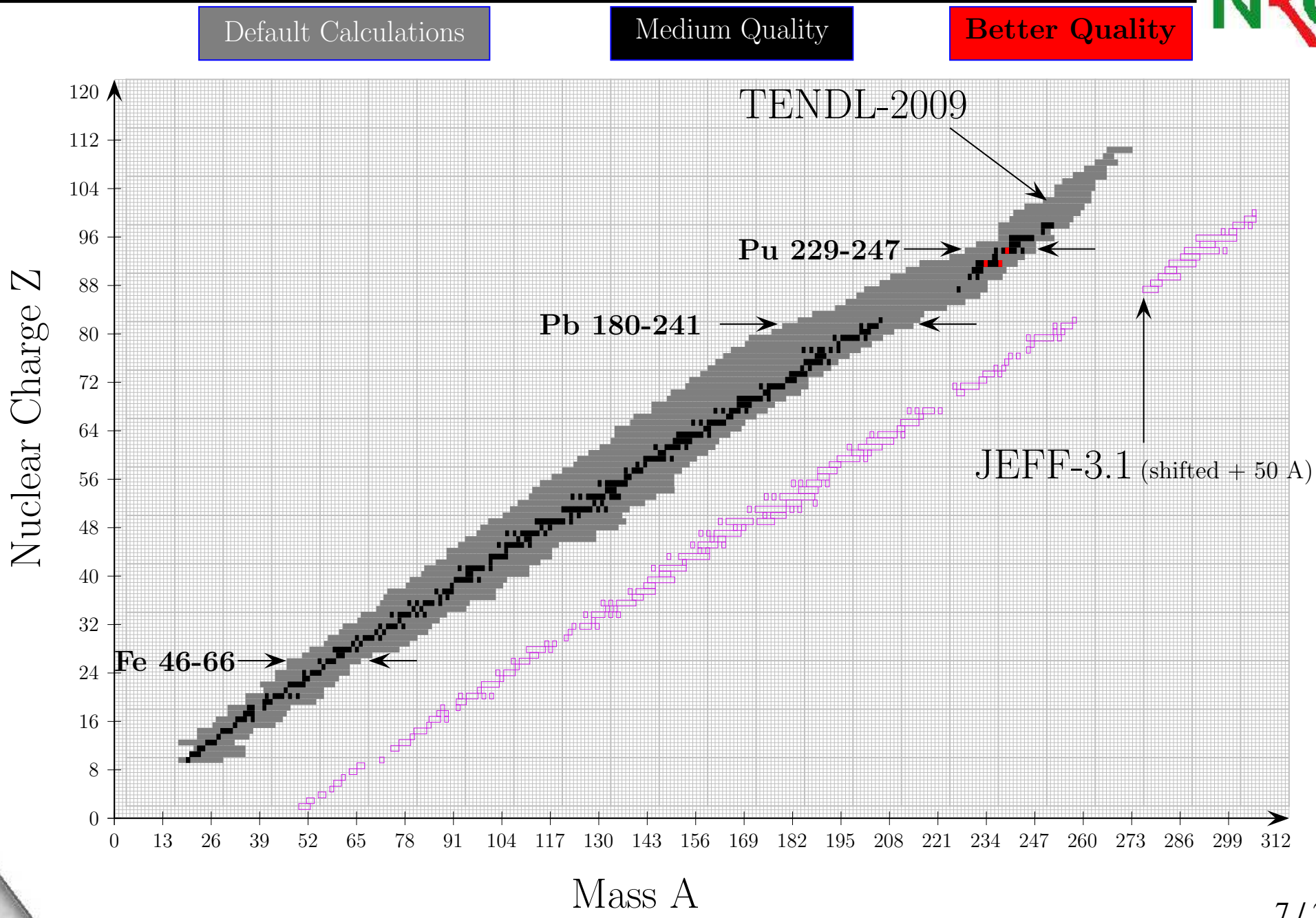
Monte Carlo: 1000 TALYS runs

Content 1- TENDL-2009

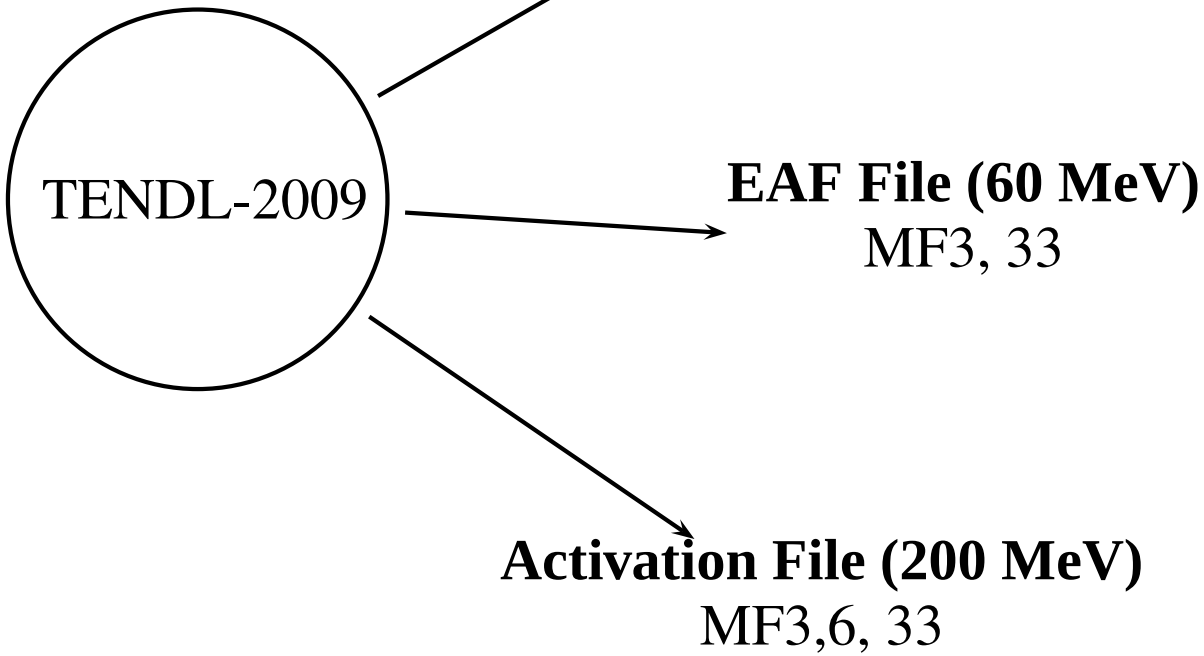
- Neutrons: ENDF files, plots, ACE files
- Protons: ENDF files, ACE files
- Alphas: ENDF files, ACE files
- ...

	Neutron	Proton	Deuteron	Triton	Alpha	Helium3	Photon
TENDL-2009	**>1000**	**>1000**	**>1000**	**>1000**	**>1000**	**>1000**	**>1000**
TENDL-2008	**348**	**344**	**336**	**339**	**342**	**338**	327
(JEFF-3.1)	*381*	*26*					
(ENDF/B-VII.0)	*393*	*48*	*5*	*3*			*163*

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



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



Content 4- TENDL-2009 Neutron library: from MF-1 to MF-34

Content of a typical file up to 200 MeV (out of $>$ 1000 files):

- 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 5- Available files

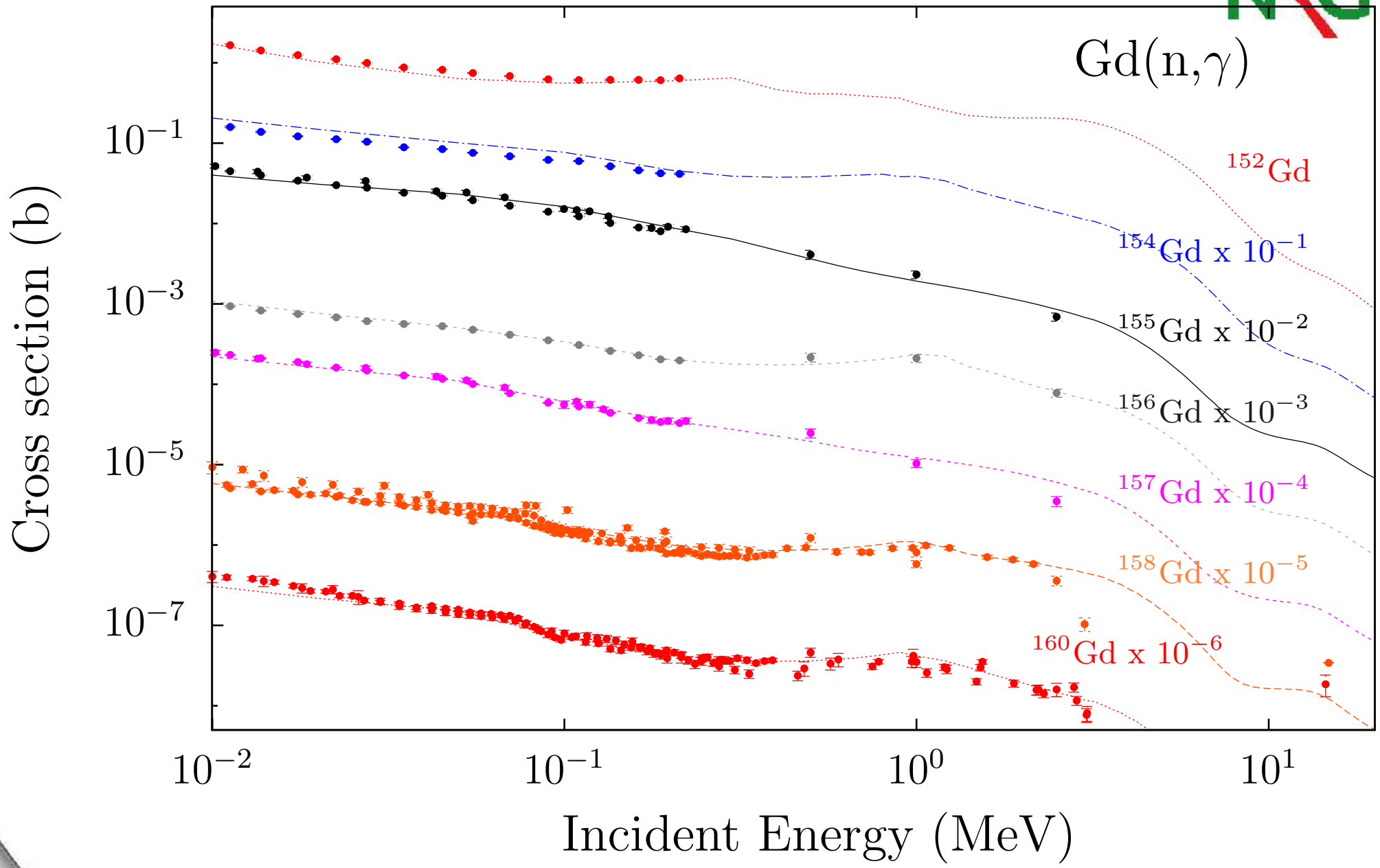
1. Tabular angular distributions
2. Tabular Gamma-ray intensities
3. Tabular partial cross sections to discrete levels
4. Tabular residual cross sections
5. Tabular cross sections
6. ENDF files
7. EAF cross section and variance files
8. Processed ACE files (with NJOY)
9. Processed AMPX files (with PUFF)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

Content 6- TENDL-2009: Actinides

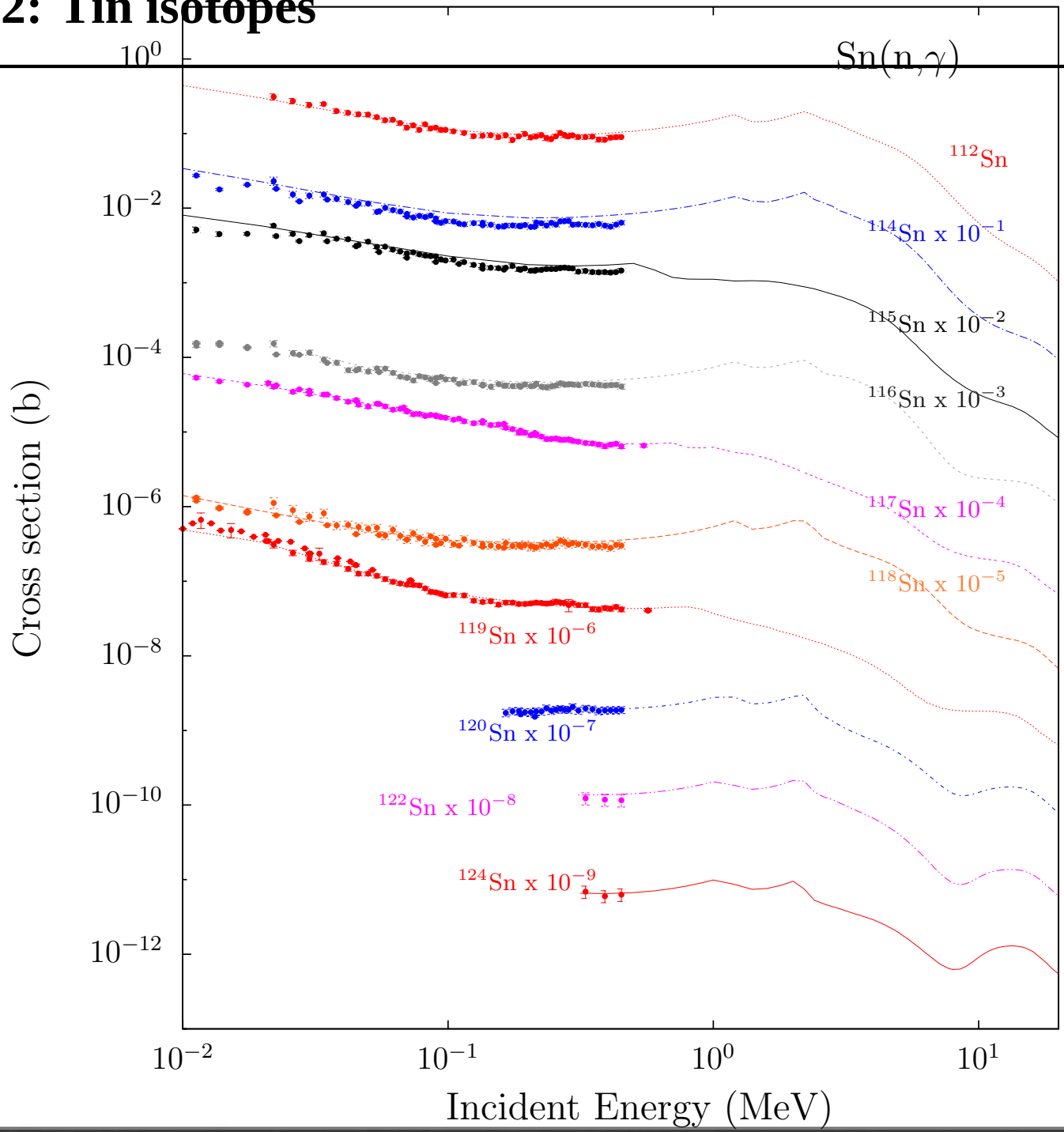
Element	Isotopes	Element	Isotopes
Th	208-227, 228-232, 233-239	Pa	213-230, 231,233, 234-239
U	222-232, 233-238, 239-242	Np	225-236, 237, 238-244
Pu	229-237, 238-244, 245-247	Am	232-238, 239-243, 245-247
Cm	238-242, 243-248, 249-252	Bk	238-248, 249, 250, 251
Cf	237-248, 249, 250-256	Es	241-253, 254, 255-257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

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

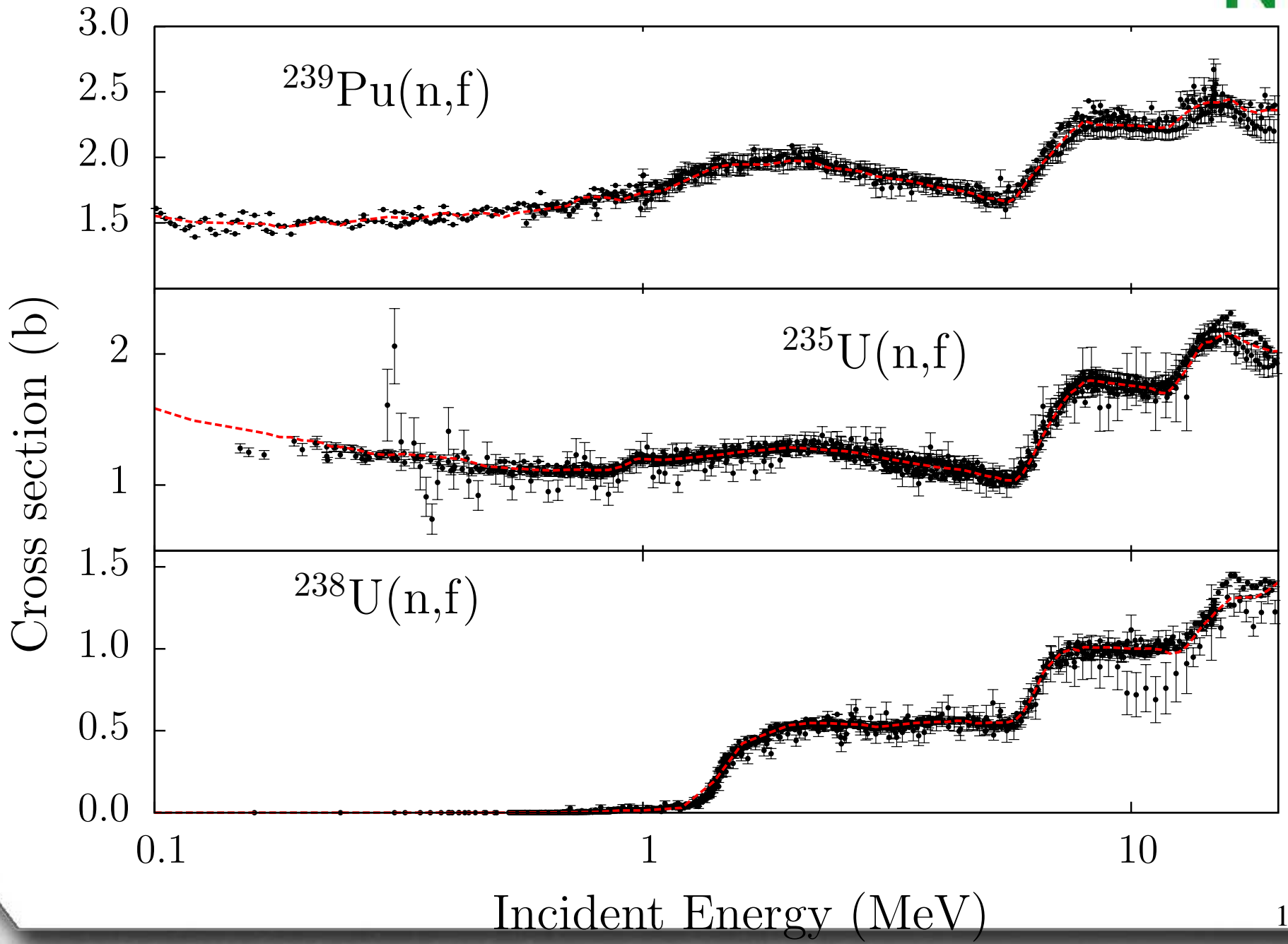
Examples 1: Gadolinium isotopes



Examples 2: Tin isotopes



Examples 3: Some actinides



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:

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

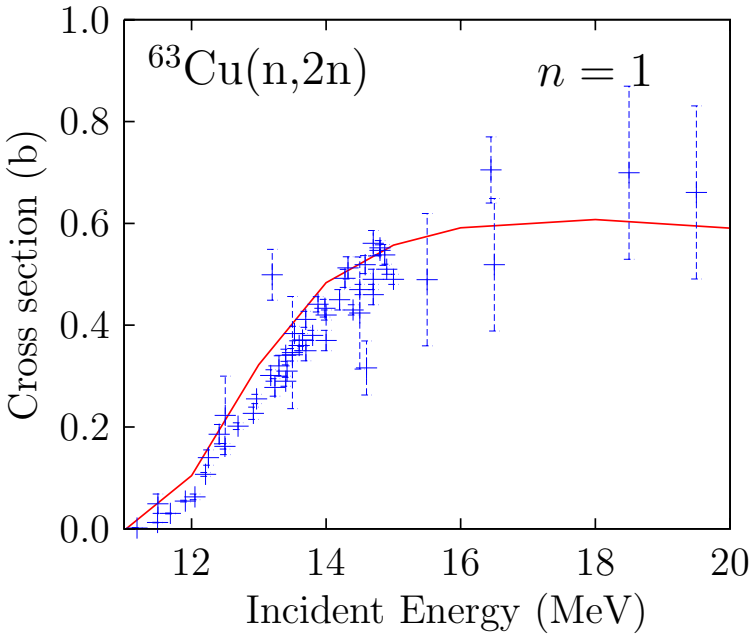
The average covariance matrix for cross sections is given by

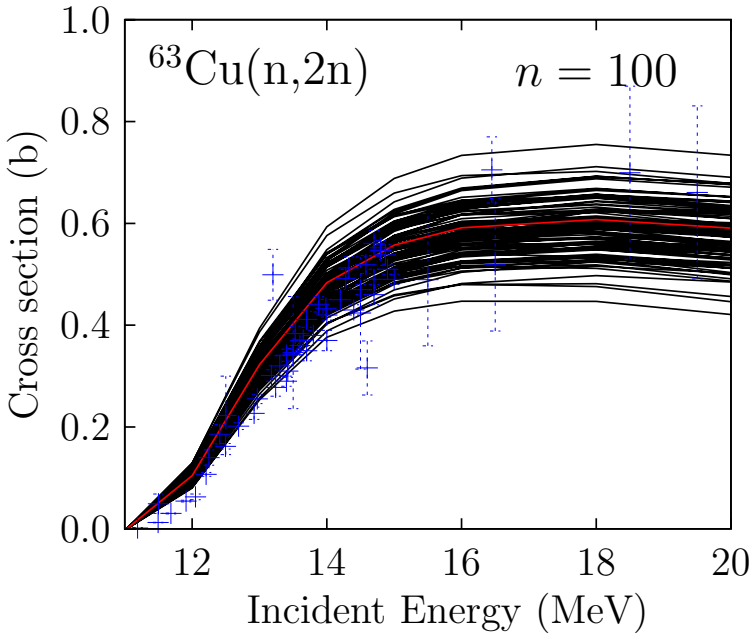
$$V_{ij} = \frac{1}{K} \sum_{k=1}^{K} (\sigma_i^{(k)} - \sigma_i^{(0)})(\sigma_j^{(k)} - \sigma_j^{(0)}), \qquad i, j = 1, N,$$

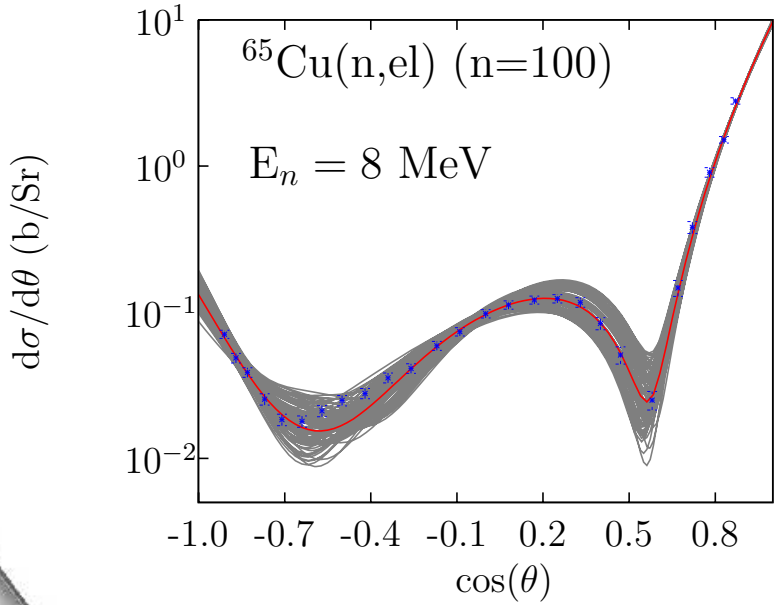
where K is the total number of TALYS runs needed for statistical convergence. The average calculated cross sections are

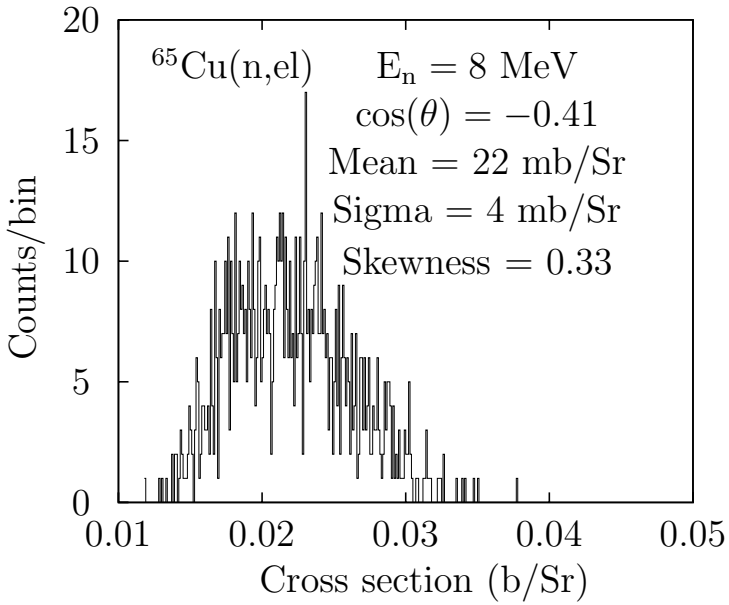
$$\bar{\sigma}_i = \frac{1}{K} \sum_{k=1}^{K} \sigma_i^{(k)}, \qquad i = 1, N,$$

Covariances: example

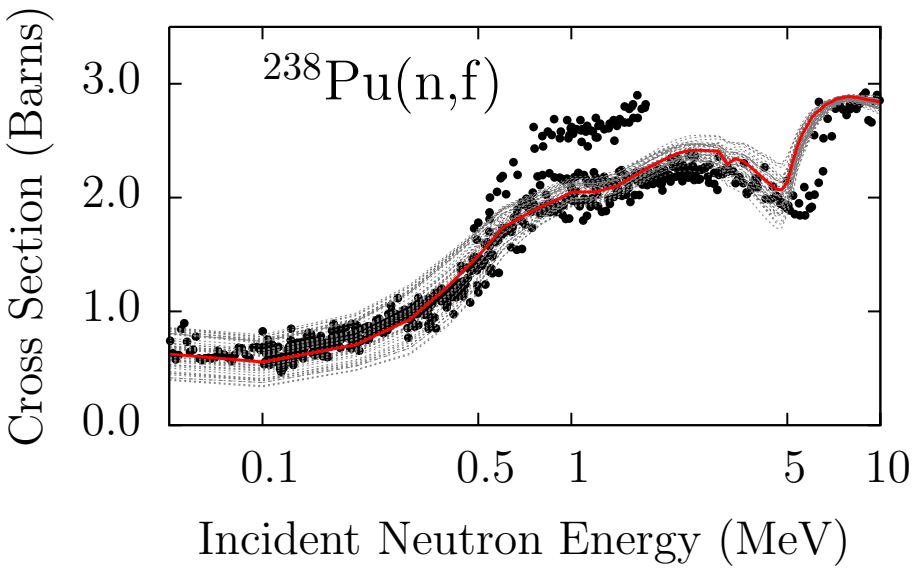


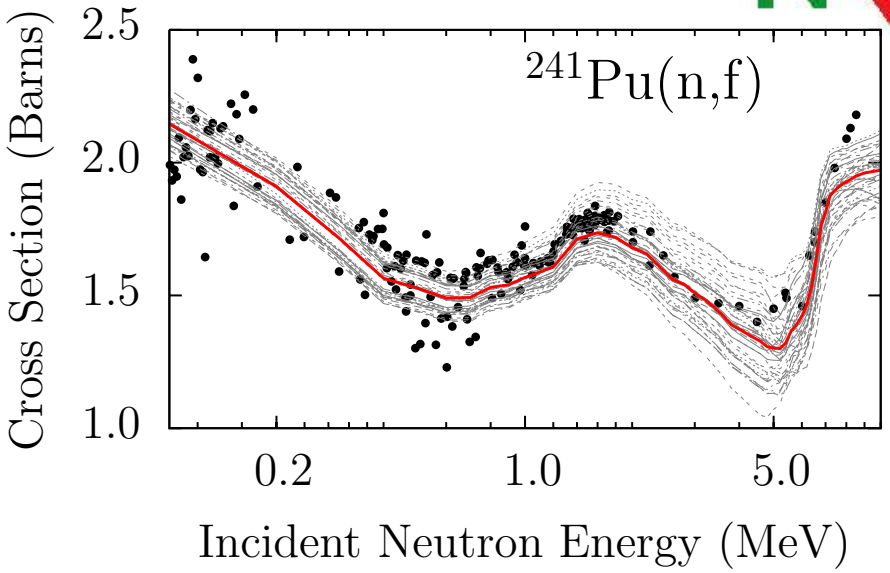


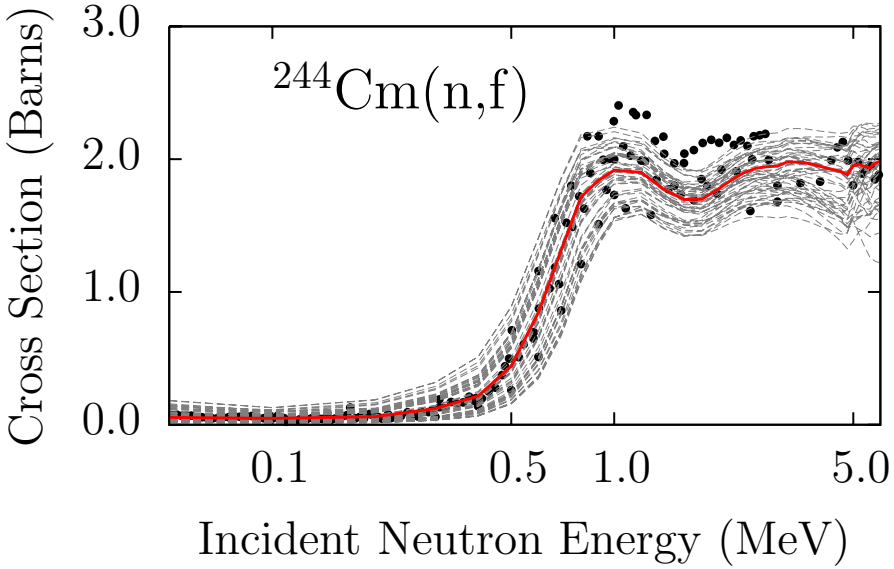


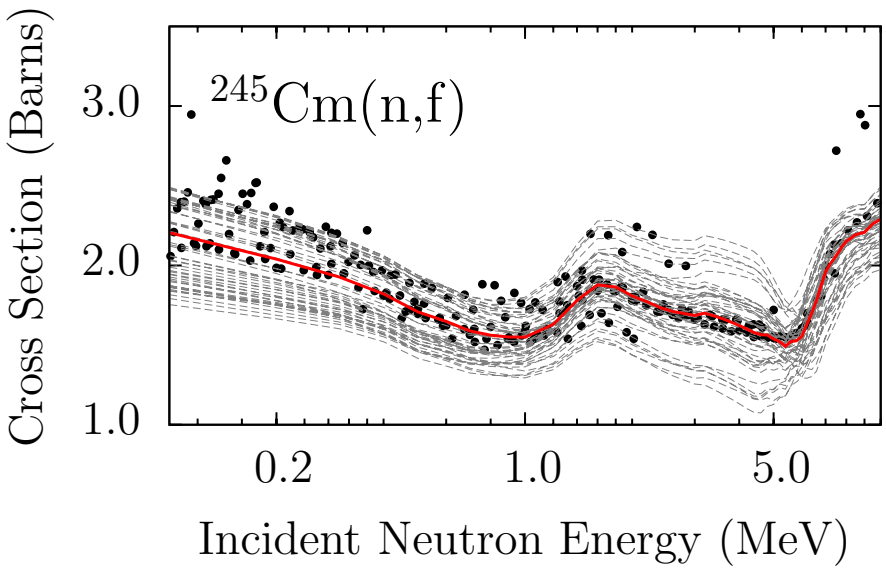


Covariances: example

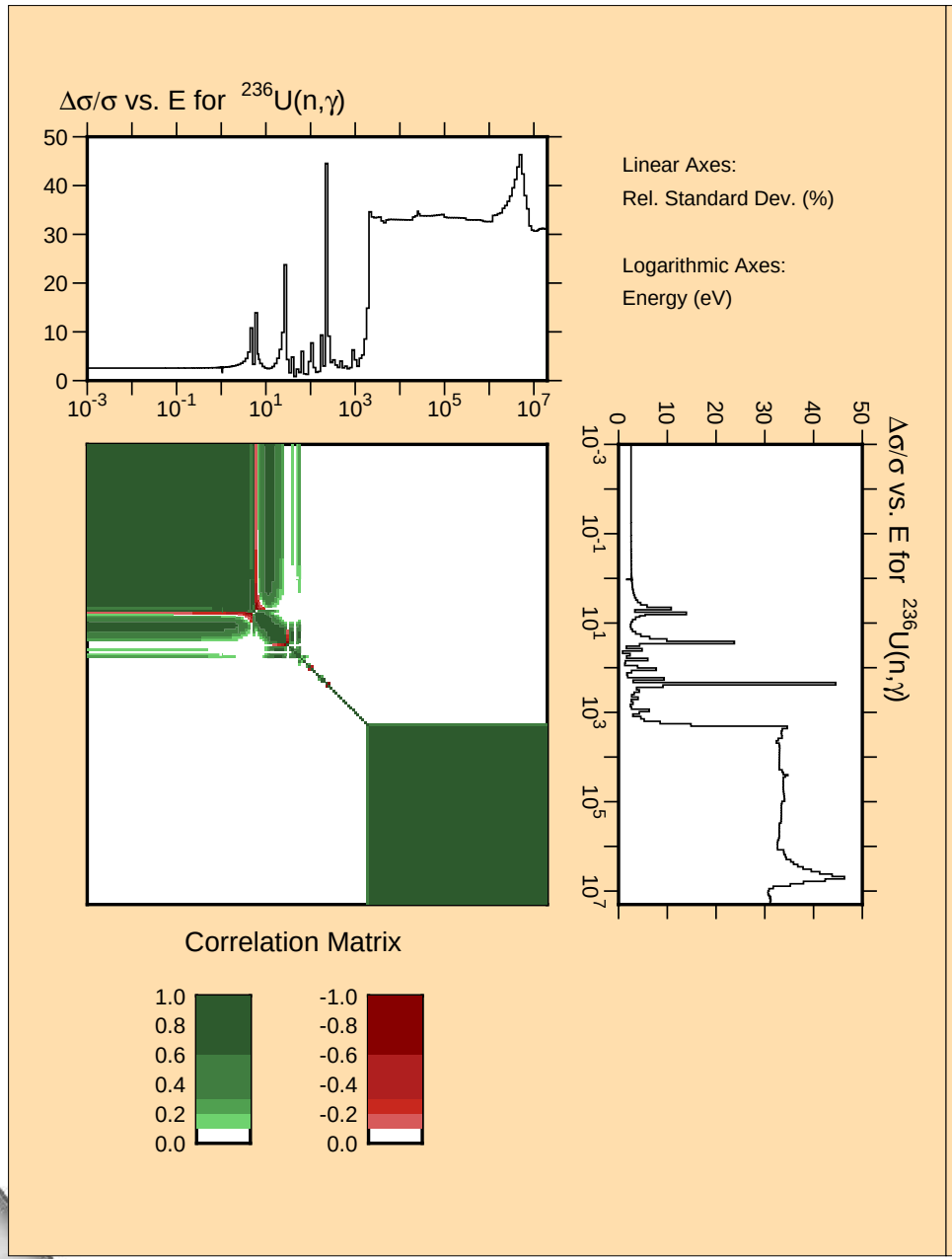


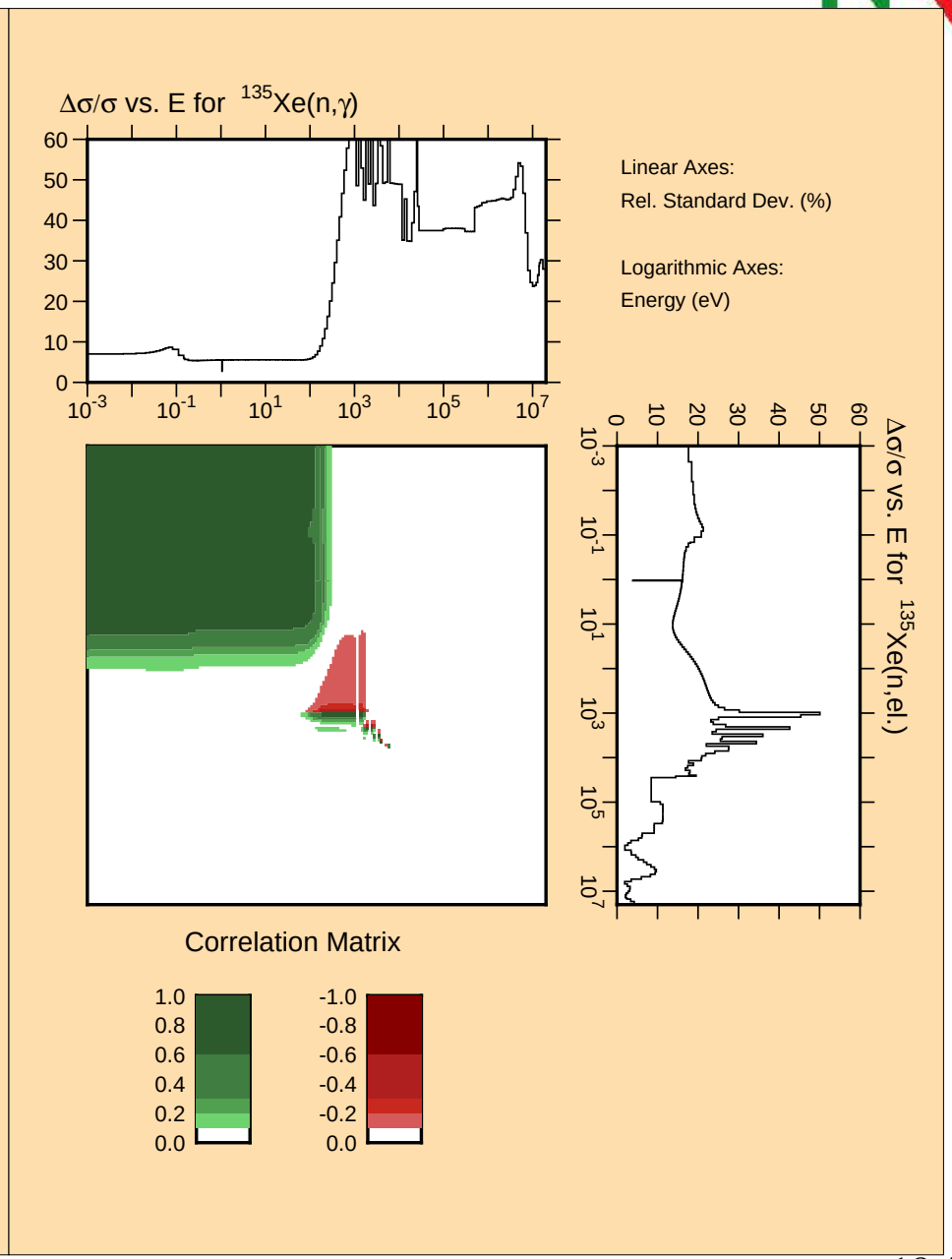






Covariances: example





TENDL-2009: validation

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

Category	Energy Range	Number	Category	Energy Range	Number
LEU	Thermal	285	^{239}Pu	Thermal	105
HEU	Thermal	122	^{239}Pu	Fast	6
HEU	Fast	64	^{239}Pu	Mixed	6
HEU	Inter	9	Other	Thermal	48
HEU	Mixed	5	Other	Fast	19
^{233}U	Thermal	13	^{233}U	Fast	4
Total		686			

Validation: global comparison of 686 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 $\chi^2_{\mathrm{ENDF/B-VII.0}}$:

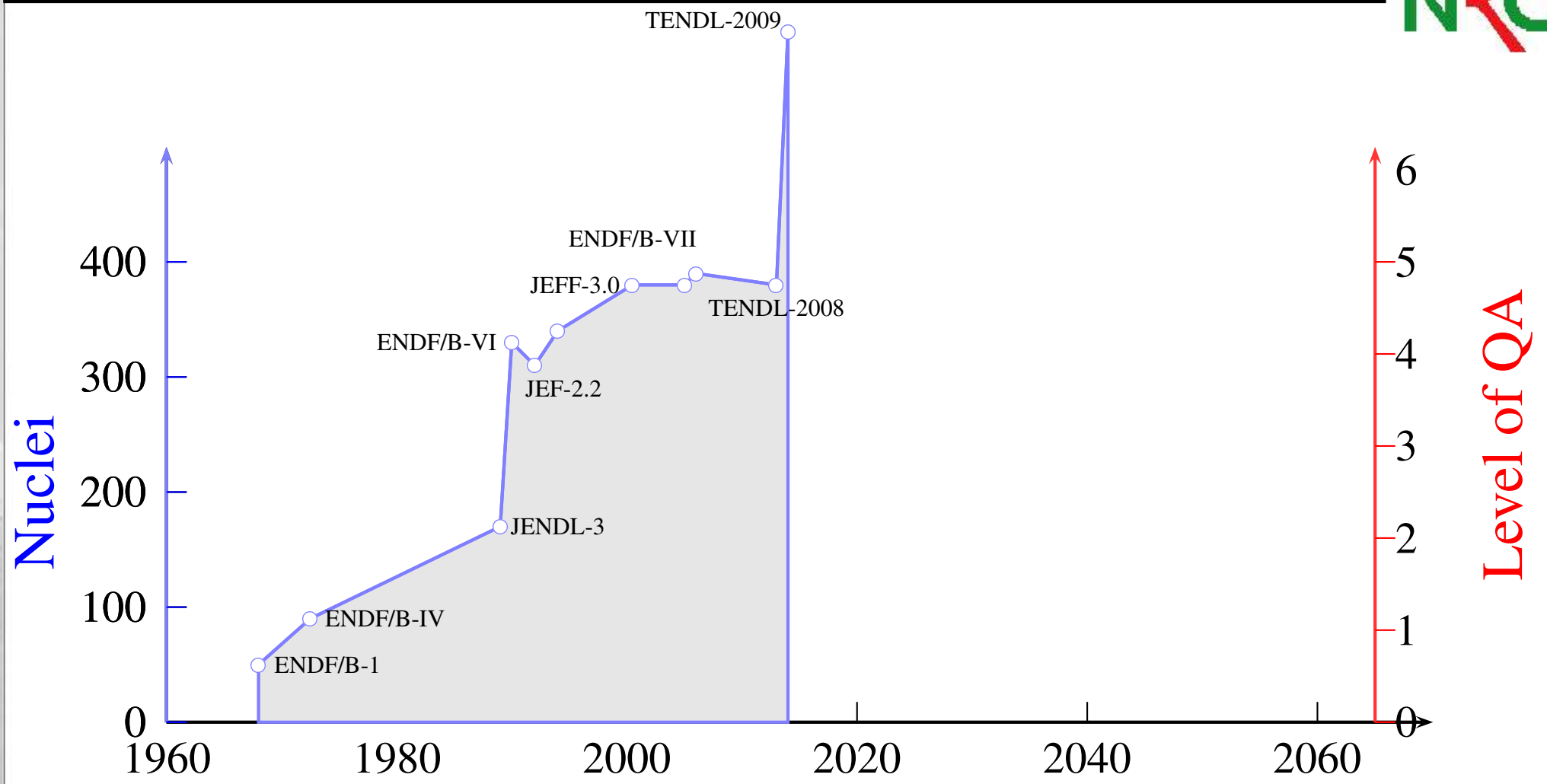
$$\chi^2_{\mathrm{Normalized,library}} = \frac{\chi^2_{\mathrm{library}}}{\chi^2_{\mathrm{ENDF/B-VII.0}}}$$

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

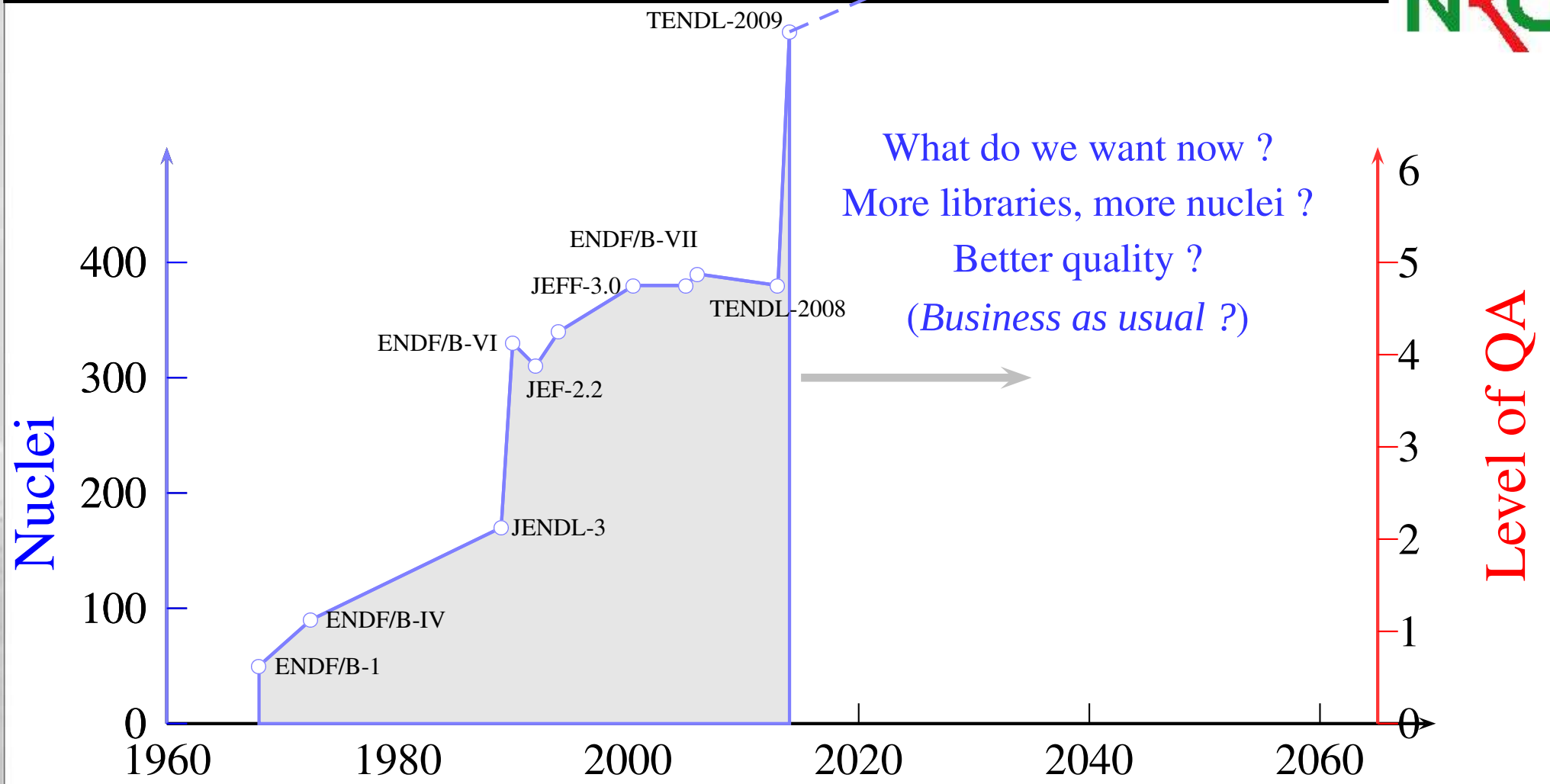
Validation: global χ^2 comparison of 686 crit-safety benchmarks

Library	Normalized χ^2_N					
	Global	LEU	HEU	^{239}Pu	Other	^{233}U
	686	285	200	117	67	17
ENDF/B-VII.0	1.00	1.00	1.00	1.00	1.00	1.00
ENDF/B-VI.8	1.19	1.68	1.24	0.88	1.12	2.52
JEFF-3.1	1.13	0.91	1.39	0.85	1.04	1.68
JENDL-3.3	1.30	1.04	1.42	1.39	1.12	0.42
TENDL-2009β	0.98	1.05	0.97	0.93	1.01	0.90

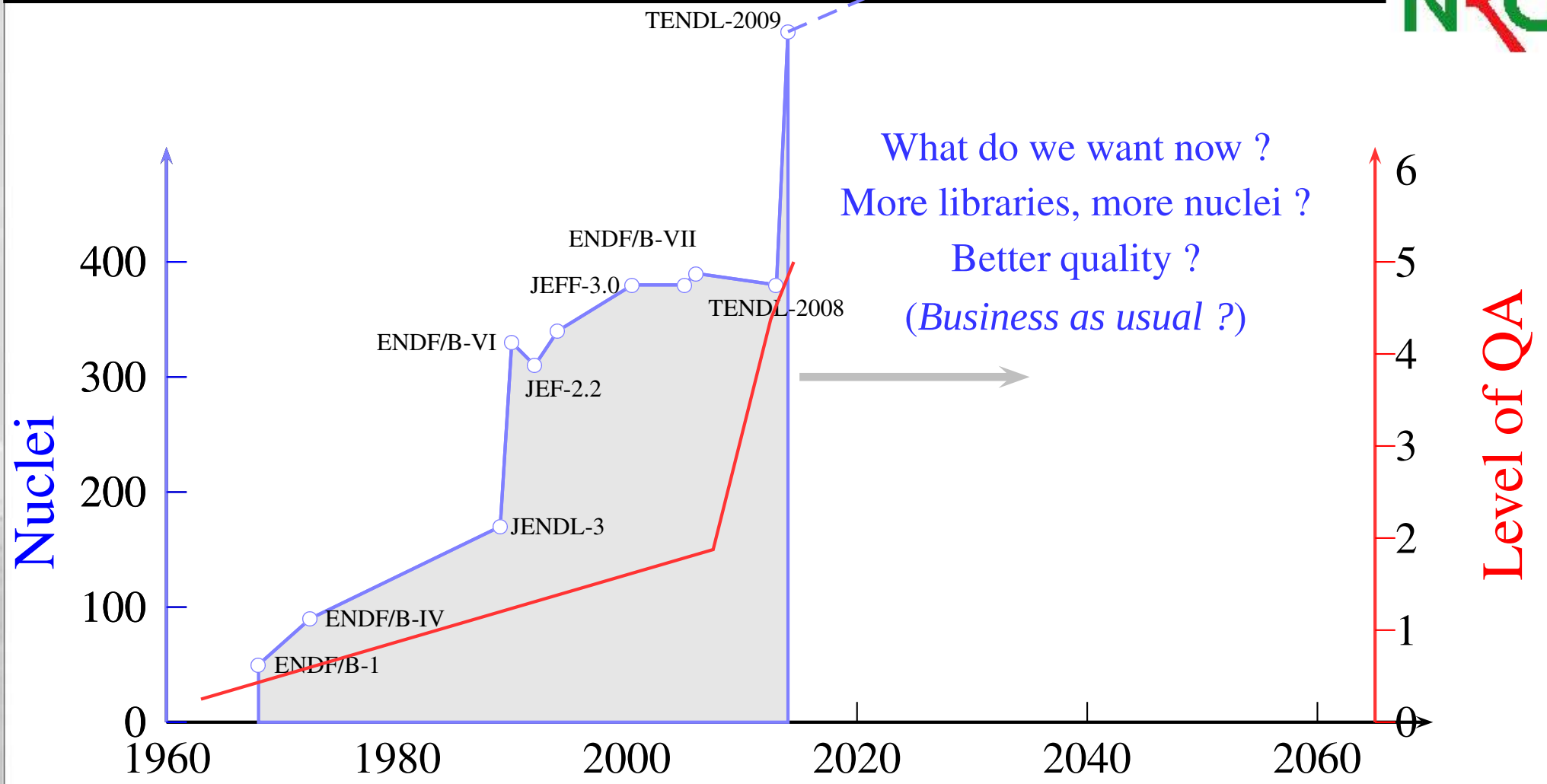
Back to the motivations: where are we ?



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

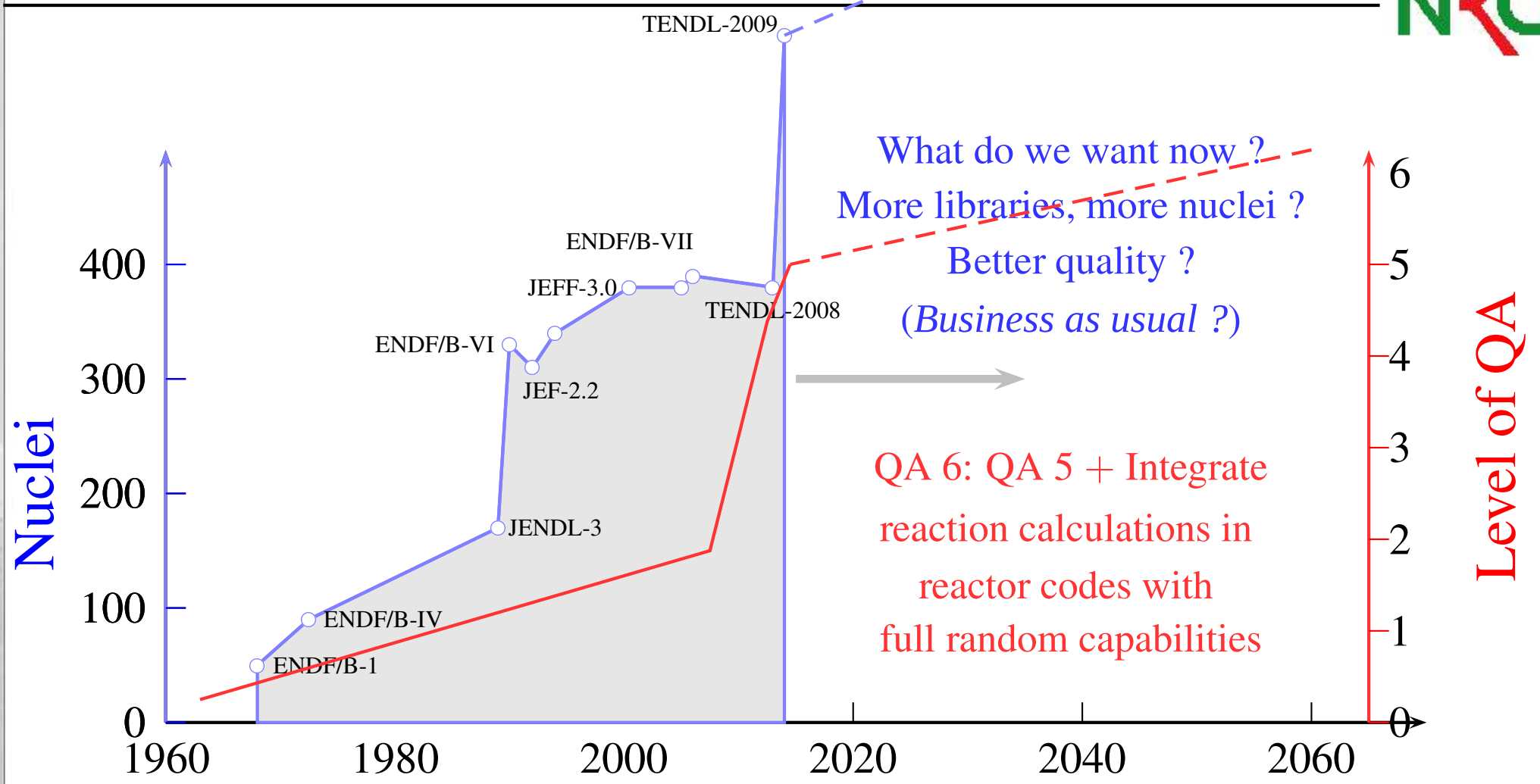
QA 2: QA 1 + Njoy, MCNP

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 with the library and reference papers)
- Best TALYS and resonance parameters fitting

Release date: End of November 2009 !

- Improve global model and uncertainties
- More extensive validation (shielding...)
- Addition of original URR