TENDL 2008-2014:
TALYS-based Evaluated Nuclear Data Library

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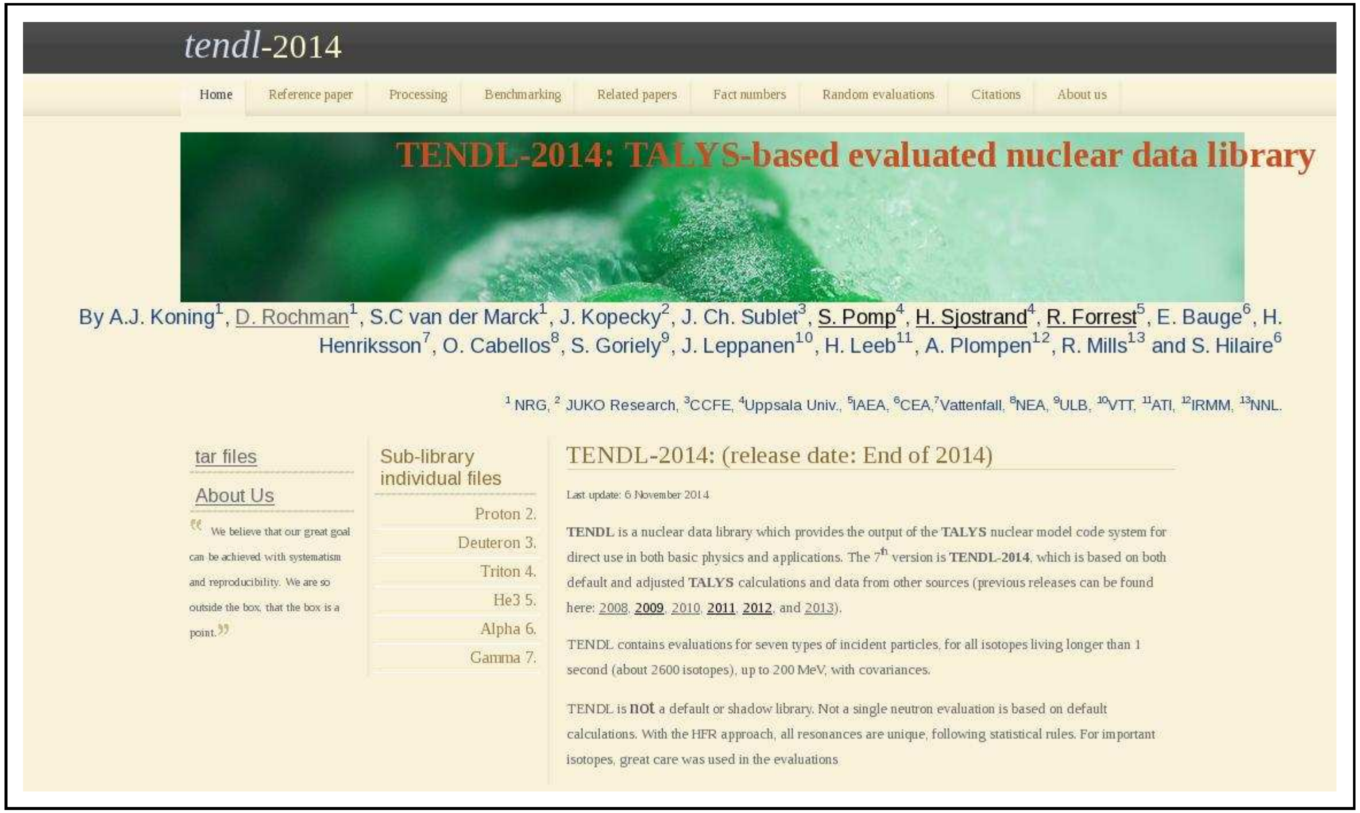
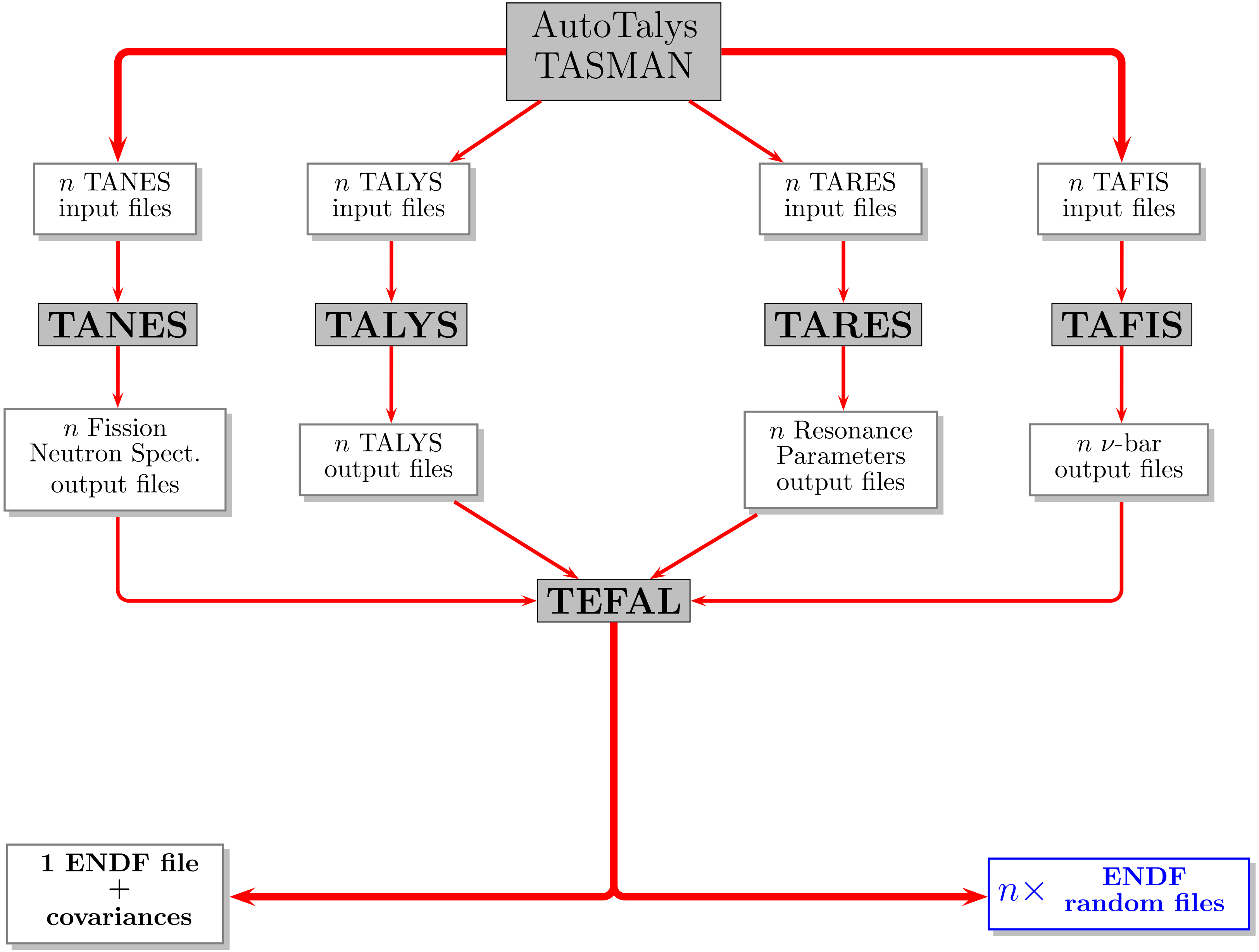


Nuclear data file evaluation and production with the TALYS system.



Possible outcomes based on the TALYS system

- Goal: improve simulations (C/E) for the European library and TENDL,
- Methods: reproductibility & completeness, development of a portable system (called T6) capable of producing TENDL + random nuclear data files and to process them for applications,
- Background: theoretical calculations (TALYS) with experimental inputs, and alternatively, TALYS normalization from other libraries

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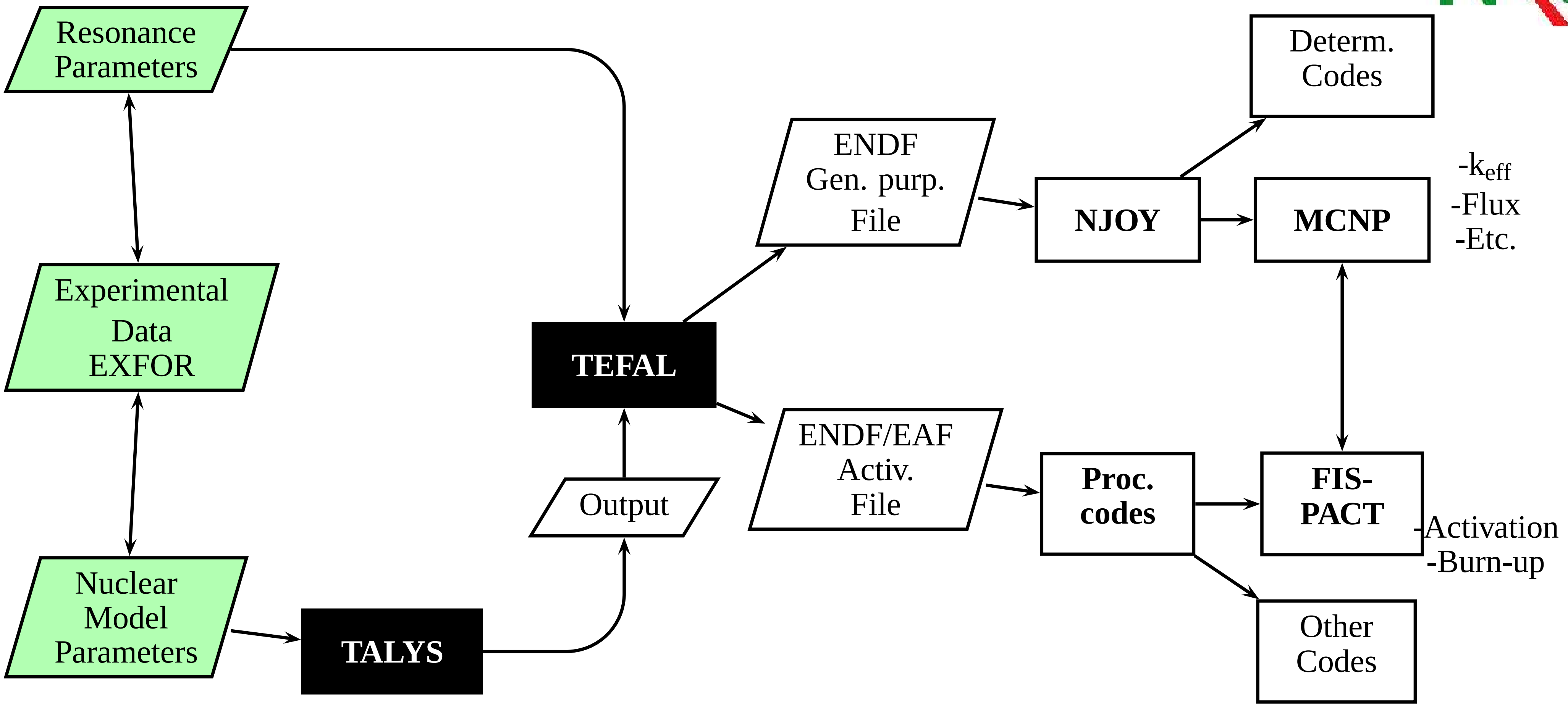
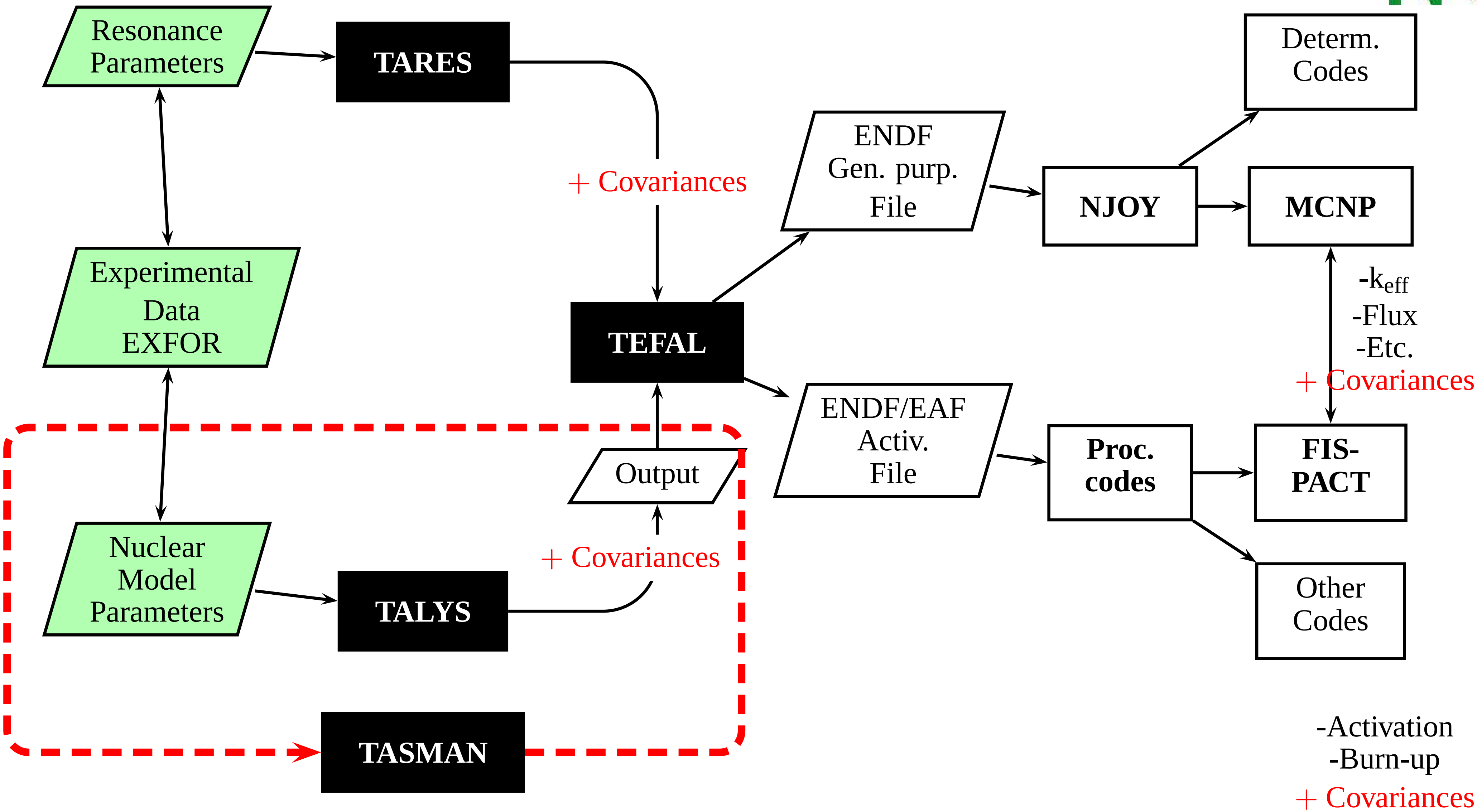
- Impact:
  - TENDL-2008 to 2014 (2600 isotopes),
  - all isotopes with covariances,
  - fully implemented in FISPACT-II,
  - more than 80 isotopes in JEFF-3.2,
  - more than 250 publications using TENDL,

- Normalized MTs:
  - MT2: 61 cases,
  - MT4: 19 cases,
  - MT16: 49 cases,
  - MT18: 26 cases,
  - MT102: 38 cases,
  - MT103: 22 cases,
  - MT107: 11 cases,

Concept: Standard nuclear data scheme



Concept: Nuclear Data Scheme with covariances



TENDL releases

- Available at www.talys.eu/
- Neutrons: ENDF files (MF1-15 and MF31-40), plots, ACE, EAF, processed files and random files (do your own Total Monte Carlo)
- Protons, deuterons, tritons, alphas, gammas: ENDF, ACE, EAF files
- Based on TALYS + automatic normalization

	Neutron	Proton	Deuteron	Triton	Alpha	Helium3	Photon	Fi. Yields	Covariances
TENDL-2014	**?**	**2629**	**2629**	**2629**	**2629**	**2629**	**2629**	**-**	**?**
TENDL-2013	**2630**	**2625**	**2625**	**2625**	**2624**	**2624**	**2626**	**-**	**2630**
TENDL-2012	**2435**	**2429**	**2428**	**2348**	**2429**	**2429**	**2430**	**-**	**2338**
TENDL-2011	**2425**	**2429**	**2419**	**2431**	**2429**	**2428**	**2428**	**574**	**2416**
TENDL-2010	**2394**	**1157**	**1159**	**1156**	**1159**	**1140**	**1152**	**529**	**1086**
TENDL-2009	**2375**	**1163**	**1164**	**1116**	**1163**	**1127**	**1165**	**509**	**1141**
TENDL-2008	348	344	336	339	342	338	327		**342**
(JEFF-3.2)	*472*								*218*
(ENDF/B-VII.1)	*423*	*47*	*5*	*3*		2	*163*	*80*	*146*
(JENDL-4.0)	*406*								*90*

Available files

❶ Tabular angular distributions
❷ Tabular Gamma-ray intensities
❸ Tabular partial cross sections to discrete levels
❹ Tabular residual cross sections
❺ Tabular cross sections
❻ ENDF files including covariances
❼ EAF cross section and variance files
❽ Processed ACE files (with NJOY)
❾ Processed covariances (tabular and plots)
❿ Random ENDF files (to get uncertainties on anything with TMC)

TENDL-2014 Neutron library: from MF-1 to MF-40, 200 MeV

NRG

- 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- 31-32-33-34-35, 40: nubar, Resonance parameter, cross section, angular distribution and fission neutron spectrum, radionuclide production.

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Nuclear Data Sheets

Nuclear Data Sheets 113 (2012) 2841–2934

www.elsevier.com/locate/nds

Modern Nuclear Data Evaluation with the TALYS Code System

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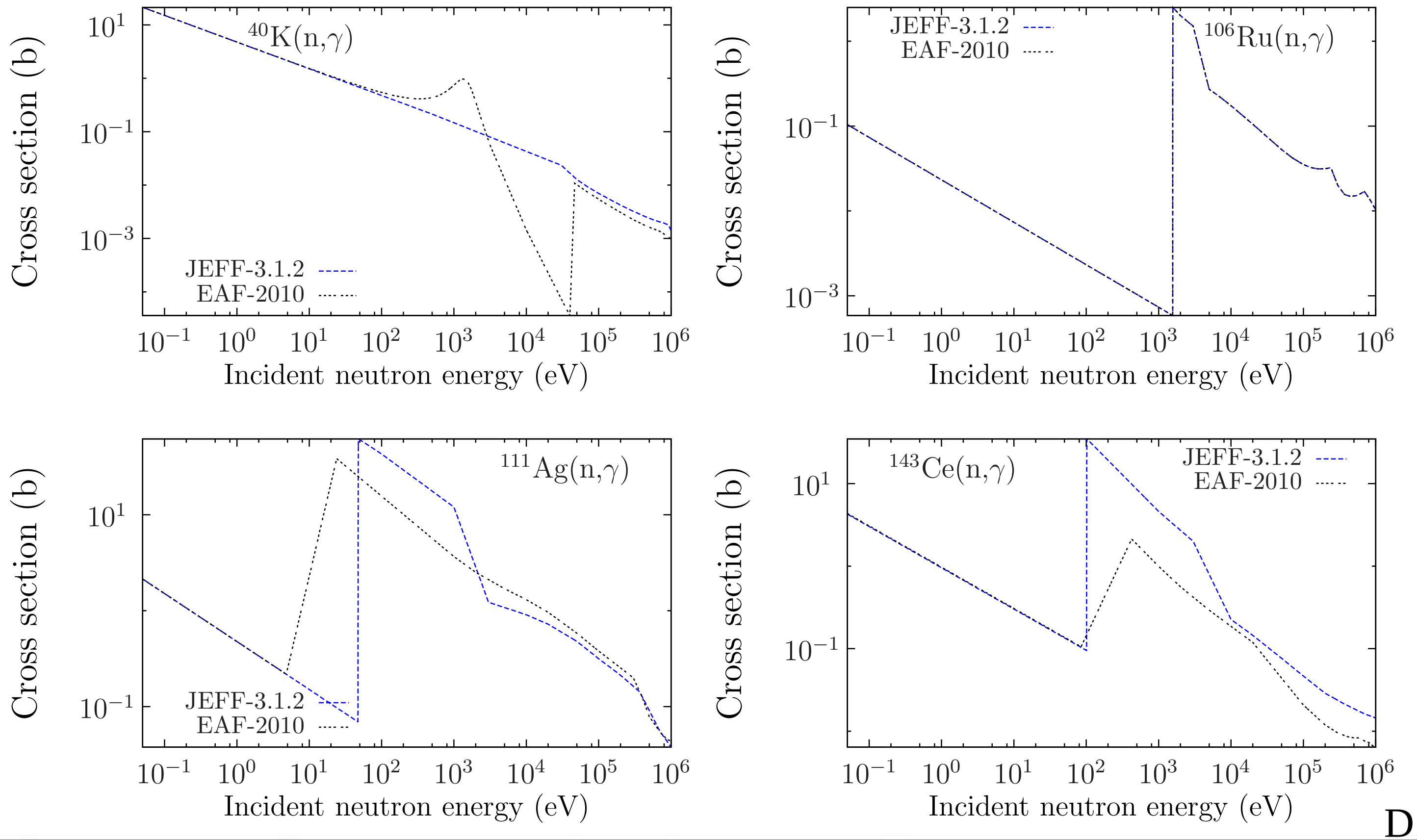
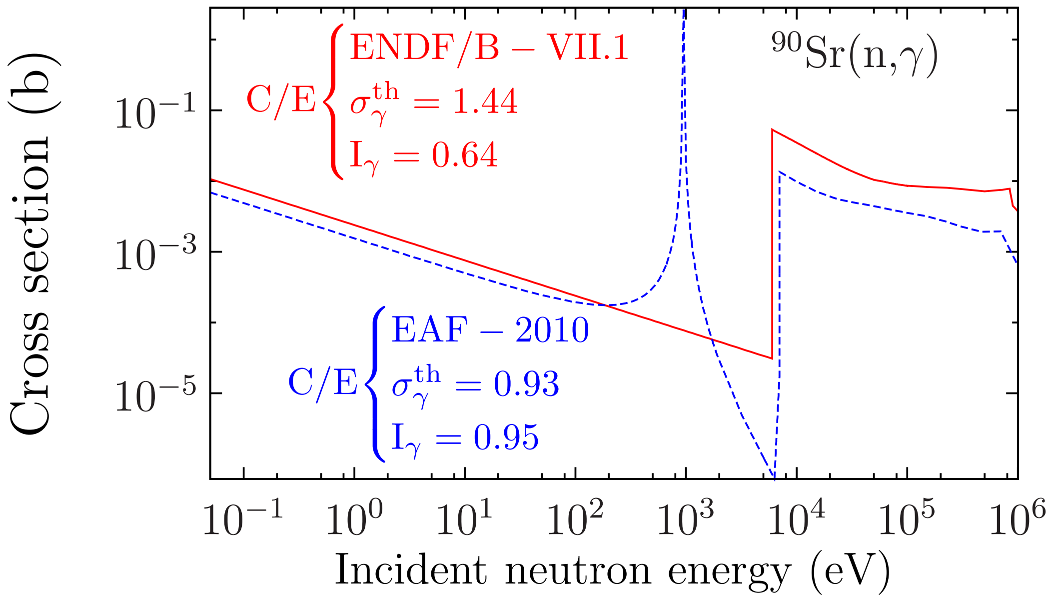
Isotopes with no or a few resonances

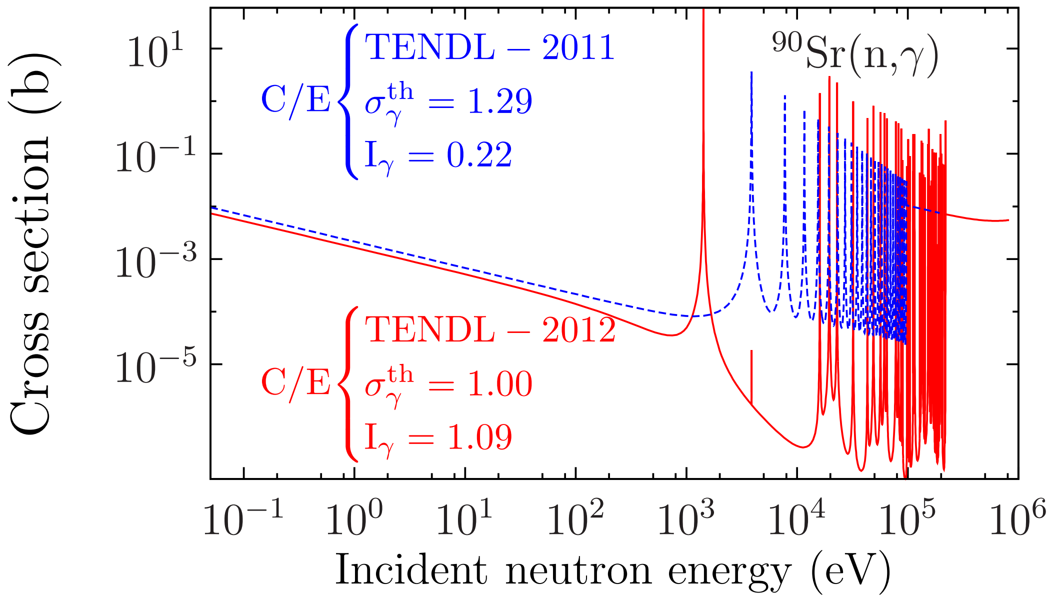
- Improve the global calculations in the resonance range for short-lived nuclides with the TALYS system
- Use CALENDF-2010 to *statistically* reconstruct the URR
- Apply the methodology to TENDL-2012 and proposed isotopes for JEFF-3.2
- Use AVEFIT if possible



Isotopes with no or a few resonances

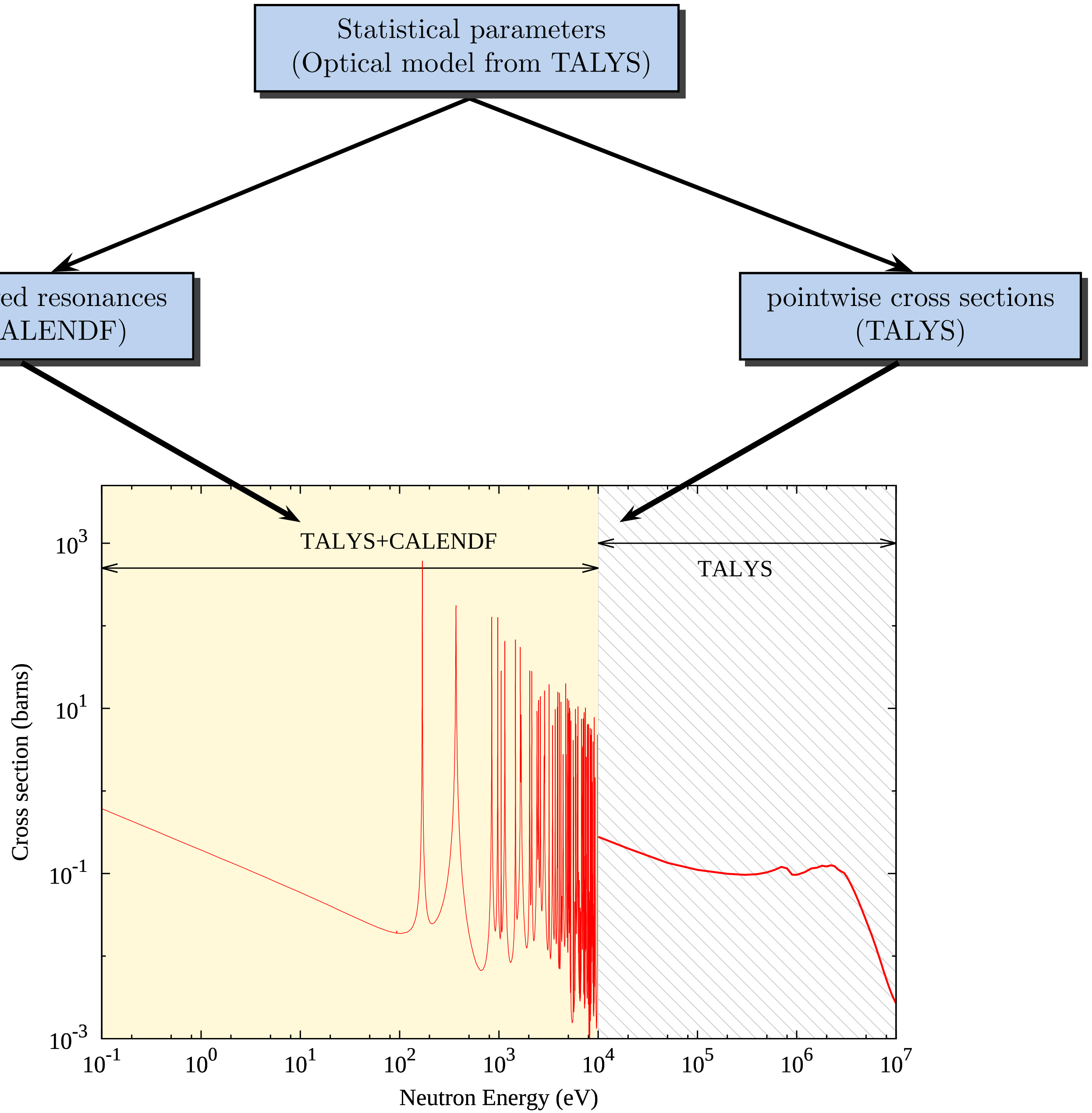
Examples of different approaches for ^{90}Sr ($h_{1/2} = 28$ sec) in the low energy region.



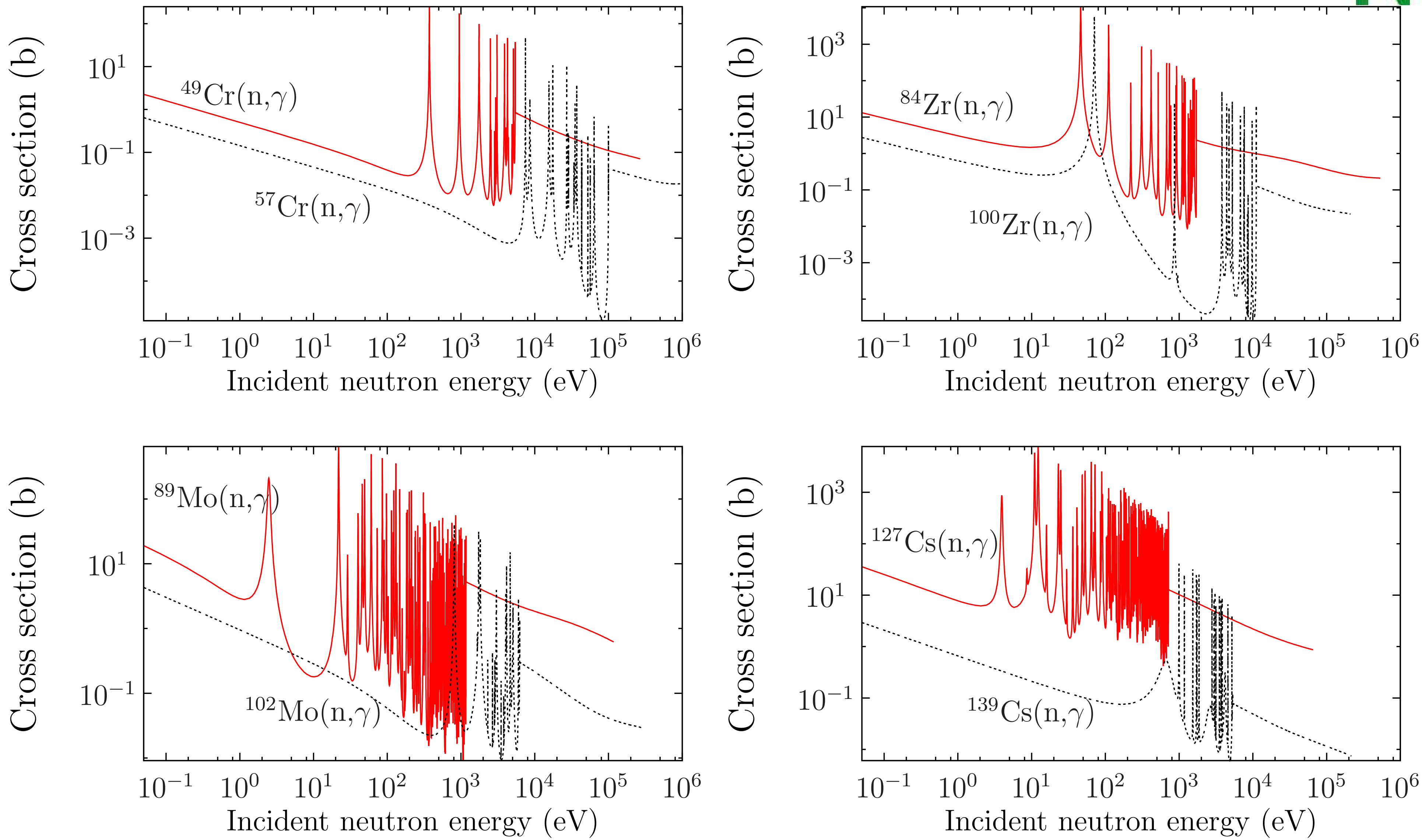


Left: basic optical model calculation for ENDF/B-VII.1 and Single Resonance Approximation (SRA) for EAF-2010. Right: multi-SRA for TENDL-2011 and the present methodology for TENDL-2012.

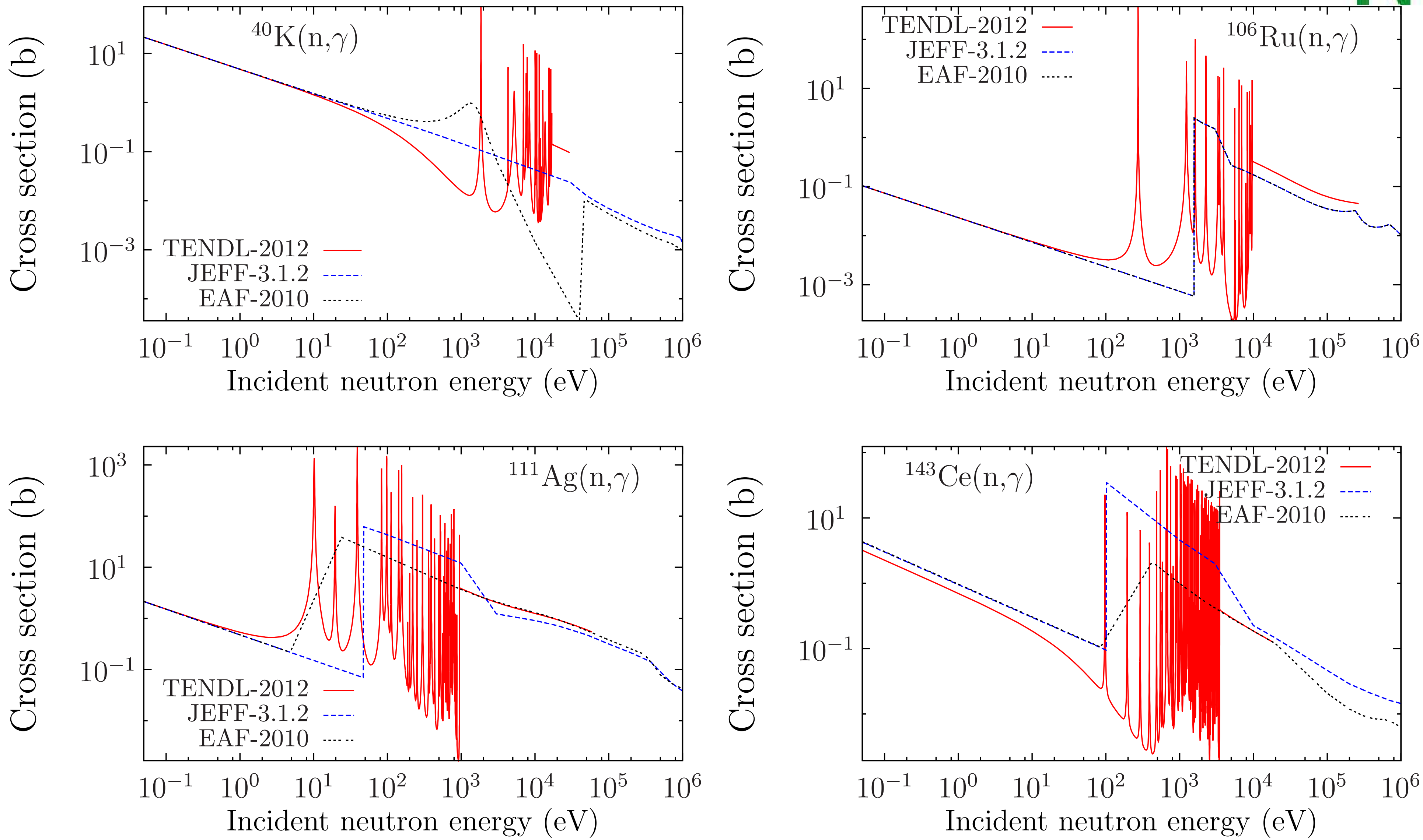
Schematic approach to use in combination TALYS and CALENDF-2010



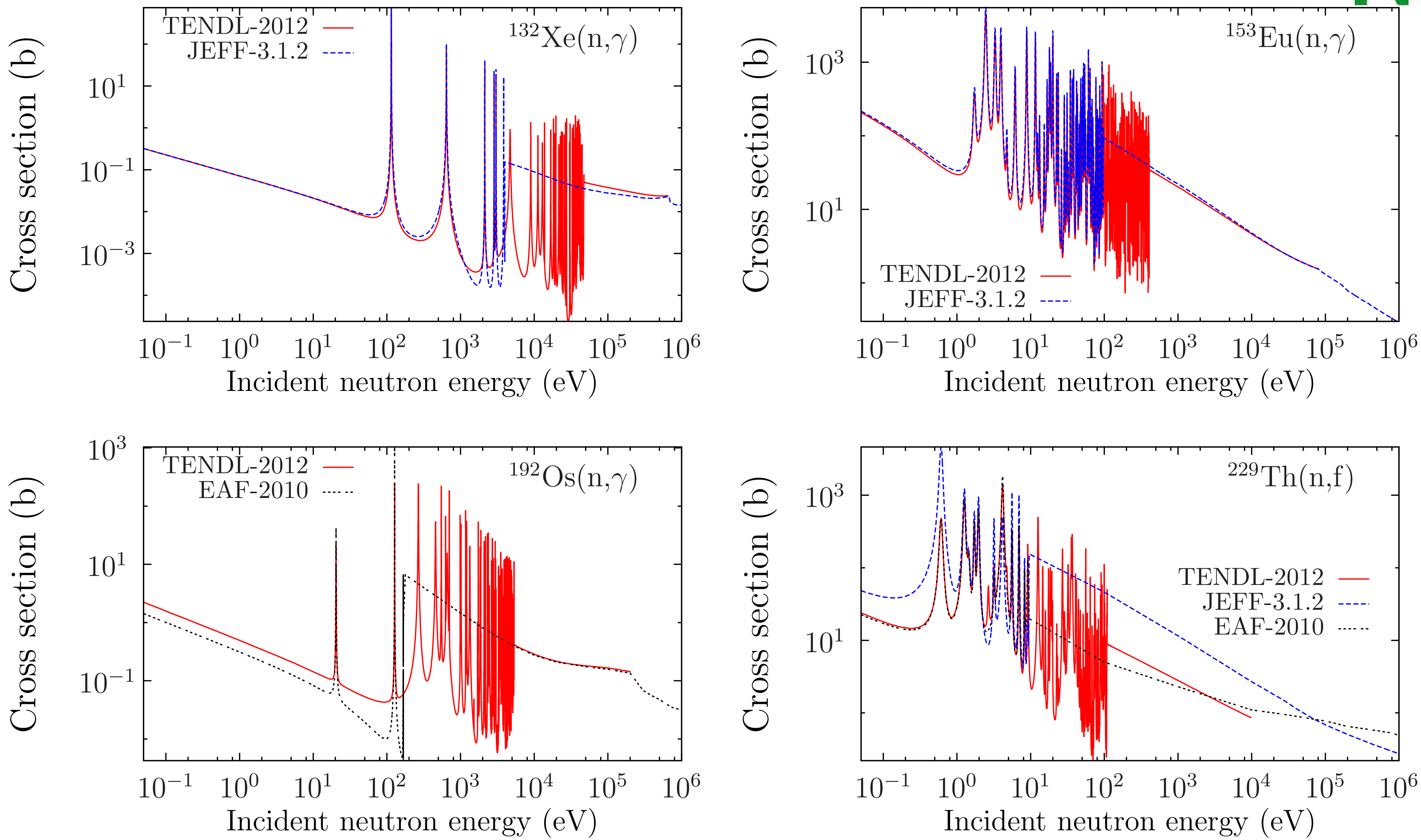
Example 1: short lived isotopes



Example 2: isotopes with known thermal cross sections



Example 3: isotopes with known resonances



Format of the covariance files

ENDF format:

- MF-31: prompt ν-bar (MF33 format) for 288 isotopes
- MF-32: compact Reich Moore or MLBW parameter covariances for 2417 isotopes
- MF-33: group cross section covariances for 2435 isotopes
- MF-34: group elastic angular distribution covariances for 2417 isotopes
- MF-35: prompt fission neutron spectrum (MF33 format) for 285 isotopes
- MF-40: activation cross section covariances for 1757 isotopes

Other formats:

- groups: 33, 44 and 187 groups for cross section covariances (matrix and plots),
- covr: 33 and 44 groups for cross section covariances,
- conversion: existing MF32 to MF33 conversion (but not used yet in TENDL),

Methods

- ☞ MF-31: Monte Carlo variations of input parameters (Los Alamos model)
- ☞ MF-32:

  1. Parameters uncertainties from EXFOR/Atlas + default,
  2. Parameter correlation obtained from the “capture kernel” measurements + default,
  3. Statistical resonances from CALENDF,
  4. Retro-active method from SAMMY,
  5. Adjustments on experimental thermal (n,γ), (n,f) and (n,el) cross sections,
  6. Adjustments on experimental resonance integral and MACS

- ☞ MF-33: Monte Carlo variations of input parameters (TALYS)
- ☞ MF-34: Same
- ☞ MF-35: Monte Carlo variations of input parameters (Los Alamos model)
- ☞ MF-40: Monte Carlo variations of input parameters (TALYS)

Resolved Resonance Region: Parameter correlation

- Short-range correlation
  Based on **capture kernel** and **Bayesian's theorem**

Resolved Resonance Region: Parameter correlation

- Short-range correlation
  Based on **capture kernel** and **Bayesian's theorem**

$$\tilde{\Psi} = \Psi - \Psi \cdot S^t \cdot \left[S \cdot \Psi \cdot S^t + \delta A\right]^{-1} \cdot S \cdot \Psi.$$

Ψ and $\tilde{\Psi}$ are the prior and posterior covariance matrices for the resonance

$$\Psi = \begin{pmatrix} \delta\Gamma_n^2 & corr\left(\Gamma_n, \Gamma_\gamma\right) \delta\Gamma_n \delta\Gamma_\gamma \\ corr\left(\Gamma_n, \Gamma_\gamma\right) \delta\Gamma_n \delta\Gamma_\gamma & \delta\Gamma_\gamma^2 \end{pmatrix},$$

S is the sensitivity matrix and S^t its transpose:

$$S = \begin{pmatrix} \frac{\partial A}{\partial \Gamma_n} \\ \frac{\partial A}{\partial \Gamma_\gamma} \end{pmatrix}. \qquad (1)$$

- Long-range correlation
  -Γ_γ-Γ_γ, E_r-E_r, R' and the retroactive method (short-long range)

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.*

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

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

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

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

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

Testing

- ☞ TMC: indirect testing with the equivalent random files in TMC,
- ☞ processing 1: automatic processing during TENDL production (NJOY),
- ☞ processing 2: processing at CCFE and testing in FISPACT-II,
- ☞ export: covariances used in other libraries (FENDL, JEFF),
- ☞ export: covariances/random files used in codes (GEANT, MCNP for charged particles, SERPENT, SCALE),
- ☞ comparison: automating comparison with experimental/evaluated results,
- ☞ comparison: covariance/TMC with PSI, AREVA, GSI and JRC Petten.

TENDL: Importing other cross sections: *autonorming*

The *autonorming* capability of the TALYS system is a key functionality in this project (see EFF-1219 for details).

- read the original cross section with its energy grid,
- import it in the TENDL evaluation (replacing the existing TALYS cross section),
- expand or simply adjust the energy grid to match the TENDL lower and higher limits,
- respect the sum rules (modifying one or more of the total, elastic and non elastic cross sections),
- keep the possibility to obtain random cross sections for the TMC uncertainty propagation.

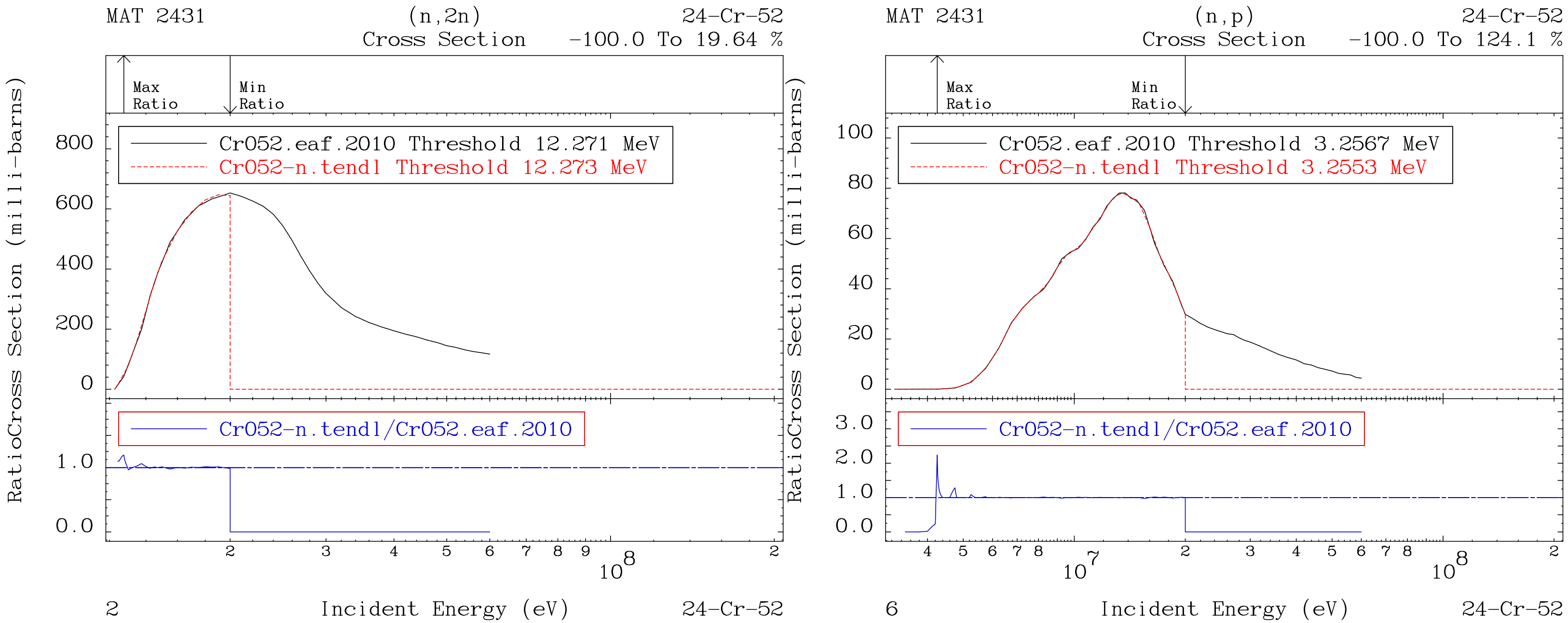
Importing other cross sections: *autonorming*

In practice, this functionality needs care to be properly implemented. In this work, it is extensively used to reproduce cross sections from the EAF-2010 library.

Main drawback: it is not possible to obtain ”better” results than the autonormed library. Even if this method can be applied to any cross sections, independently of the values of the original TALYS cross sections, it is better to *autonorm* cross sections which are already close to the imported ones. In order to minimize the modifications to other channels because of the sum rule, the cross section to be replaced should first be adjusted to values which are in agreement to the imported ones.

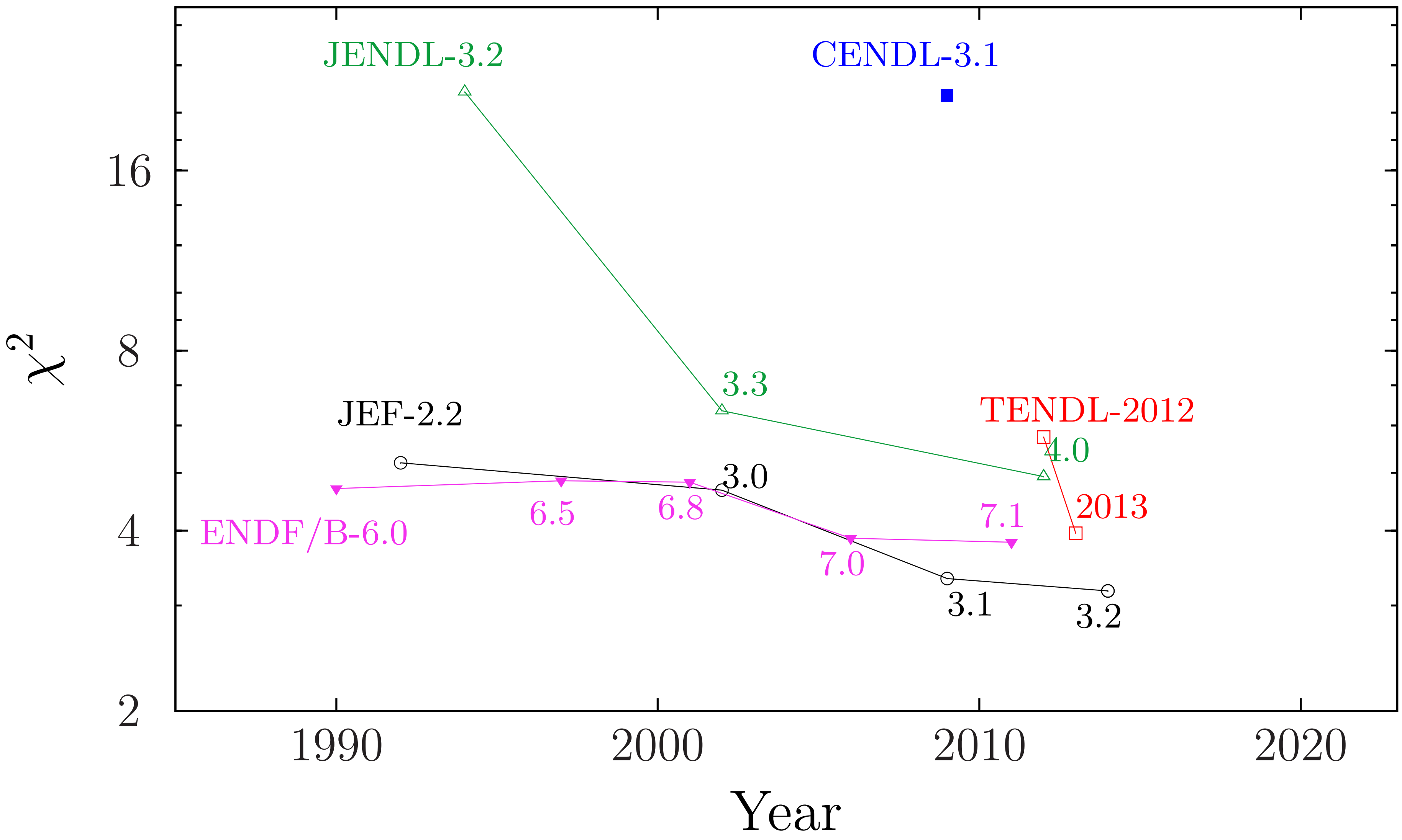
This can be achieved by adjusting the TALYS parameters so that the right cross section values are obtained. The prior agreement between the two sets of cross sections does not need to be perfect, but small differences (less than 5 %) assures that the modifications to other channels (such as elastic), or to related quantities (such as angular distributions, particle emissions) do not jeopardize physical consistency.

Importing other cross sections: *autonorming*



How well do we work ?

^{239}Pu criticality benchmarks $\chi^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{C_i - E_i}{\Delta E_i}\right)^2$ n=400



Conclusions and Future improvements

- TENDL, covariances, TMC: parallel developments,
- TENDL is now a collaborative effort between 7 groups (NRG, CCFE, JUKO, Uppsala Univ., IAEA, Vattenfall, CEA),
- Possibility to adopt an entire existing data library (e.g. JEFF-3.2) and make it complete,
- More extensive validation (burn-up...) with uncertainties with TMC,
- Improve global model and uncertainties,
- Completeness, based on reproductibility idea (t6.tar)

☺And finally nuclear data world domination (and world peace).