Covariances for the TENDL library

D. Rochman for the TENDL team

Nuclear Research and Consultancy Group,

NRG, Petten, The Netherlands

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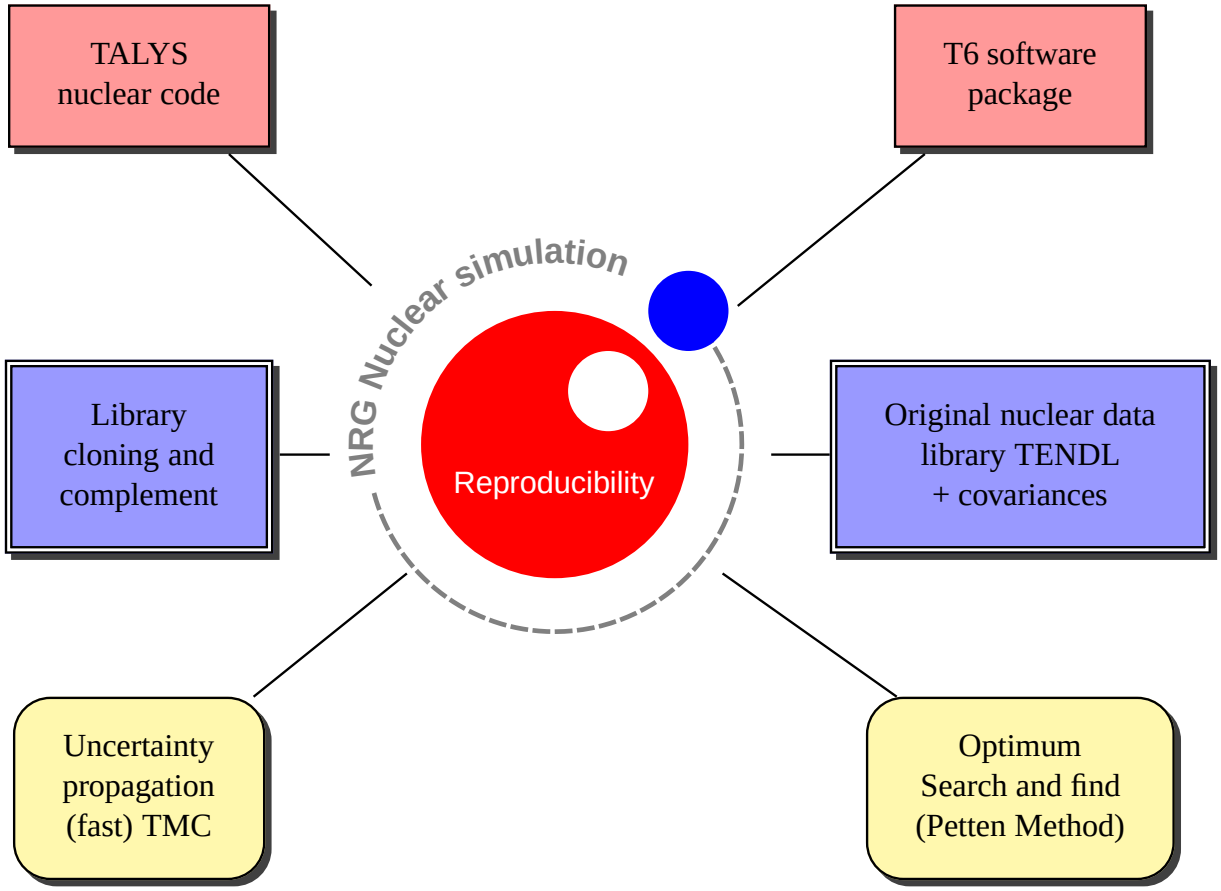
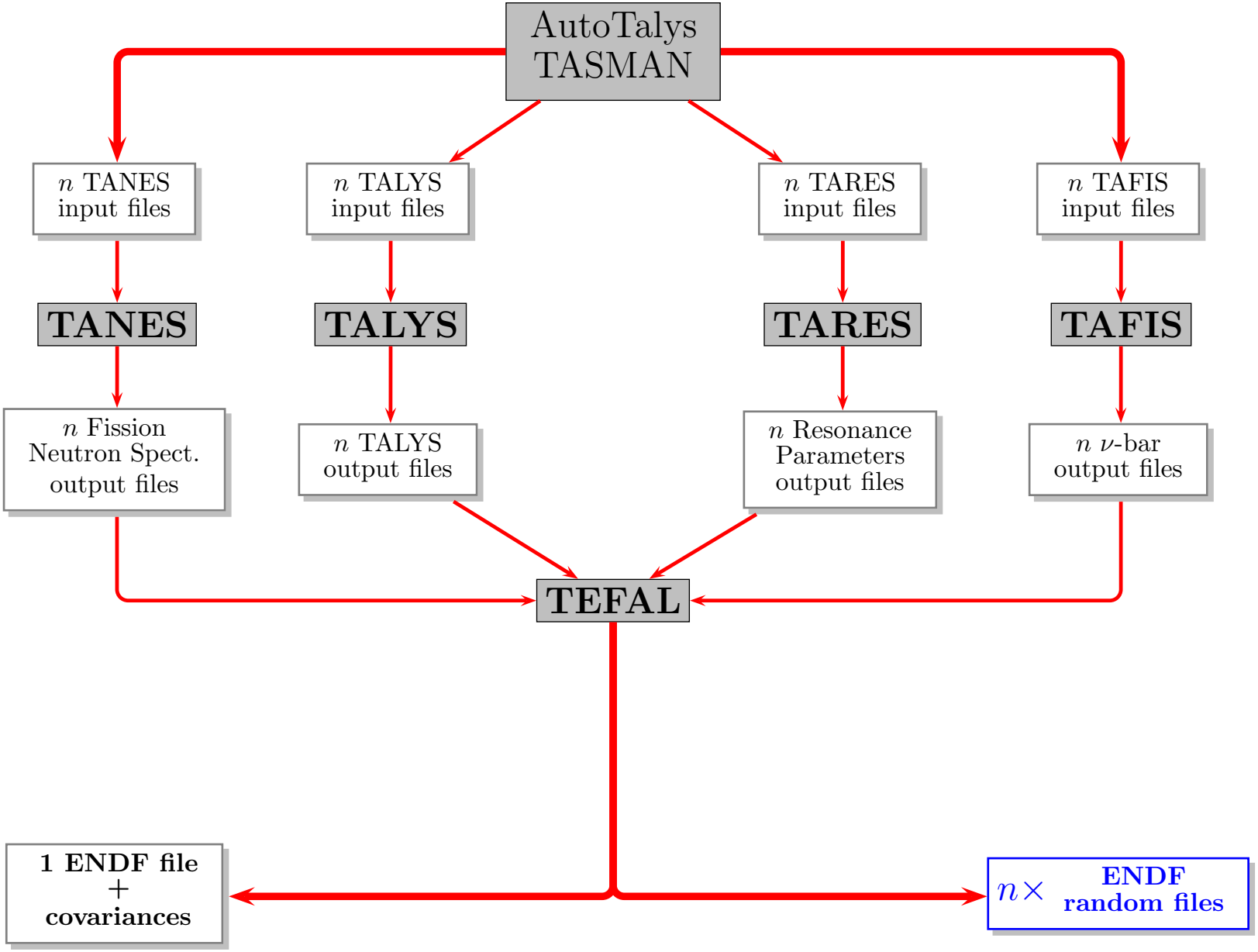


Nuclear data file evaluation and production with the TALYS system.



Background: TENDL-2012 covariances (www.talys.eu/tendl-2012)

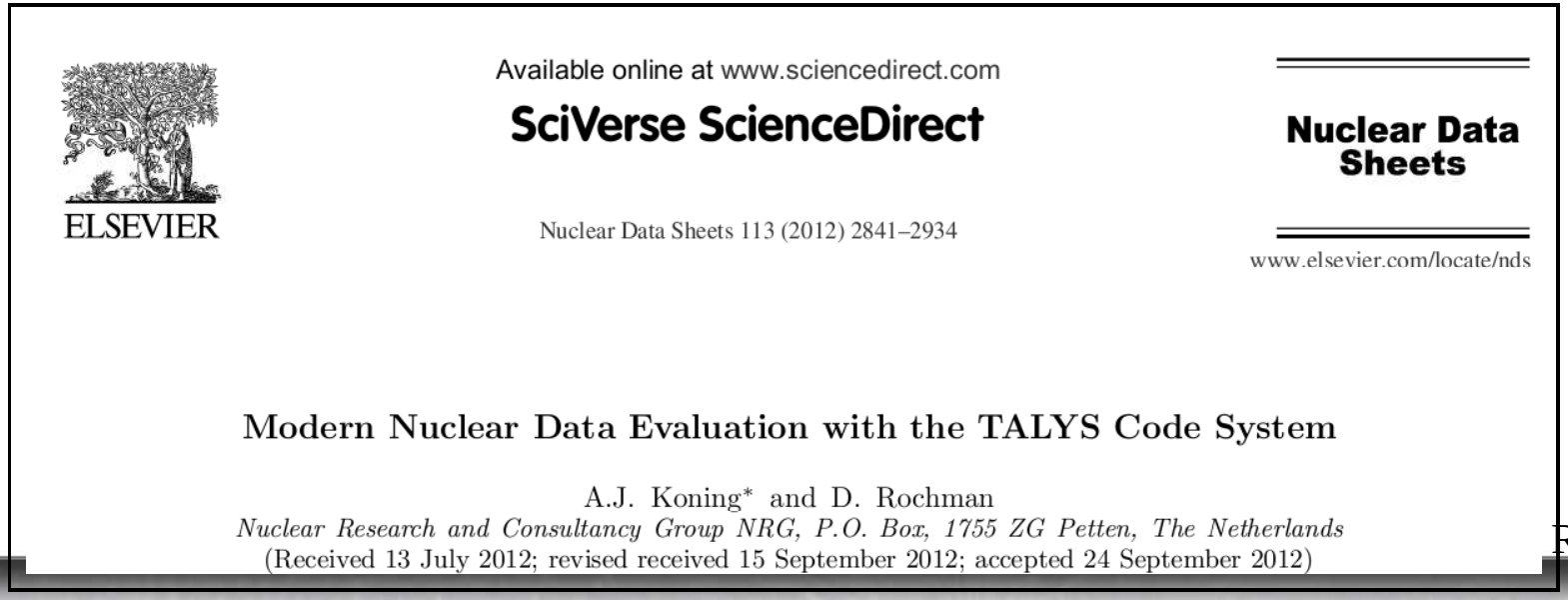
- Collaboration between NRG, CCFE, JUKO Research, Uppsala University, IAEA/NDS, CEA Bruyeres-le-Châtel and Vattenfall
- Neutrons: ENDF files (MF1-15 and MF31-40), plots, ACE, EAF, processed files
- random files (do your own Total Monte Carlo)
- Based on TALYS + automatic normalization
- Imported files: ^{1,2,3}H, ^{3,4}He, ^{6,7}Li, ^{9}Be, ^{10,11}B, ^{nat}C, ^{14,15}N, ^{16}O, ^{19}F, ^{235,238}U, ^{239}Pu

	Neutron	Proton	Deuteron	Triton	Alpha	Helium3	Photon	Fi. Yields	Covariances
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-3.1.2)	*381*	*26*						*44*	*32*
(ENDF/B-VII.1)	*423*	*47*	*5*	*3*		2	*163*	*80*	*146*
(JENDL-4.0)	*406*								*90*

Content 3- TENDL-2012 Neutron library: from MF-1 to MF-40

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-4-5: Elastic angular distribution (Legendre Polynomials) + Prompt/delay FNS
- MF-6: Double differential distributions and spectra for (n,2n), ..., (n,α_i)
- MF- 8-10-12-15: Isomeric xs, gamma yields, angular distributions and spectra
- MF- 31-32-33-34-35-40: nubar, Resonance parameter, cross section, elastic angular distribution and fission neutron spectrum covariances



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Modern Nuclear Data Evaluation with the TALYS Code System

A.J. Koning* and D. Rochman

Nuclear Research and Consultancy Group NRG, P.O. Box, 1755 ZG Petten, The Netherlands

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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. Adjustements on experimental thermal (n,γ), (n,f) and (n,el) cross sections,
  6. Adjustements 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.*

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

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

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

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.

Conclusions and Future improvements

- The development of covariances is parallel to the development of the TENDL libraries ,
- 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-3.1.1) and make it complete,
- More extensive validation (burn-up...) with uncertainties with TMC,
- Improve global model and uncertainties,
- Convert MF32c to MF33 ?
- Include delayed fission neutron spectrum uncertainties.

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