# GND: Purpose of the new data structure

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- The essential points in the nuclear data chain
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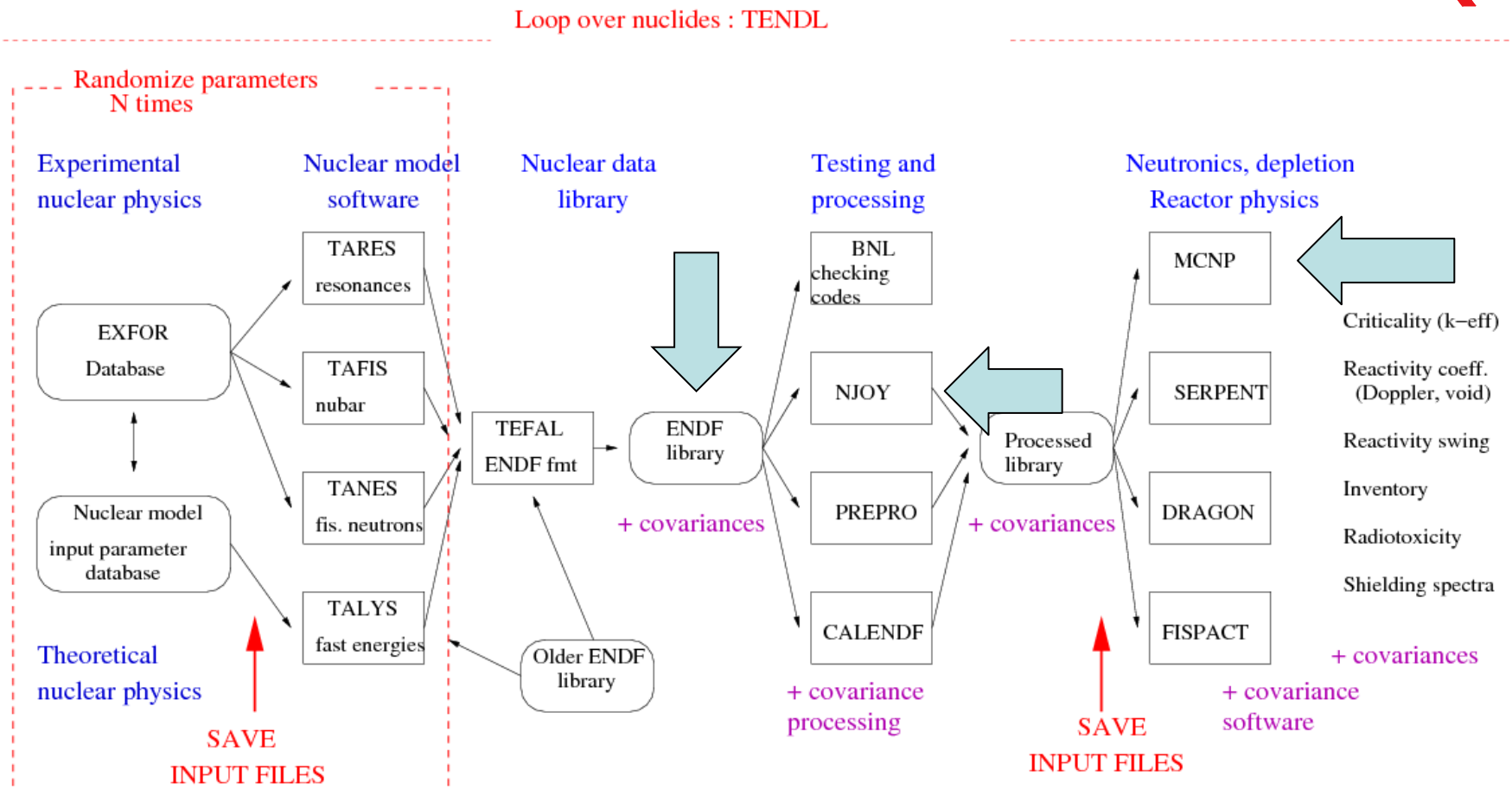
# Essential points in the nuclear data chain




Cost: $$ $$$ $$$$

## TALYS Evaluated Nuclear Data Library: TENDL-2012

- Neutron, proton, deuteron, triton, Helium-3, alpha and gamma data libraries.
- 2430 targets (all isotopes with lifetime > 1 sec.)
- Complete reaction description in ENDF-6 format: MF1-MF40, up to 200 MeV
- MCNP-libraries ("ACE-files"), PENDF files and multi-group covariance data

Default: Global calculations by TALYS-1.48 and TARES (resonances)

which are overruled by

Adjusted TALYS calculations (340 input files) and Resonance Atlas-based TARES calculations

which are overruled by

TALYS-normalization to ~200 (experimental) evaluated reaction channels from other libraries (e.g. IRDFF, light nuclides, main channels of "big 3")

# Basic format and physics verification

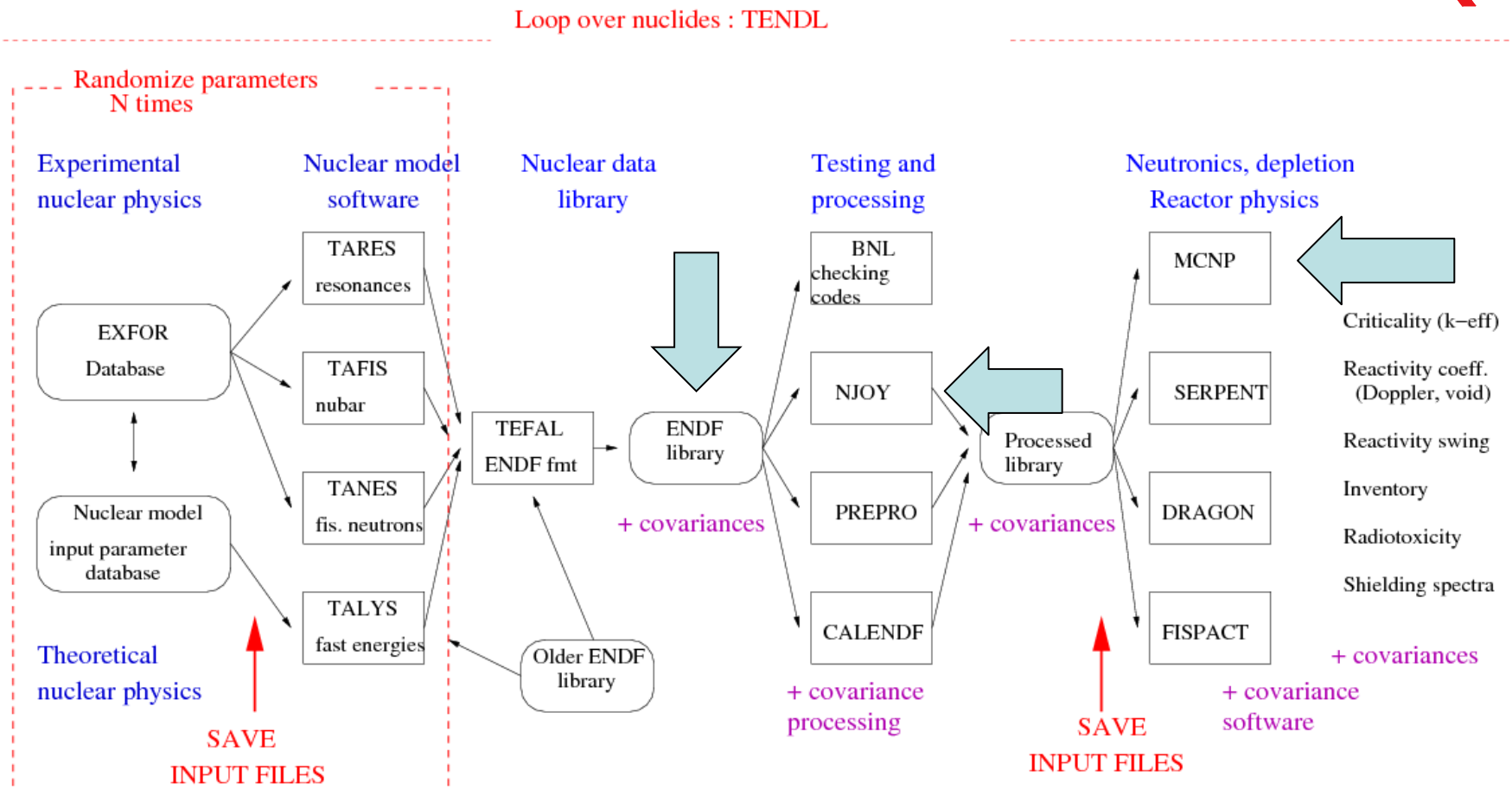
2430 (nuclides) x 7 (projectiles) data libraries are tested with:

- CHECKR, FIZCON, PSYCHE and INTER
- FUDGE (is ENDF2GND2ENDF = ENDF ?)
- PREPRO-2010
- NJOY-99.364
- MCNPX-2.7

Scripts which search for all the possible warning and error messages by the above codes have been used. Now all problems for these 17010 data libraries are (almost) gone.

Checking all plots is more time consuming and boring……but it should be done.

# Essential points in the nuclear data chain

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# Classification of nuclear reactions

From the TALYS manual:

$$\sigma_{tot} = \sigma_{el} + \sigma_{non-el}.$$

Elastic angular distribution can again be unambiguously provided

Remaining question: Do we again have a cut in the energy grid between the resonance range and the pointwise range: MF2/MF3

Most ambiguity arises for the components of the non-elastic cross section.

# Classification of nuclear reactions

$$\sigma_{non-el} = \sum_{i_n=0}^{\infty}\sum_{i_p=0}^{\infty}\sum_{i_d=0}^{\infty}\sum_{i_t=0}^{\infty}\sum_{i_h=0}^{\infty}\sum_{i_\alpha=0}^{\infty}\sigma^{ex}(i_n, i_p, i_d, i_t, i_h, i_\alpha),$$

e.g. the $(n, 2np)$ cross section is given by $\sigma^{ex}(2, 1, 0, 0, 0, 0)$

With a further subdivision:

$$\sigma_{n,n'} = \sigma^{disc}_{n,n'} + \sigma^{cont}_{n,n'},$$ MT4=MT51-90 + MT91

$$\sigma^{disc}_{n,n'} = \sum_{i=1}^{N}\sigma^{i}_{n,n'}.$$ MT51-90

This already gives rise to inconsistencies (sum rules etc.). Should all partial cross sections be given as ratios?

# Classification of nuclear reactions

Alternative: breakdown in residual production cross sections:

$$\sigma_{non-el} = \sum_Z \sum_N \sigma_{prod}(Z,N).$$

(3.25)
$$\sigma_{prod}(Z,N) = \sum_{i_n=0}^{\infty}\sum_{i_p=0}^{\infty}\sum_{i_d=0}^{\infty}\sum_{i_t=0}^{\infty}\sum_{i_h=0}^{\infty}\sum_{i_\alpha=0}^{\infty} \sigma^{ex}(i_n,i_p,i_d,i_t,i_h,i_\alpha)\delta_N\delta_Z\,,$$

where the Kronecker delta's are defined by

(3.26)
$$\begin{aligned}
\delta_N &= 1 \text{ if } i_n + i_d + 2i_t + i_h + 2i_\alpha = N_C - N \\
&= 0 \text{ otherwise} \\
\delta_Z &= 1 \text{ if } i_p + i_d + i_t + 2i_h + 2i_\alpha = Z_C - Z \\
&= 0 \text{ otherwise,}
\end{aligned}$$

$(Z_C, N_C)$. As an example, consider the $n + {}^{56}\text{Fe} \rightarrow {}^{54}\text{Mn} + x$ reaction. The exclusive cross sections that add up to the $^{54}$Mn production cross section are $\sigma_{n,2np}$, $\sigma_{n,nd}$, and $\sigma_{n,t}$, or $\sigma^{ex}(2,1,0,0,0,0)$, $\sigma^{ex}(1,0,1,0,0,0)$, and $\sigma^{ex}(0,0,0,1,0,0)$, respectively.

One could also use ratios here. For most important channels this is trivial

In ENDF-6 format, total particle production is obtained as follows

$$\sigma_{n,xn} = \sum_{i_n=0}^{\infty}\sum_{i_p=0}^{\infty}\sum_{i_d=0}^{\infty}\sum_{i_t=0}^{\infty}\sum_{i_h=0}^{\infty}\sum_{i_\alpha=0}^{\infty} i_n \sigma^{ex}(i_n, i_p, i_d, i_t, i_h, i_\alpha), \tag{3.20}$$

i.e. in the more common notation,

$$\sigma_{n,xn} = \sigma_{n,n'} + 2\sigma_{n,2n} + \sigma_{n,np} + 2\sigma_{n,2np} + .... \tag{3.21}$$

Which also starts to give problems at high energies. Can we get rid of the MT5 switch by using a different reaction classification?

# Associated issues

- The current ENDF-6 format is very unforgiving. One set of zeroes at the wrong place and the whole (processing) machinery stops
- Should we make nuclear data evaluation more idiot-proof, and perform default operations on a GND library if certain info is not given? E.g. no angular distribution means isotropy.

# Important spin-offs

- Easier plotting of any data curve
- Automatic comparison with EXFOR will be more general and easier:
  - For cross sections (MF3) this can (and is) already done, since there is basically one format option

  (7 400 000 data points in EXFOR, 2 500 000 can be automatically compared with ENDF-6 data libraries)
  - For secondary distributions like DDX, angular distributions, gamma production etc. there is too much liberty for the evaluator, and that liberty has been used in the past.
  - Translation to one unified GND format will enable easier comparison of libraries with EXFOR, and thus more efficient evaluation of data