Nuclear reaction data in GND

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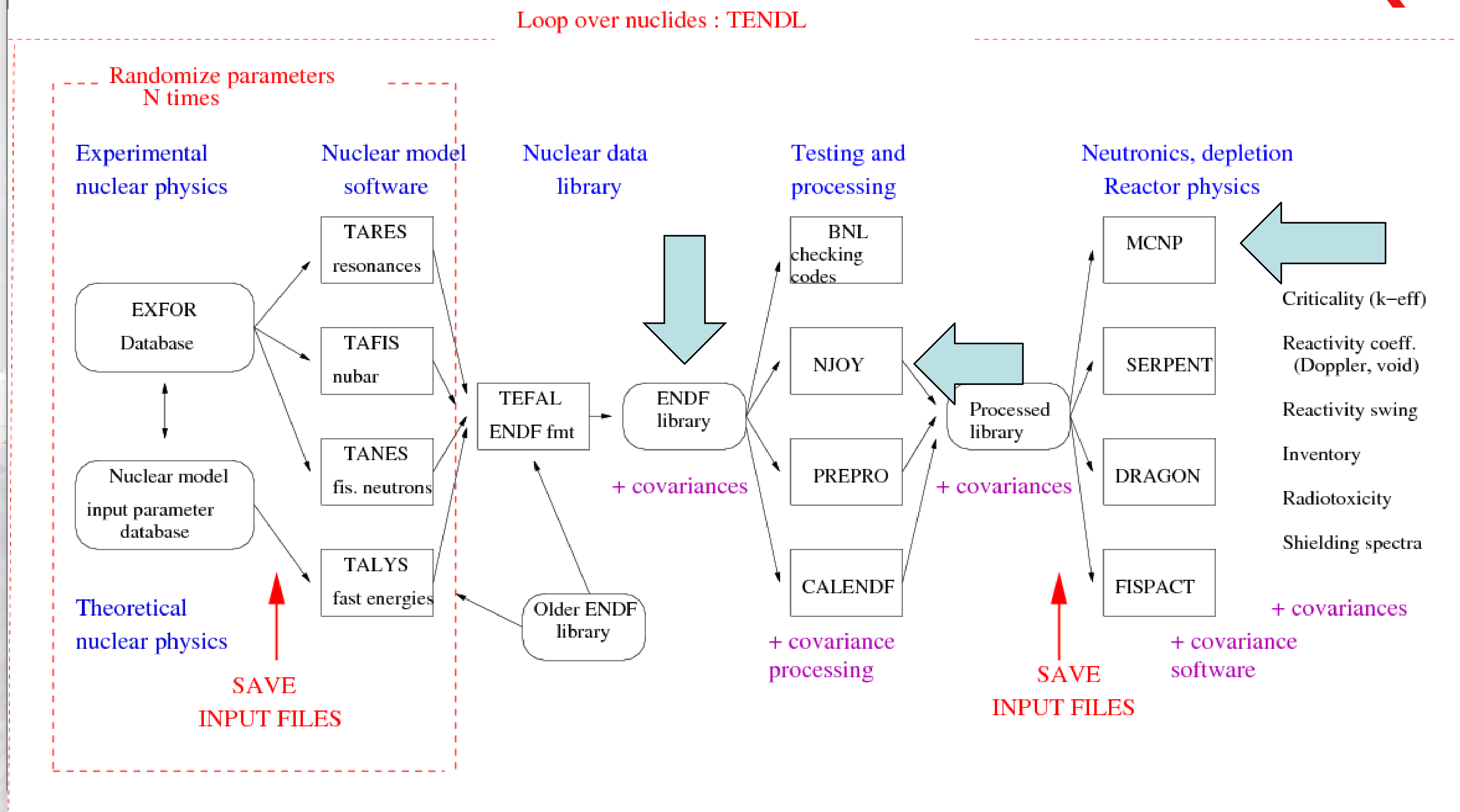
WPEC SG38 Meeting, OECD/NEA Data Bank

May 21-22 2013, Issy-les-Moulineaux

Contents

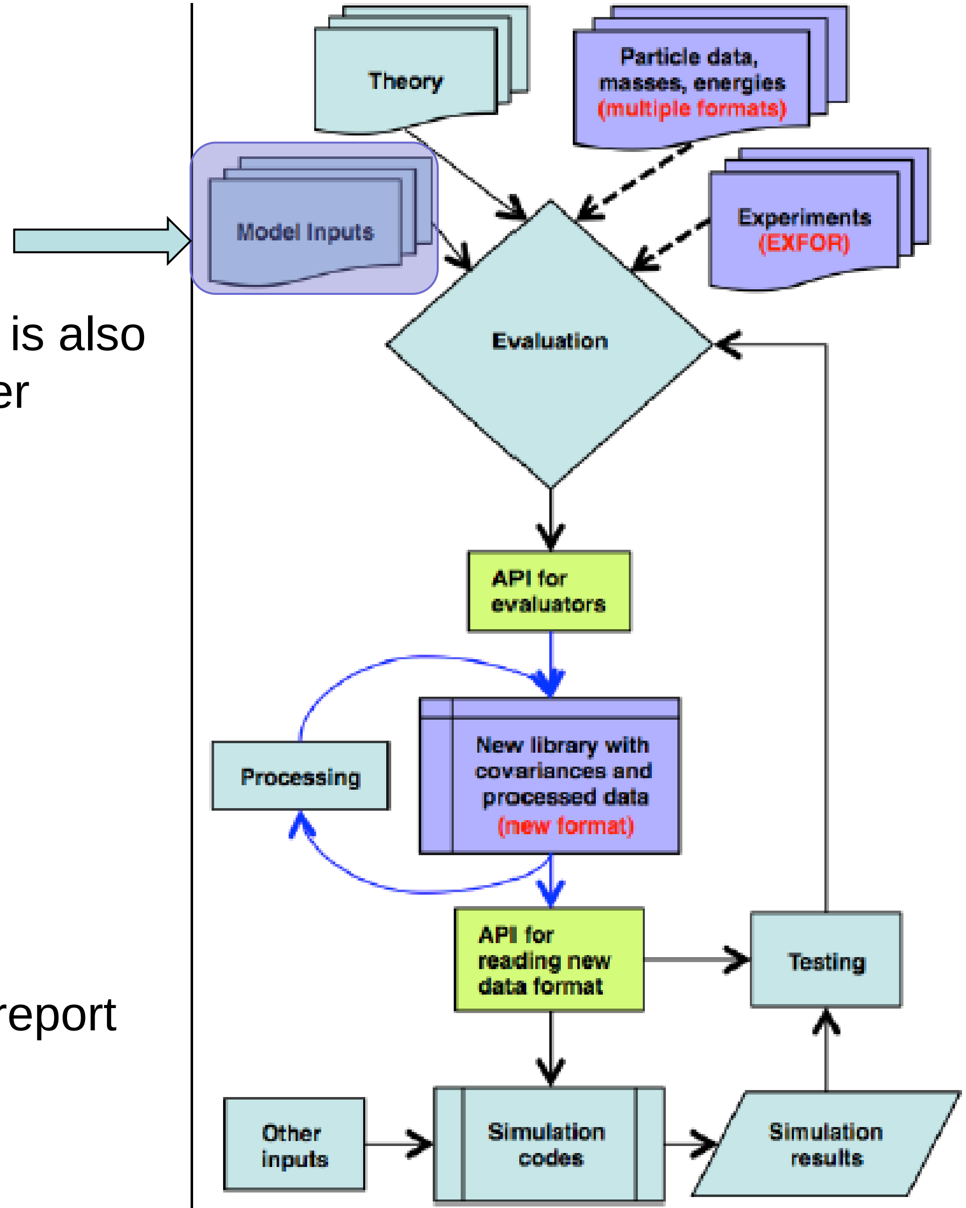
- Introduction
- Defaults
- Covariance data
- Other issues

Essential points in the nuclear data chain



Cost: $$ $$$ $$$$

In TENDL, this is also a data container



(b)

Fig 3b of SG38 report

Defaults

- There are many unnecessary differences among ENDF files for particle masses, nuclear masses (and thus Q-values) discrete level energies.
- Danger of current ENDF files: “if data is not given, the process doesn’t happen”. E.g. no gamma data: no energy balance, macroscopic quantity seems (falsely) insensitive to gamma data, etc.
- Should we make nuclear data evaluation more idiot-proof, and perform default operations on a GND library if certain info is not given? This requires extra intelligence for the processing step.

Defaults for nuclear properties

Possibility: Evaluator gives projectile + Z + A (+ isomer):

- Particle masses, nuclear masses, lifetime, discrete levels, etc. from **hardwired** link to particle database (the same for the whole world), more discussion in Task 5.
- Evaluator has the possibility to overrule these by giving the info explicitly in the evaluation.
- Next, for e.g. an (n,2n) table the evaluator needs to provide only the x-y values.

Defaults for reactions

Possible defaults:

- No angular distribution: isotropy or energy-dependent shape
- No isomeric branching: take branching from discrete level file
- No secondary spectrum: take some average physics-based shape
- No gamma data: ?

Of course, all of the above should no longer occur in modern files: nuclear model codes provide everything!

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. Also, handling of background cross sections for MT1,2,3,18,102,103,107 has given rise to problems in the past. Can we get rid of that?

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:

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

$$\sigma_{n,n'}^{disc} = \sum_{i=1}^{N} \sigma_{n,n'}^{i}.$$ 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

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

(3.26)

(Z_C, N_C). As an example, consider the $n + {}^{56}\text{Fe} \to {}^{54}\text{Mn} + x$ 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

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

i.e. in the more common notation,

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

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

Covariance data

- Uncertainties and their correlations are trivial for Total Monte Carlo: simply store N random libraries (each with possibly a weight). This will also work for GND.

Covariance matrices:

- Many important correlations are taken into account in the current ENDF-6 format, but
  - Most important omission: MF37 (covariance of thermal scattering data)
  - Complex, error-prone format
  - No MF42-45, the omission of MF36 can only be partly covered by MF35 and MF40
  - Are we sure that we include all important correlations?

Possible way out: make an indexing scheme that allows to correlate any data point to any other data point

Covariance data

Possible way out: make an indexing scheme that allows to correlate any data point to any other data point

xs 1 xs 1 Variance

xs 1 xs 2 Covariance

…..

xs 1 xs N Covariance

xs 2 xs 2 Variance

…..

- Use defaults, e.g. one may use variance only, implying 0 correlation
- Allow for cross-energy, cross-channel and cross-nuclide correlations by starting each list with nuclide-1, channel-1, nuclide-2, channel-2
- Requires new processing modules.

Other issues

- Will it be possible to combine partial reaction channels from different evaluations without penalty? E.g. take (n,2n) from France, (n,n') from Japan, etc.
- Define sum rules based on user-defined priority, e.g. flag that the total cross section deserves the highest degree of confidence, while the partial channels should "adapt".
- Include new information currently not available in ENDF-format:
  - nu instead of nubar, as a function of fission fragment and also with a probability table for the (integer) number of neutrons from fission.
  - A simple format for correlated emitted particles
  - Etc.