Nuclear reaction data in GND

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Essential points in the nuclear data chain

Loop over nuclides: TENDL

Randomize parameters N times

Experimental nuclear physics

- EXFOR Database
  - Nuclear model input parameter database
  - Nuclear model software
    - TARES resonances
    - TAFIS nubar
    - TANES fis. neutrons
    - TALYS fast energies

Nuclear model software

- TEFAL ENDF fmt
- Older ENDF library

Nuclear data library

- ENDF library + covariances
- BNL checking codes
- NJOY
- PREPRO
- CALENEFD
- Processed library + covariances

Testing and processing

- CALF
- SAVE INPUT FILES

Save input files

Neutronics, depletion

- Reactor physics
  - MCNP
  - SERPENT
  - DRAGON
  - FISPACT

- Criticality (k-eff)
- Reactivity coeff. (Doppler, void)
- Reactivity swing
- Inventory
- Radiotoxicity
- Shielding spectra + covariances

Theoretical nuclear physics

- SAVE INPUT FILES

Cost: $$ $$$ $$$$
In TENDL, this is also a data container
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

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

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

With a further subdivision:

\[ \sigma_{n,n'} = \sigma_{\text{disc}}^{n,n'} + \sigma_{\text{cont}}^{n,n'}, \]

MT4=MT51-90 + MT91

\[ \sigma_{\text{disc}}^{n,n'} = \sum_{i=1}^{N} \sigma_i^{n,n'}. \]

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:

\[
\sigma_{\text{non-el}} = \sum_{Z} \sum_{N} \sigma_{\text{prod}}(Z, N).
\]

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

where the Kronecker delta’s are defined by

\[
\delta_N = 1 \text{ if } i_n + i_d + 2i_t + i_h + 2i_{\alpha} = N_C - N
\]
\[
= 0 \text{ otherwise}
\]

\[
\delta_Z = 1 \text{ if } i_p + i_d + i_t + 2i_h + 2i_{\alpha} = Z_C - Z
\]
\[
= 0 \text{ otherwise},
\]

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

\[
\sigma_{n,xn} = \sum_{i_n=0}^{\infty} \sum_{i_p=0}^{\infty} \sum_{i_d=0}^{\infty} \sum_{i_t=0}^{\infty} \sum_{i_h=0}^{\infty} \sum_{i_\alpha=0}^{\infty} i_n \sigma_{\text{ex}}(i_n, i_p, i_d, i_t, i_h, i_\alpha),
\]

i.e. in the more common notation,

\[
\sigma_{n,xn} = \sigma_{n,n'} + 2\sigma_{n,2n} + \sigma_{n,np} + 2\sigma_{n,2np} + ....
\]

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.