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Data Lessons Learned from Cinder 202x's Modernization

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Introduction

- Cinder 202x is a nearly complete rewrite of Cinder 2008
- A key new feature is automatic library generation from ENDF-formatted data
- Issues in the libraries and formats have required many workarounds
- This presentation will go through some of these issues

Inconsistent Metastables and Levels

This is the main issue found during development.

- `MF=6` uses metastable index (`LIP`)
- `MF=9,10` and reactions like (n, n') use level number (`LFS`)
- `MF=8 MT=X` has file/reaction mapped to residual nucleus energy
- `MF=8 MT=457` has energy, metastable index, and level number
- All of these are regularly inconsistent with each other for one reason or another

The following examples all come from JEFF-4.0[1].

JEFF-4.0 was chosen as the primary test case due to its overall data quality and completeness.

[1] Joint Evaluated Fission and Fusion Project (2025). *JEFF-4.0 Evaluated Data: Neutron Data.* Data set. DOI: 10.82555/e9ajn-a3p20.

Inconsistent Metastables and Levels - Example 1

Data: JEFF-4.0, ^{127}In `MT=4` producing ^{127}In

Reaction:

Level #	E (keV)
0	0.0
1	408.9
9	1863.0

$(\mathrm{n}, \mathrm{n}')$

$\longrightarrow$

`MF=8 MT=457` ^{127}In:

Level #	E (keV)
0	0.0
1	460.0

Insufficient information in ENDF to determine the resulting physical state of Level #9.

We cannot assume it will decay to ground either.
According to ENSDF, $^{127\mathrm{m}2}$In decays 100% through β^-.

Inconsistent Metastables and Levels - Example 2

Data: JEFF-4.0, ^{127}In `MT=102` producing ^{128}In

Reaction:

Level #	E (keV)
0	0.0
3	340.0

(n, γ)

$\longrightarrow$

`MF=8 MT=457` ^{128}In:

Level #	E (keV)
0	0.0
1	247.9
2	320.0

Unclear if Level #3 is missing in `MF=8`, or if it should be #1 or #2.

Inconsistent Metastables and Levels - Example 3

Data: JEFF-4.0, ^{158}Tb `MT=17` producing ^{156}Tb

Reaction:

Level #	E (keV)
0	0.0
3	88.4
9	200.1

$(\mathrm{n}, 3\mathrm{n})$

$\longrightarrow$

`MF=8 MT=457` ^{156}Tb:

Level #	E (keV)
0	0.0
2	60.0
4	88.4

Here, ^{156}Tb has a level at $(49.63 + x)$ keV. The decay library and the reaction library have a different value of x, which changes the order.

This prevents using sort order to match levels.

Metastable and Level Summary

- 6073 (!) level-related issues processing JEFF-4.0
- Reaction and decay libraries are inconsistent
- Reaction data from different years / different libraries are inconsistent
  This inconsistency is amplified when integrating model-based libraries such as TENDL.
- Level indices have *no* physical meaning
  (They can only be used to locate the `MF=8` entry in the same file)
- Level energies can change as new data comes in
- Quantum numbers can be unknown or uncertain

What do I (ideally) want?

A single database of levels, shipped with the library, that **all** values are indexed unambiguously against. When it is updated, reaction libraries are updated alongside.

Beta Decay Data

Data provided in ENDF:

- Mode of decay (β^-, β^+, electron capture)
- Energy of the decay (assumed to be Q for beta decay)
- Transition type

Consider ^{210}Bi β^- decay

ENDF/B-VIII.0[2]:

- β^- decay
- $E = 1.1621$ MeV
- Type = 1
  (allowed or super-allowed)

ENSDF[3]:

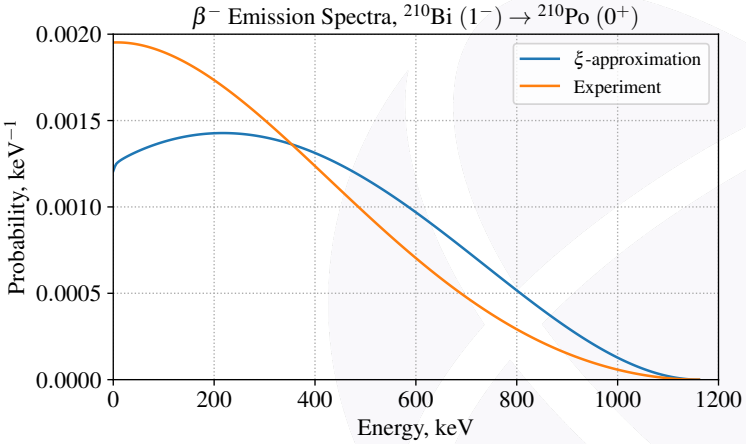
- β^- decay
- $E = 1.1612$ MeV
- $^{210}\text{Bi}\ (\text{J}^\pi = 1^-) \rightarrow {}^{210}\text{Po}\ (\text{J}^\pi = 0^+)$
  (1st forbidden non-unique)

[2] D.A. Brown et al. (2018). "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data". In: *Nuclear Data Sheets* 148, pp. 1–142. ISSN: 0090-3752. DOI: https://doi.org/10.1016/j.nds.2018.02.001

[3] M. Shamsuzzoha Basunia (2014). "Nuclear Data Sheets for A = 210". In: *Nuclear Data Sheets* 121, pp. 561–694. DOI: 10.1016/j.nds.2014.09.004

Beta Decay Data

ENDF/B-VIII.0 appears to use the ξ-approximation, where n-th forbidden non-unique is converted to $(n-1)$-th forbidden unique. This approximation can be poor[4,5]:



[4] X. Mougeot (2019). "Towards high-precision calculation of electron capture decays". In: *Applied Radiation and Isotopes* 154, p. 108884. ISSN: 0969-8043. DOI: https://doi.org/10.1016/j.apradiso.2019.108884.

[5] A. Grau Carles (2005). "Beta shapefactor determinations by the cutoff energy yield method". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 551.2, pp. 312–322. ISSN: 0168-9002. DOI: https://doi.org/10.1016/j.nima.2005.05.070.

Options to Improve Beta Decay

Put the whole emission spectra instead of just the endpoint energy/type:

- Loses β-ν correlation
- Allows directly adding experimental data to the file
- Covariance handling is simple

Add fitted shape function coefficients:

- Requires defining a beta decay model to fit them to
- Current approach used in Betashape

Just use ENSDF data:

- No covariance at all (yet?)
- Requires a library to indicate which ENSDF version to use
- Requires more interpretation decisions to be made

What do I (ideally) want?

Putting the whole spectrum is easiest and requires no format changes.

Decay Heating

Computing decay heating in neutron transport without double-counting is not easy due to delayed neutrons.

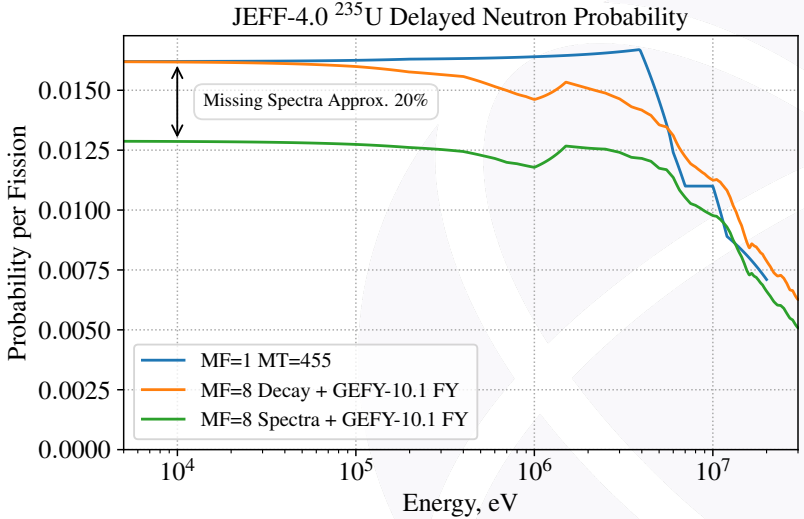
Transport needs to use `MF=1 MT=455` delayed neutrons:

- `MF=8` delayed neutron spectra is incomplete
- FPY data, excluding some libraries like GEFY, are not energy-dependent

Cannot subtract out delay neutron heat from total decay heat:

- Insufficient data to compute neutron energy from $(\beta^-, x\text{n})$ decays
- `NC=3` decay energy data does not provide delayed neutron energy separately
- No one uses `NC=17` format

Decay Heating



[6] Karl-Heinz Schmidt, Beatriz Jurado, and Kilian Kern (June 2025). *GEF-based Fission-Fragment Yield Library in ENDF Format*. Version 10.1. URL: https://www.khschmidts-nuclear-web.eu/GEFY.html

Decay Heating Summary

What do I (ideally) want?

The best option is energy-dependent FPY and enough neutron emission spectra to use for transport, but that requires far more data than we currently have.

Conversion to the `NC=17` decay heat format would reduce, but not eliminate, the need for approximations.

Ambiguous Elastic Scattering on Metastables in ENDF-102

`MT=2`:

- (z, z_0)
- “Elastic scattering cross section for incident particles”

`MT=50`

- (y, n_0)
- “leaving the residual nucleus in the ground state”
- “Not allowed for incident neutrons; use MT=2”

`MT=51`

- (z, n_1)
- “with residual in the 1st excited state”

For metastables, all libraries I’ve looked at keep `MT=2` as elastic and set `MT=51` as production of ground, adjusting `MT=52-90` correspondingly.

Miscellaneous Other Issues

General fission:

- I would like fragment-correlated data
- Covariance data would also be useful

Spontaneous fission:

- Most libraries other than JEFF are missing spontaneous fission decay heat on ^{252}Cf
- All libraries are missing prompt beta from spontaneous fission heat
  (GEF doesn't support computing them)

Other decay library issues:

- `MF`=38 decay covariance data probably should exist
- The format does not specify how to write "observationally stable"
  ENDF/B-VIII.1 approach: nuclide marked unstable with $T_{1/2} = 0$.

These are only the issues I've encountered so far.

Conclusions

While there is a lot of interest in expanding reaction channels, there is a long way to go before we have a great transmutation library.

We need:

- A consistent way to handle excited states
- Improved particle emission data (β spectra, more data)
- More complete delayed heat data
- More rigor when it comes to our formats
  A format is only useful if we all agree on what it contains!

Thank you for your time.