MT=900-999 proposal & Sum Rules

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Use of MT=900+ for primary gamma two-body channels, MT=102 being derived from these for backward compatibility

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Formats to specify primary capture gammas

- *Primary* gammas:
  - Each primary gamma can be its own two-body reaction (z,g) with the residual being left in the excitation state for that primary gamma
    - Primary gammas have energy that rises with incident projectile energy
  - The residual is then decayed using transition probabilities to produce the correlated *secondary* (discrete) gammas on an event-by-event bases
    - e.g, n + O16 -> primary gamma + (O17_e3 -> O17 + transition gammas)
    - Secondary gammas have energies that are fixed, independent of projectile energy.
- ENDF format:
  - The ENDF format currently does not allow for correlated primary/secondary gammas.
  - MT=102 format is complicated as it must describe both primary and secondary gammas.

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History: new specification for primary gammas

- History
  - MT=102 used traditionally in ENDF format for capture reactions.
  - Two-body reactions for particle products exist for n,p,d,t,h and a. But not for gammas (g) !
  - MT=102 different from other summing channels 4, 103, 104, 105, 106, 107 for n, p, d, t, h and a, as these are sums of two-body channels
- Proposal (more details later)
  - Use MT=900-998 for the first 99 discrete primary gammas needed
  - Use MT=999 as continuum channel for any further primaries
- I proposed this at MiniCSEWG meeting at LLNL in April 2023
  - Acceptance delayed so backward compatibility can be guaranteed.
  - Too late for ENDF/B-VIII.1
  - But still should be useful for experimentalists, evaluators and data users

Current ENDF/B-VIII.0 with primary γ channels

n-001_H_002.endf: 1 primary - only explicit two-body primary.
n-003_Li_006.endf: 2 primaries
n-003_Li_007.endf: 2
n-005_B_010.endf: 6
n-005_B_011.endf: 6
n-006_C_012.endf: 2
n-007_N_014.endf: 11 (rather old)
n-014_Si_029.endf: 23
n-014_Si_030.endf: 8
n-017_Cl_035.endf: 69
n-017_Cl_037.endf: 22

GRIN ENDF/B-VIII.1 candidates:
C13: 4 primaries
O16: 2
F19: 29
Si28: 13

All of these are candidates for conversion to MT=900-999.
Evaluations in red can be converted unambiguously
More will be added from GRIN project.
Much better to use in R-matrix fits rather than Reich-Moore sums

Proposal: MT=900-999 for primary capture gammas

- Use new MT numbers 900-999 to describe all primary gammas:
  - MT=102 becomes a summed-cross-section channel like 4, 103-107.
  - Can be reconstructed from 900-999 if present
- New MT Definitions for ENDF6 manual Appendix B:
  - MT=900: Production of a primary-γ particle leaving the residual nucleus in the ground state
  - MT=901-998 Production of a primary-γ particle, with residual in 1^{st} to 98^{th} excited state
  - MT=999: Production of a primary-γ particle in the continuum not included in the above discrete representation.
  - MT=102: Radiative capture: production of one or more gammas (photons) plus a residual. Redundant: sum of MT=900-999, if they are present.
- For backward compatibility:
  - In a PREPRO-like step before processing with older codes, make another file version by
    Reconstructing MT=102 with distributions and delete MT 900s.
    (See code MT900s2MT102.py later).

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Consequences for Gamma Data

If using new MT numbers, then

- The secondary decay gammas must be specified either:
  1. **by transition probability arrays with MF=12 data (preferred),** or
  2. separately for each of discrete MT channels (900-998), or
  3. in a continuum distribution for MT channels 999.
- All the primary gammas MT=900-998 are 2-body channels.
  - Can use MT=999 :
    - for channels not covered by MT 900 to 998 [MT 91 for MT 50 to 90 for (n,n')]
    - if primary channels not known for a gamma
    - If data only gives continuum distribution of gamma production
- MT=102 can now be derived from the new channels if present
  - If 900-999 not present, just put inclusive data & distributions in MT=102 as now.

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Code assistance

We give a FUDGE translation code gnds-capture.py

- that converts MT=102 to MT=900-998, 999 primary and secondary data
- Works well so far for ENDF/B-VIII.0 and VIII.1 versions of neutrons on Li6, Li7, B10, C12.

And a FUDGE code MT900s2MT102.py to reconstruct MT=102 from 900-999 & delete these, for backward compatibility.

- Like a PREPRO module making a intermediate version

Published ENDF evaluations should <u>not</u> have <u>distributions</u> with <u>both</u> MT=102 and 900-999, to avoid any double counting.

- That is, define like MT=103 – 107 for charged particles

Conclusion

- Proposal for explicit description of primary capture gammas from two-body reaction channels
  - No change needed for GNDS 2.0 (only for ENDF6 format)
  - Need relativistic kinematics or at least distinct treatment of photons.
- Resonance parameters should be specified for each channel: for each MT 900 to 998 as needed.
  - No longer for Reich-Moore ‘absorption’ to give summed capture gammas
- Codes (processing and transport) need to be updated to handle these MTs.
  - Demonstration files available for n + H2, Li6, Li7, B10, C12, C13, O16
- If gamma-then-particle emission, particle resonance width has to be assumed zero (discrete) if MT=900-998. MT=999 is ok.
  - For example the He5 resonance in d + t → gamma + (He5 → He4 + n)

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Where we left off

David Alan Brown @dbrown · 11 months ago Owner

@beck6 @thompson97, After the discussion at CSEWG on 15 Nov. 2023, it is clear that a careful description of the sum rules for the MT=9XX is needed, especially when MT=999 is used. In particular, for MT=900-998, only one primary gamma is present and the primary gamma's multiplicity is 1 for these MT's. MT=999 will include all primary gammas that could not be accommodated with their own channel. As a result, care must be taken with the primary gamma multiplicity. The total primary gamma multiplicity for MT=999 must be <=1 (since some primaries might be missing). This may confuse users since the average user may expect the primary gamma multiplicities to be 1 for MT=999 as well. This I believe was the origin of the discussion at CSEWG.

The total thermal capture cross section should of course match the sum of the partial MT=9XX cross sections. However, the sum of multiplicities is a little more complex as well as the averaged MT=102 outgoing particle distribution. These other sum rules (for multiplicities and distributions) should also be spelled out in the ENDF manual if they aren't already.

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Where we left off

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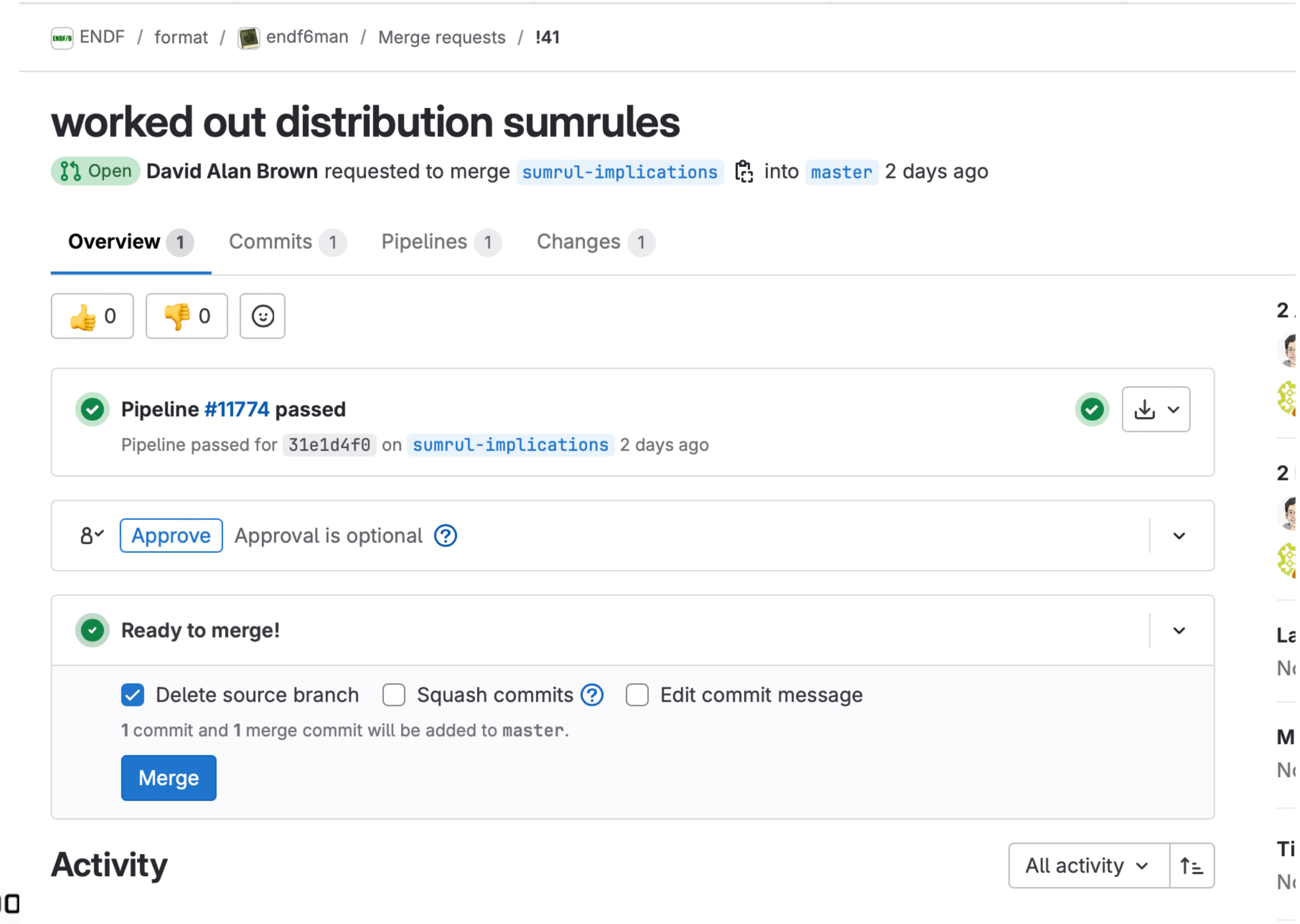
Takeaways:
- **Need to describe the sumrule**
- **Need to remind user about multiplicity trickiness**

Note: these issues are not specific to the MT=9XX format proposal and are relevant for all ENDF sumrules

distribution. These other sum rules (for multiplicities and distributions) should also be spelled out in the ENDF manual if they aren't already.

Merge Request 41



I volunteered Caleb & Doro to review

It is not a format proposal, but simply explains how ENDF sumrules impact outgoing multiplicities & distributions

These sum rules have implications for outgoing particle multiplicities and distributions users who wish to "sum-up" exclusive reactions to make the inclusive reaction defined by the sum rule. For the sake of simplicity, assume we consider only neutron incident particles. For a sum rule defined in Table 14 or in Chapter 23, we may write

$$\sigma_0(E) = \sum_{MT} \sigma_{MT}(E) \tag{1}$$

for the cross sections and

$$\frac{dn_{i,0}}{dE'd\mu'} = \sum_{MT} f_{MT}(E) \frac{dn_{i,MT}}{dE'd\mu'} \tag{2}$$

for the number of particles of interest i scattering into scattering cosine μ' with energy E' (assuming azimuthal symmetry). Here $f_{MT}(E)$ is the fraction of the reactions in the sum proceeding through a given MT and is clearly $f_{MT}(E) = \sigma_{MT}(E)/\sigma_0(E)$. We may write each of the $dn_i/dE'd\mu'$'s' as

$$\frac{dn_i}{dE'd\mu'} = y_i(E) f_i(\mu', E, E') \tag{3}$$

where the particle yield (or multiplicity) for particle i is $y_i(E)$ and the outgoing energy angle distribution is $f_i(\mu', E, E')$. Inserting Eq. 3 into 2 and integrating over all outgoing energies and angles, we obtain the sum rule for particle yields/multiplicities:

$$y_{i,0}(E) = \sum_{MT} \frac{\sigma_{MT}}{\sigma_0} y_{i,MT}(E). \tag{4}$$

Inserting Eq. 3 into 2 and dividing through by the total yield, we find

$$f_{i,0}(\mu', E, E') = \sum_{MT} \frac{\sigma_{MT}}{\sigma_0} \frac{y_{i,MT}(E)}{y_{i,0}(E)} f_{i,MT}(\mu', E, E'). \tag{5}$$

In many cases the yields are straightforward, however the gamma yields may be non-trivial in the case that the yields must be computed by doing a "mini-gamma cascade" using the branching ratio matrix in MF=12.