Translating ENDF/B-VIII into GND

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FUDGE tool rePrint.py translates ENDF-GNDS and back

- Translation code is strict (perhaps even pedantic!) about following ENDF-6 format manual: helps uncover data quality issues

  - Identified and fixed many problems especially during the last hackathon (August 2017). Examples:

    - internal inconsistencies (common problems included inconsistent isomer indices, discrepancies between files 2 and 32),

    - missing or incorrect MAT numbers,

    - incorrect target ZA numbers, etc.

- Re-translating back to ENDF-6 helps check how well GNDS preserves the original evaluation.

Translating ENDF-VIII-b5+ (rev 1388) to GNDS

- Sub-libraries currently being translated:

    - Incident n, p, d, t, He3, alpha, gamma and electron data

    - standards

    - photo-atomic

    - atomic relaxation   (writing back to ENDF-6 not yet implemented)

    - thermal_scattering

    - decay   (writing back to ENDF-6 not yet implemented)

- Not yet translated

    - Neutron-induced and spontaneous fission yields

        - nfy and sfy translation is simple, but need to finalize how to store them in GNDS

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Status of neutron sub-library:

- 557 / 557 files translated ✅

- 653969 / 15,982,667 lines (about 4%) have at least one difference after translating back to ENDF-6

  - Most differences are trivial, often the result of not running STANEF. Example from Kr79:

  - Another common cause for differences: duplicate points are dropped by FUDGE during translation, can cause many lines to differ

Other common reasons for differences after rePrint.py

- When duplicate (x,y) points appear in TAB1, the translator drops the second point where possible. Can result in many diffs that are not important!

- ENDF stores mass (AWR) many times, GND picks the most frequently-used value and only stores that.

- Small (few eV) domain mismatch between cross section and multiplicity/distribution
  - Re-written file uses MF3 domain everywhere
  - Larger mismatch is treated as an error

- INTG records (compact correlation matrix in MF32) are inconsistent: some files store 0 correlations explicitly, other files use blank spaces instead

Status of neutron sub-library (continued):

- Important differences between original and re-translated files include:

  - MOD1 numbers in the MF1 MT451 directory: currently not preserved during translation

  - Sub-actinide fission cross sections (MF10 / MT18).

    - Planned resolution: store these in the 'incompleteReactions' section, need to update FUDGE to handle that

  - Some rarely-used covariance formats (LB=8 and LB=9) are currently skipped during translation.

    - Planned resolution: make special interpolation rules. When grouping, size of covariance must vary either inversely (LB=8) or directly (LB=9) with size of the group

  - P(nu) (MF6 / MT18)

    - Two options for handling this:

      - store P(nu) as a pdf similar to P(E' | E), or

      - break fission into multiple reactions, one for each prompt neutron multiplicity.

Status of photo-nuclear sub-library:

- 163 / 163 files translated ✅

  - 46458 / 2,830,869 lines differ (1.6%)

- Most differences appear to be duplicate points removed by FUDGE. Example from Pu241:

Status of charged-particle sub-libraries:

- Incident protons: 49 / 49 files translated ✅

  - 637 / 677839 lines differ (0.1%)

- Incident deuterons: 5 / 5 ✅

  - 50 / 5164 lines differ (1%)

- Incident tritons: 5 / 5 ✅

  - 38 / 9179 lines differ (0.4%)

- Incident helions: 3 / 3 ✅

  - 12 / 10161 lines differ (0.1%)

- Incident alphas: 1 / 1 ✅

  - 0 / 101 lines differ (0%)

Status of other sub-libraries:

- Incident electrons: 100 / 100 files translated ✅

    - ~272,000 / 303,923 lines differ (90%)

        - Nearly all differences due to not running STANEF

- Photo-atomic: 100 / 100 files translated ✅

    - ~210,000 / 286,928 lines differ (90%)

        - STANEF not run

- Standards: 8 / 8 ✅

    - 52 / 11,053 lines differ (0.5%)

- Thermal scattering: 35 / 35 ✅

    - 264 / 3,279,002 lines differ (0.0008%)

- Atomic relaxation: 100 / 100 ✅

    - Translation back to ENDF-6 not yet supported

- Decay: 3821 / 3821 ✅

    - Translation back to ENDF-6 not yet supported

Some files still have problem data

- The translator complains about some data issues, but can "recover" from them with the proper flag

- Missing evaluation date in MT451
  - GND requires evaluation date. n + Pu239 fails without '--skipBadDate'

- Unnormalizable continuum gammas in MF6
  - GND stores gammas like MF12,15 does, thus MF6 gamma data must be converted to MF12,15 like data
  - At some incident energies, the continuum gamma spectrum integrates to 0 and cannot be normalized as needed for MF12 like data.
  - Translator crashes unless option --continuumSpectraFix is set
  - Affected isotopes:
    — n + Cl35, Ca42-46, As73, Pb204-207
    — p + Be9

- Still many problems with energy balance!

More detail on continuum gamma problem

- In MF6, continuum, primary and discrete gammas are all listed together for each incident energy, along with total multiplicity for all gammas

  - Each primary & discrete has a probability, continuum has a spectrum

  - Some continuum spectra are all 0s

    — probability distribution at these incident energies cannot be normalized

  - Probability can go from non-zero to zero and back multiple times:

p + Be9 MT=5 continuum gamma probability
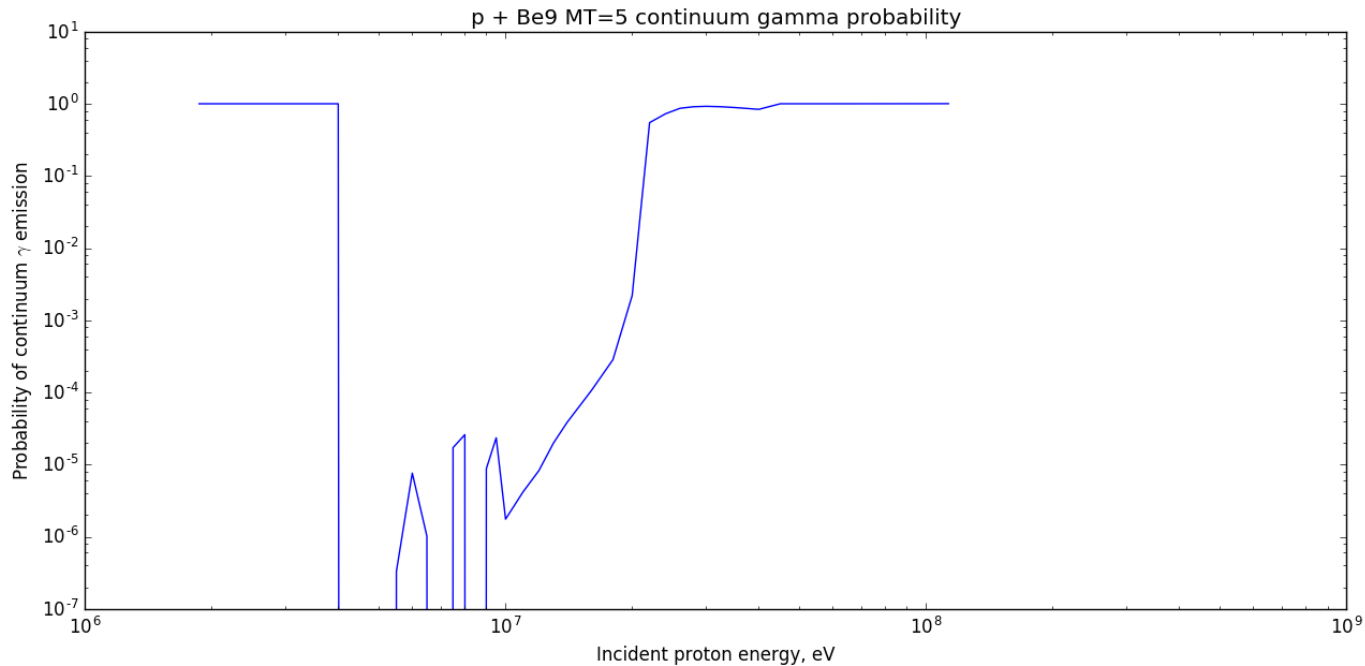
Patching continuum gamma problems

- When option --continuumSpectraFix is supplied, the translator replaces 0-norm continuum spectra with a delta function, weighted by total gamma multiplicity

p + Be9 MT=5 continuum gamma multiplicity (after fixes)

After the fix, multiplicity drops here to 10^{-23} rather than 0
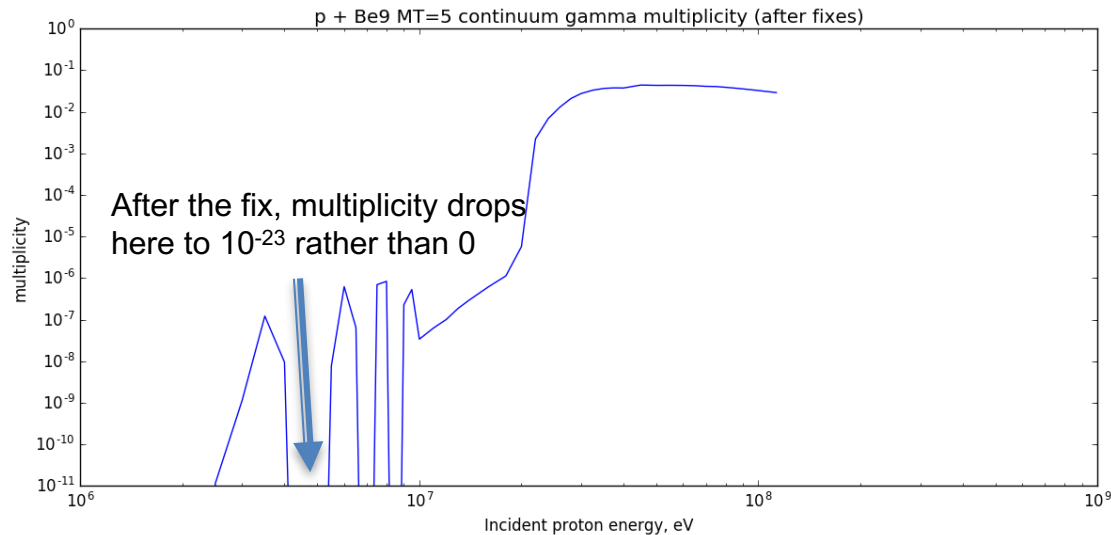
- This is just a temporary work-around. Gamma spectra need more attention!