Issues with ENDF-VIII candidate evaluations

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Testing rev. 807 from the NNDCforge repository (Thursday April 7)

- What evaluations cause trouble for Fudge translation?
- Use Fudge physics testing with error sensitivity turned down, to detect ‘worst cases’ of unnormalized distributions, energy imbalance, etc.
- A few other long-standing issues

Step 1: test Fudge-GND translation

- Translate neutron, gamma, proton, deuteron, triton, helium3, standards, photoat, atomic_relax and electron sub-libraries

- neutrons: 5 failures
  - O16, W182-186
- protons: 2 failures
  - H2 and Pb207
- Other sublibraries are fine

n-008_O_016

- Two discrepancies in new CIELO evaluation:
  - For MT=103, MF=13 and 14 disagree about what level the 277.4 keV gamma is emitted from. ENSDF supports MF=13, recommend we adopt that for MF=14 as well.
  - For MT=107, the MF=3 cross section starts at 2.355 MeV but the MF=13 gamma production cross sections all start at 2.3545 MeV. Recommend making MF=13 thresholds equal to MF=3
- Minor format issues: MF 13/14 should use LP=1 for gammas whose parent is known
  - This is an issue in many ENDF files.
- See tracker item #980, including suggested patch file

Documentation in ENDF manual on LP in sections 12 and 13.

ES_k energy of the level from which the photon originates. If the level is unknown or if a continuous photon spectrum is produced, then $ES_k \equiv 0.0$ should be used.

EG_k photon energy for LP=0 or 1 or Binding Energy for LP=2. For a continuous photon energy distribution, $EG_k \equiv 0.0$ should be used.

LP indicator of whether or not the particular photon is a primary:

LP=0 origin of photons is not designated or not known, and the photon energy is EG_k;

LP=1 for non-primary photons where the photon energy is again simply EG_k;

LP=2 for primary photons where the photon energy EG'_k is given by

$$EG'_k = EG_k + \frac{AWR}{AWR + 1} E_n.$$

[MAT, 12, MT/ Eg_k, ES_k, LP, LF, NR, NP/ E_{int} / $y_k(E)$] TAB1

1.105000+7	1.105000+7	0	2	1	76	72513	4
1.105000+7	1.105000+7	1	2	1	76	72513	4

Example from Li6 with LP set to 1 when it should be 0.

4.776000+5 0.000000+0 1 2 1 2 32512102

Bad level index in MF=12 for neutrons/n-050_Sn_113

- ENDF documentation 12.2.2 states:

NS Number of levels below the present one, including the ground state. (The present level is also uniquely defined by the MT number and by its energy level).

5.011300+4 1.119350+2 2 1 2 0502812 51

- All MTs for MF=12 region have this issue:
  - 51-82, 601-639 and 801-817
- Yes there are others: e.g., neutrons/n-054_Xe_131.

n-074_W_182, 183, 184, 186: MF=8 and 10 are used to store experimental fission cross section

- Discussion with A. Trkov:
  - "Measurements of the fission cross section of W-isotopes exist. The question is how to include them in the ENDF files... I included fission into MF10... there is a small inconsistency if ENDF-6 rules are followed very strictly: ZAP (i.e. ZA of the residual) is undefined for fission. I set it to zero. My logic was the gamma-photon as a residual is physically meaningless, therefore ZAP=0 is simply a flag that the residual is undefined. Strictly speaking, this convention should be added to the ENDF-6 manual"
  - Should we adopt this convention (and document in the manual)?

p-001_H_002

- A primary gamma is listed in MF=6 MT=102, but the primary energy does not increase with incident energy

```
 0.000000+0 0.000000+0          1          2          1          2 128 6102
          2          2                                                128 6102
 0.000000+0 1.000000+5          1          0          2          1 128 6102
-5.493539+6 1.000000+0                                              128 6102
 0.000000+0 1.500000+8          1          0          2          1 128 6102
-5.493539+6 1.000000+0                                              128 6102
```

Last value should be -1.053728+8 to account for incident energy?

- Could be our misunderstanding of format manual (we only have a few examples where primary gammas are listed in MF=6)

ND Number of discrete energies given.

The first ND≥0 entries in the list of NEP energies are discrete, and the remaining (NEP-ND)≥ 0 entries are to be used with LEP to describe a continuous distribution. Discrete primary photons should be flagged with negative energies.

- NNDCforge tracker #979 has our proposed fix

p-082_Pb_207

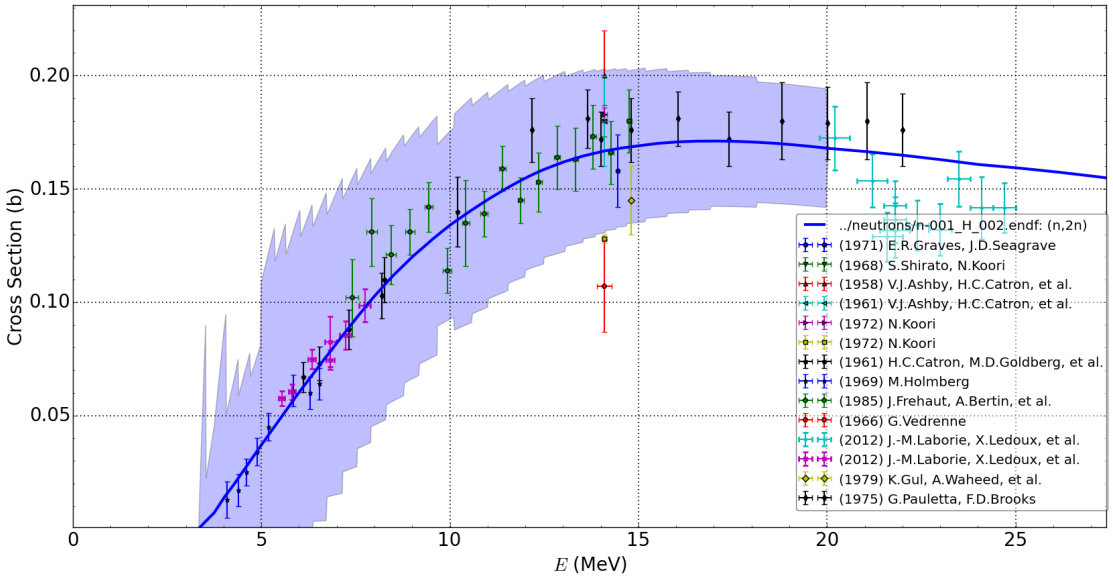
- Outgoing products in MF=6 MT=5 include Bi194, outgoing energy spectrum for that product has several problems
  - For incident proton energy = 150 MeV, outgoing energies are not in ascending order
  - At the same incident energy, outgoing spectrum is FAR from normalized (integral = $2.35*10^6$)!
- NNDCforge tracker #669 has tentative, partial fix

Missing covariances?

- Some important covariance matrices disappeared in CIELO updates!
  - Latest Fe56 and Pu239 evaluations contain no covariance data
  - MF=33 MT=1,2,4,16,17 all disappeared from new U238 evaluation

Questionable covariances

- In n-001_H_002, the covariance matrix for (n,2n) is computed from other matrices: MT1 – MT2 – MT102. Experimental data suggests smaller uncertainty would be appropriate:



Sample warnings from Fudge physics checking (neutron sub-library)

- Negative elastic cross sections in resonance region for Ar40, Gd152 and Dy160. In each case, ‘background’ cross section in MF=3 is negative, overwhelms resonance contribution

  - Ar40: dips negative near 978.3 keV
  - Gd152: dips negative 14 times between 33 eV and 2.2 keV
  - Dy160: 7 times between 330 eV and 1.85 keV

32 evaluations need denser energy grids in URR

- ENDF manual suggests giving 3-10 points per decade, points shouldn't differ by more than factor of 3
  - When energy grids are sparser than that, reconstruction codes give different results (looked at NJOY, AMPX, PREPRO and Fudge)
  - Why not thicken URR grid (using evaluator's recommended interpolation)?
- Energy grid differences by factor of 3 or more:
  - As74, Kr82, Nb94, Nb95, Mo99, Sn123, Sb125, Te127m, Te129m, I131, Cs136, Ba140, Ce139, Nd147, Pm148, Pm149, Pm151, Sm153, Eu152-156, Gd153, Gd154, Gd157, Tb160, Dy156, Dy158, Ho166m, Er167

Probability distributions dropping below -0.01:

- Y90: in MT=53, $energy_{in}$ = 15,17,18 MeV
- Te132: MT=52, $energy_{in}$ 18 MeV
- Xe136: MTs 51, 54, 56, 57
- Ho165: MTs 2 and 51
- Hf177 and Hf179: MT=2
- Au197: MTs 2 and 53 (worst case: P = -0.223 for MT53)
- U239: MT = 2, MTs 62-81
- U240: MTs 51 and 52
- U241: MT = 2, MTs 51-72

Other random questions (mainly about neutron sub-library) from me + other nuclear data users at LLNL:

- Evaluations for Ne isotopes?
- P31 lumps all inelastic into MT=91, can we break that up into discrete states?
- Expanded covariance estimates
  - N14?
  - Charged-particle sub-libraries?