

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

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:

36079.0000	78.2421200	0	0	0	03628	3	2	3.607900+4	7.824212+1	0	0	0	03628	3	2	
0.0	0.0	0	0	1	573628	3	2	0.000000+0	0.000000+0	0	0	1	573628	3	2	
57	2	0	0	0	03628	3	2	57	2	0	0	0	03628	3	2	
1.00000E-5	0.0	.025300000	0.0	100.000000	0.0	3628	3	2	1.000000-5	0.000000+0	2.530000-2	0.000000+0	1.000000+2	0.000000+03628	3	2
100.000000	52.0808100	200.000000	49.3543100	500.000000	35.70030003628	3	2	1.000000+2	5.208081+1	2.000000+2	4.935431+1	5.000000+2	3.570030+13628	3	2	
700.000000	31.6789000	1000.000000	27.9247000	2000.000000	21.94510003628	3	2	7.000000+2	3.167890+1	1.000000+3	2.792470+1	2.000000+3	2.194510+13628	3	2	
5000.000000	16.2542000	7000.000000	14.6939000	10000.000000	13.30650003628	3	2	5.000000+3	1.625420+1	7.000000+3	1.469390+1	1.000000+4	1.330650+13628	3	2	
20000.00000	11.2684000	50000.000000	9.57599100	70000.000000	9.159290003628	3	2	2.000000+4	1.126840+1	5.000000+4	9.575991+0	7.000000+4	9.159290+03628	3	2	
100000.0000	8.79341900	200000.0000	7.86655100	300000.000000	6.857660003628	3	2	1.000000+5	8.793419+0	2.000000+5	7.866551+0	3.000000+5	6.857660+03628	3	2	
400000.0000	6.00801000	500000.000000	5.26864000	700000.000000	4.224850003628	3	2	4.000000+5	6.008010+0	5.000000+5	5.268640+0	7.000000+5	4.224850+03628	3	2	
850000.0000	3.63748000	1000000.000000	3.20748000	1300000.000000	2.633530003628	3	2	8.500000+5	3.637480+0	1.000000+6	3.207480+0	1.300000+6	2.633530+03628	3	2	
1500000.0000	2.37814000	1800000.000000	2.08964000	2000000.000000	1.939980003628	3	2	1.500000+6	2.378140+0	1.800000+6	2.089640+0	2.000000+6	1.939980+03628	3	2	
2250000.0000	1.80180000	2500000.000000	1.70878000	2750000.000000	1.647130003628	3	2	2.250000+6	1.801800+0	2.500000+6	1.708780+0	2.750000+6	1.647130+03628	3	2	
3000000.0000	1.60169000	3200000.000000	1.59124000	3400000.000000	1.590400003628	3	2	3.000000+6	1.601690+0	3.200000+6	1.591240+0	3.400000+6	1.590400+03628	3	2	
3600000.0000	1.59717000	3800000.000000	1.60986000	4000000.000000	1.627070003628	3	2	3.600000+6	1.597170+0	3.800000+6	1.609860+0	4.000000+6	1.627070+03628	3	2	
4200000.0000	1.64761000	4400000.000000	1.67050000	4600000.000000	1.694960003628	3	2	4.200000+6	1.647610+0	4.400000+6	1.670500+0	4.600000+6	1.694960+03628	3	2	
4800000.0000	1.72033000	5000000.000000	1.74608000	5500000.000000	1.809550003628	3	2	4.800000+6	1.720330+0	5.000000+6	1.746080+0	5.500000+6	1.809550+03628	3	2	
6000000.0000	1.86824000	7000000.000000	1.96137000	8000000.000000	2.015870003628	3	2	6.000000+6	1.868240+0	7.000000+6	1.961370+0	8.000000+6	2.015870+03628	3	2	
9000000.0000	2.03251000	10000000.000000	2.01679000	11000000.000000	1.975610003628	3	2	9.000000+6	2.032510+0	1.000000+7	2.016790+0	1.100000+7	1.975610+03628	3	2	
12000000.0000	1.91598000	13000000.000000	1.84444000	14000000.000000	1.766490003628	3	2	1.200000+7	1.915980+0	1.300000+7	1.844440+0	1.400000+7	1.766490+03628	3	2	
15000000.0000	1.68634000	16000000.000000	1.60716000	17000000.000000	1.531420003628	3	2	1.500000+7	1.686340+0	1.600000+7	1.607160+0	1.700000+7	1.531420+03628	3	2	
18000000.0000	1.46114000	19000000.000000	1.39783000	20000000.000000	1.342540003628	3	2	1.800000+7	1.461140+0	1.900000+7	1.397830+0	2.000000+7	1.342540+03628	3	2	
0.000000+0	0.000000+0	0	0	0	03628	3	0	0.000000+0	0.000000+0	0	0	0	03628	3	0	

- 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:

9.424100+4	2.389860+2	0	0	1	09443	5	16	9.424100+4	2.389860+2	0	0	1	09443	5	16
0.000000+0	0.000000+0	0	1	1	29443	5	16	0.000000+0	0.000000+0	0	1	1	29443	5	16
	2	2	0	0	09443	5	16		2	2	0	0	09443	5	16
1.177400+7	1.000000+0	2.000000+7	1.000000+0		9443	5	16	1.177400+7	1.000000+0	2.000000+7	1.000000+0		9443	5	16
0.000000+0	0.000000+0	0	0	1	99443	5	16	0.000000+0	0.000000+0	0	0	1	99443	5	16
	9	2	0	0	09443	5	16		9	2	0	0	09443	5	16
0.000000+0	1.177400+7	0	0	1	39443	5	16	0.000000+0	1.177400+7	0	0	1	39443	5	16
	3	2	0	0	09443	5	16		3	2	0	0	09443	5	16
0.000000+0	0.000000+0	2.000000-5	5.000000+4	4.000000-5	0.000000+09443	5	16	0.000000+0	0.000000+0	2.000000-5	5.000000+4	4.000000-5	0.000000+09443	5	16
0.000000+0	1.200000+7	0	0	1	929443	5	16	0.000000+0	1.200000+7	0	0	1	919443	5	16
	92	2	0	0	09443	5	16		91	2	0	0	09443	5	16
1.000000-5	0.000000+0	1.000000-5	0.000000+0	2.832120+2	1.478777-89443	5	16	1.000000-5	0.000000+0	2.832120+2	1.478777-8	5.664241+2	2.955908-89443	5	16
5.664241+2	2.955908-8	8.496361+2	4.431394-8	1.132848+3	5.905238-89443	5	16	8.496361+2	4.431394-8	1.132848+3	5.905238-8	1.699272+3	8.848001-89443	5	16
1.699272+3	8.848001-8	2.265696+3	1.178421-7	3.398544+3	1.763701-79443	5	16	2.265696+3	1.178421-7	3.398544+3	1.763701-7	4.531393+3	2.346373-79443	5	16
4.531393+3	2.346373-7	5.664241+3	2.926446-7	6.797089+3	3.503929-79443	5	16	5.664241+3	2.926446-7	6.797089+3	3.503929-7	7.929937+3	4.078831-79443	5	16
7.929937+3	4.078831-7	9.062785+3	4.651162-7	1.132848+4	5.788143-79443	5	16	9.062785+3	4.651162-7	1.132848+4	5.788143-7	1.359418+4	6.914945-79443	5	16
1.359418+4	6.914945-7	1.585987+4	8.031639-7	1.812557+4	9.138295-79443	5	16	1.585987+4	8.031639-7	1.812557+4	9.138295-7	2.039127+4	1.023498-69443	5	16
2.039127+4	1.023498-6	2.265696+4	1.132178-6	2.492266+4	1.239874-69443	5	16	2.265696+4	1.132178-6	2.492266+4	1.239874-6	2.718836+4	1.346594-69443	5	16

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:

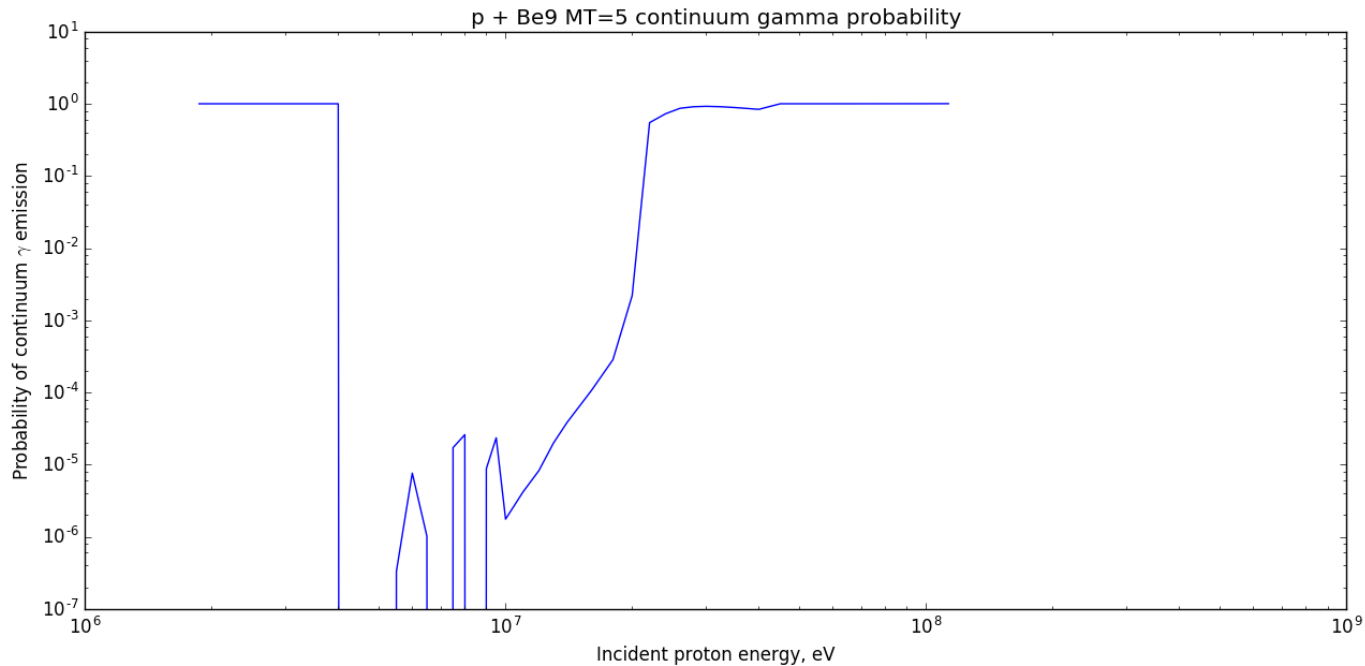
- Incident electrons: 100 / 100 files translated 
 - ~272,000 / 303,923 lines differ (90%)
 - Nearly all differences due to not running STANEF
- Photo-atomic: 100 / 100 files translated 
 - ~210,000 / 286,928 lines differ (90%)
 - STANEF not run
- Standards: 8 / 8 
 - 52 / 11,053 lines differ (0.5%)
- 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!

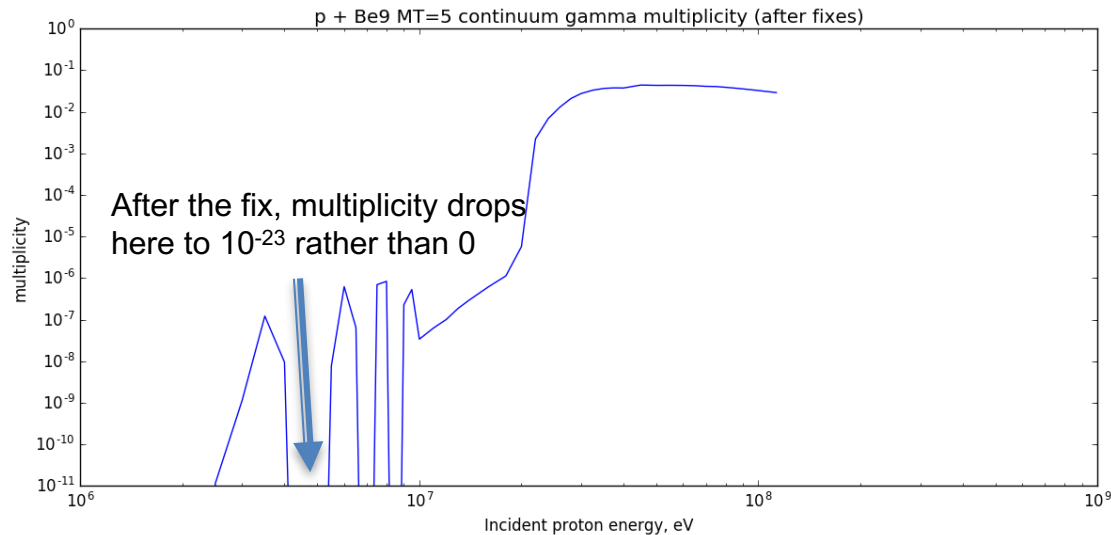
More detail on continuum gamma problem

- 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:



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



- This is just a temporary work-around. Gamma spectra need more attention!