Enabling gamma cascades in GNDS

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+ GRIN collaboration

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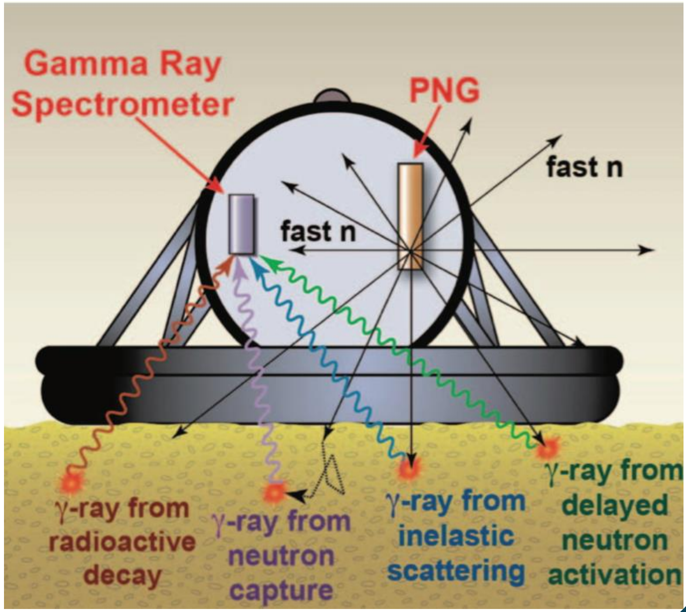
GRIN- Gamma Rays Induced by Neutrons

✓ A project to help improving gamma-ray data libraries and enable inline gamma cascades in transport codes

Target users:

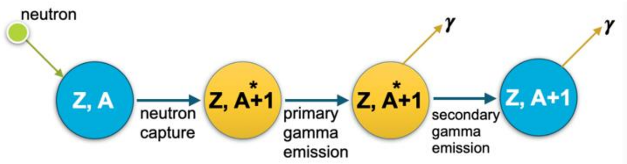
- **"Traditional"** users call for a precise particle-γ spectrum to perform material identification.
- **"Event-by-event"** users need the **correlations between scattered neutrons, gammas emitted from nuclear de-excitations**. Current evaluated data in ENDF libraries are not sufficient and must be extended.

- **Capture, Inelastic and Decay Gammas**
  Nuclear fingerprints
- **Subject to**
  - Thorough experimental knowledge;
  - Precise models and evaluations;
  - Incorporation of data into evaluated files;

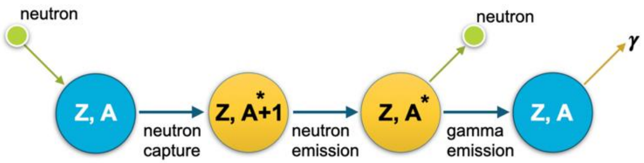


Neutron Induced Reactions and Gamma-Ray cascades

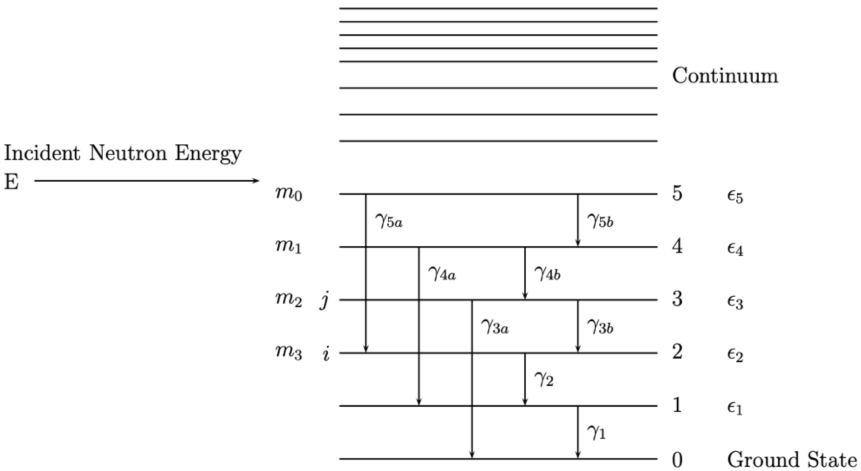
Thermal neutron capture gammas



Inelastic reaction gammas

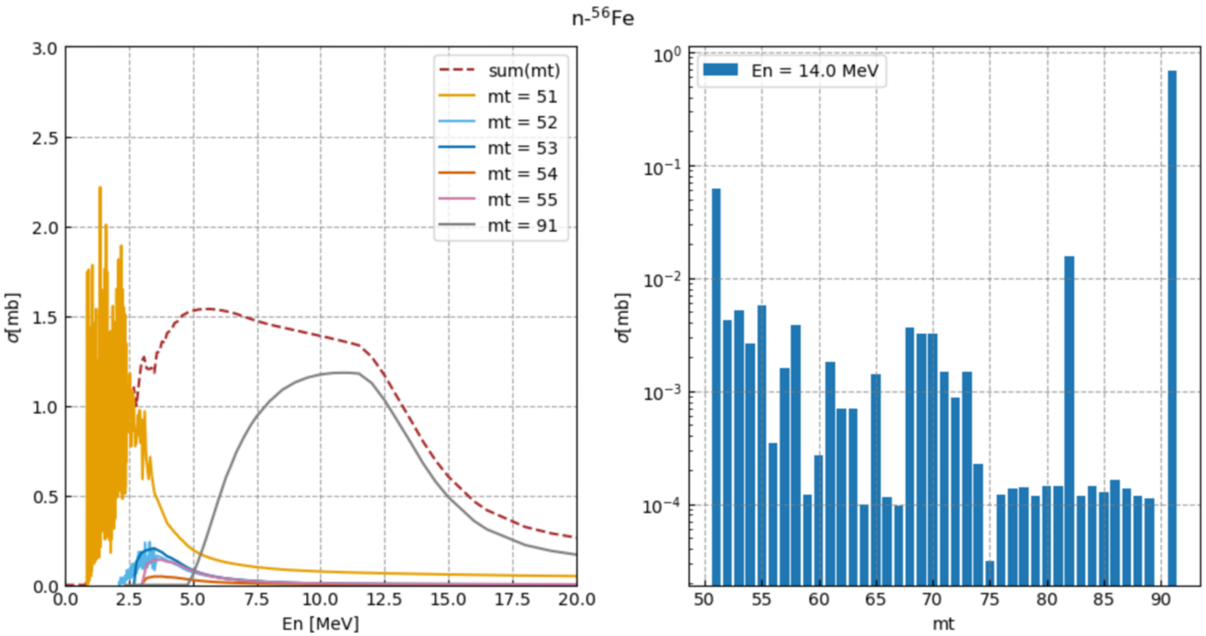


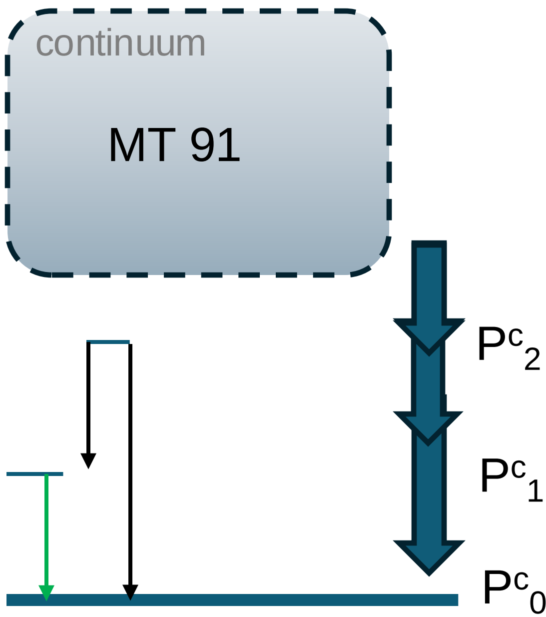
Reactions are different but the decay process is similar



- Inelastic reactions involve target **(A)** states while capture populates compound system **(A+1)** levels

Inelastic Cross Sections in an ENDF file



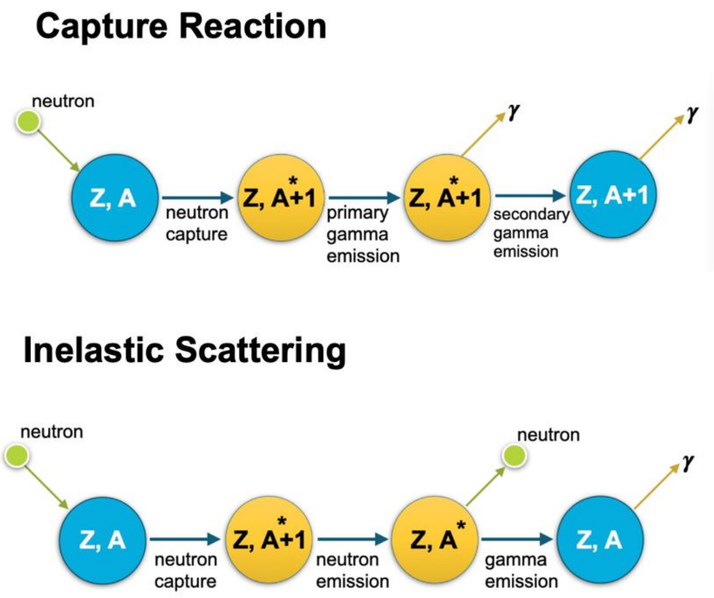


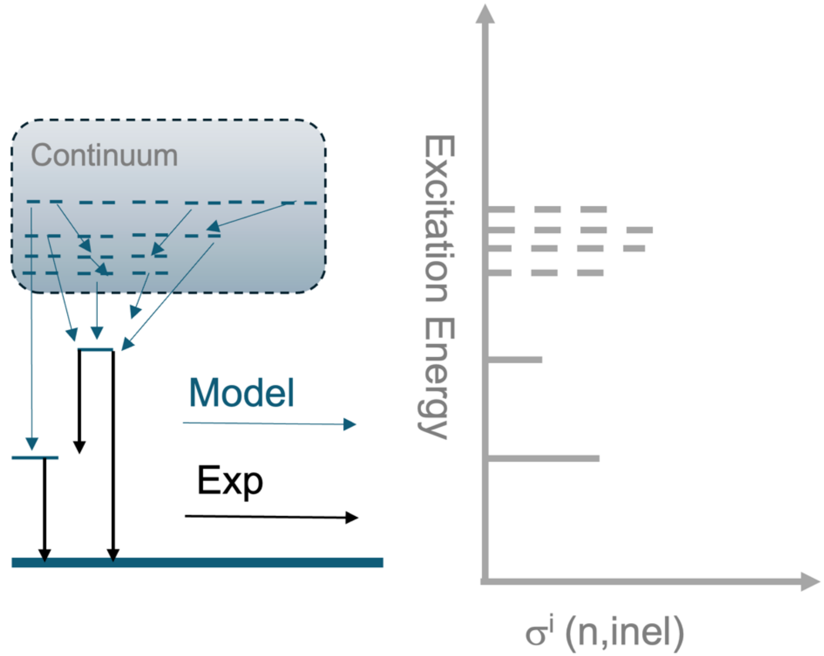
$\sigma(n,n'g) = \sigma\,(n,n'_{lev=1}) + \sigma^{c}(n,n'_{from\ above})$

^{56}Fe Excited states
mt < 91 : discrete
mt = 91: continuum

ENDF does not know how discrete levels are fed from the continuum

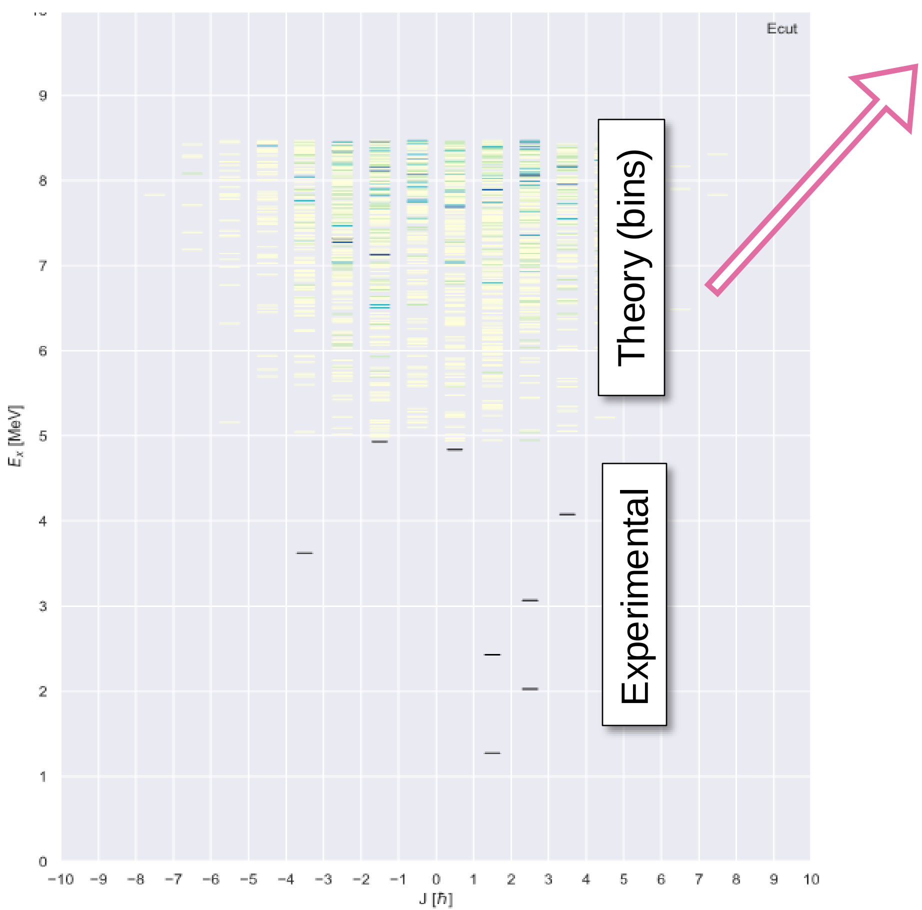
Neutron Induced Reactions and Gamma-Ray cascades





- ✓ We need all levels (including "bins” for the continuum)
- ✓ Population of each level as a function of incident energy
  - Capture is “easy” since one or two states are populated (s wave)
  - Inelastic is more complicated with a distribution of populated states

Levels and branching ratios



- Continuum discretized: The bins in the continuum are generated with level densities

$$\rho(E, J, \pi) = \rho(E)f(J)\pi(E)$$

  - Each bin can be populated in a reaction.
    -- similar to (n,n') to each discrete level

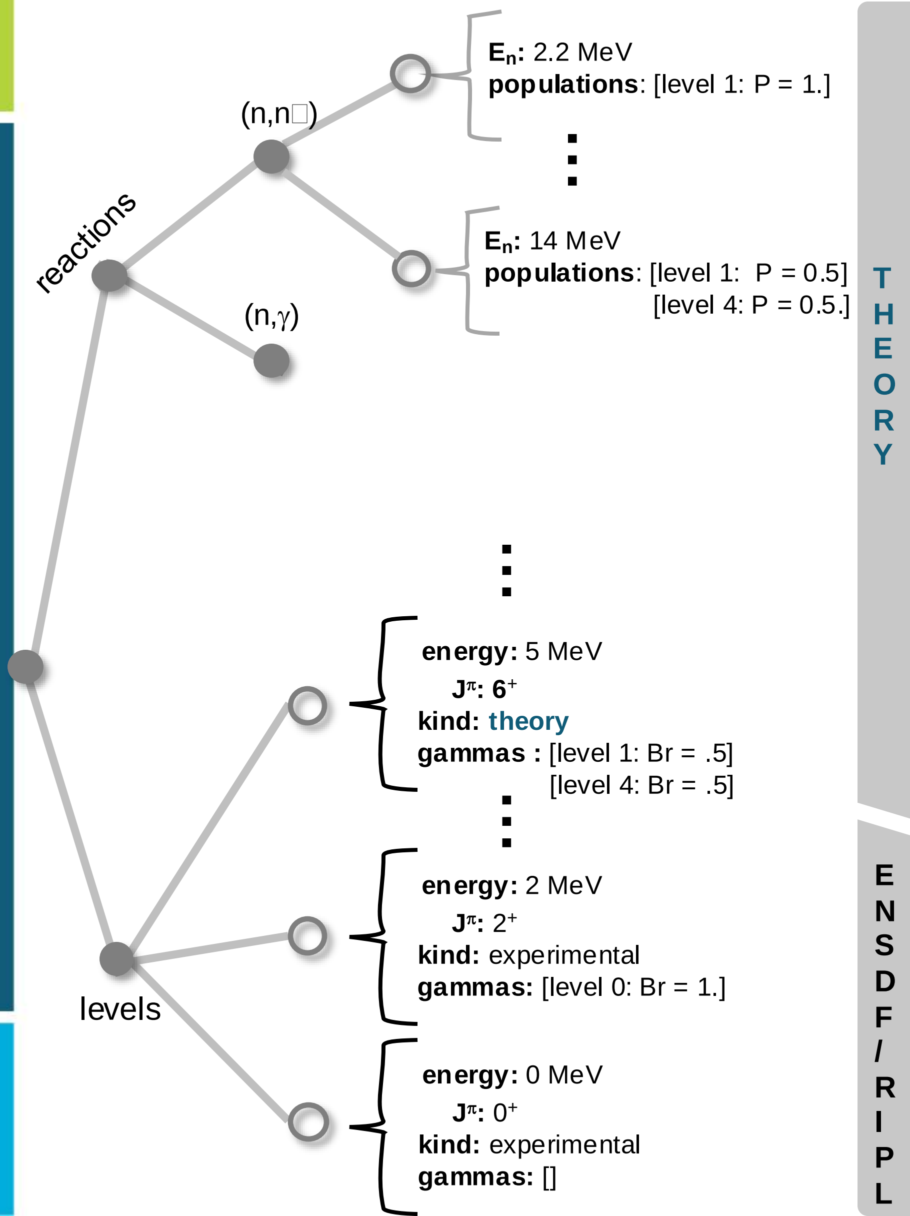
- The branching ratios are computed with PSF

✓ All of these can be found in reaction codes

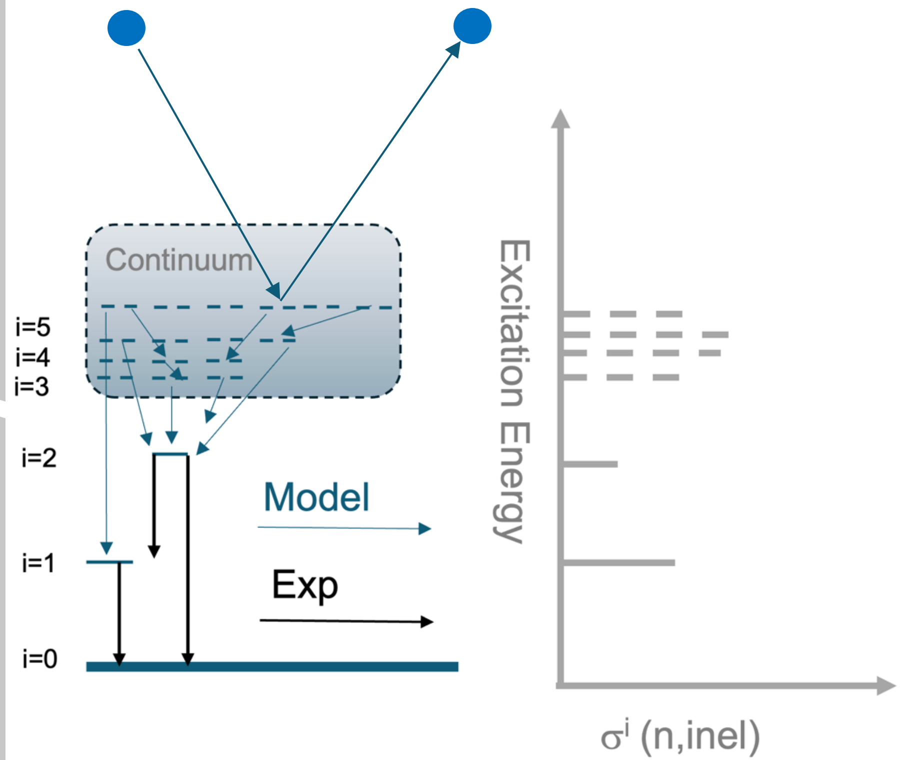
Experimental From IAEA/NDS RIPL

Reference Input Parameter Library Derived from ENSDF

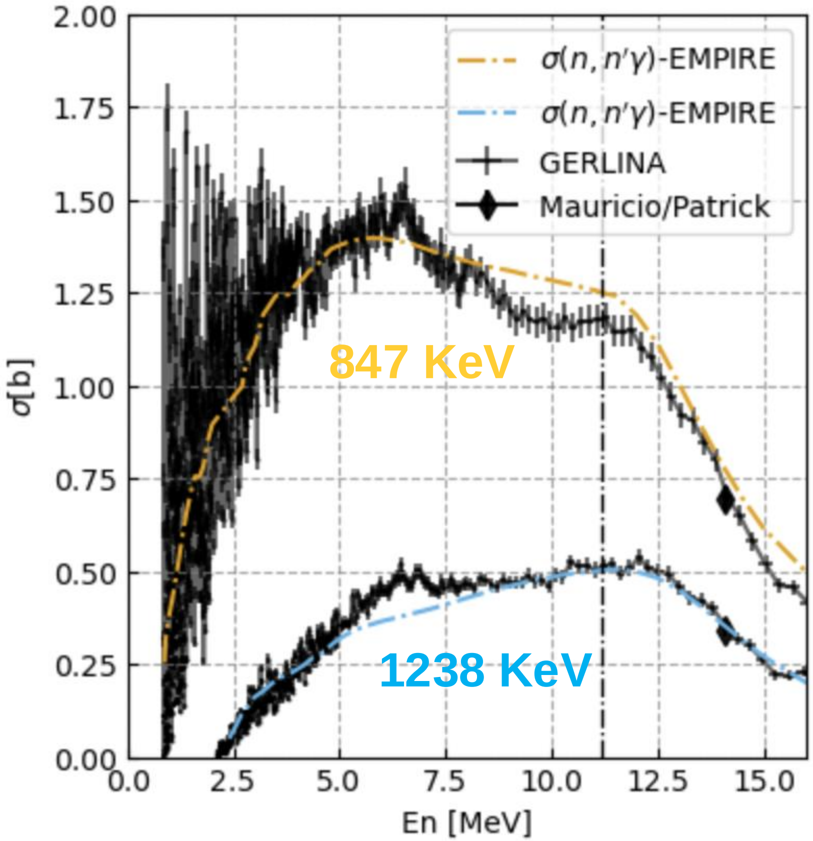
In-line Gamma-Ray cascades

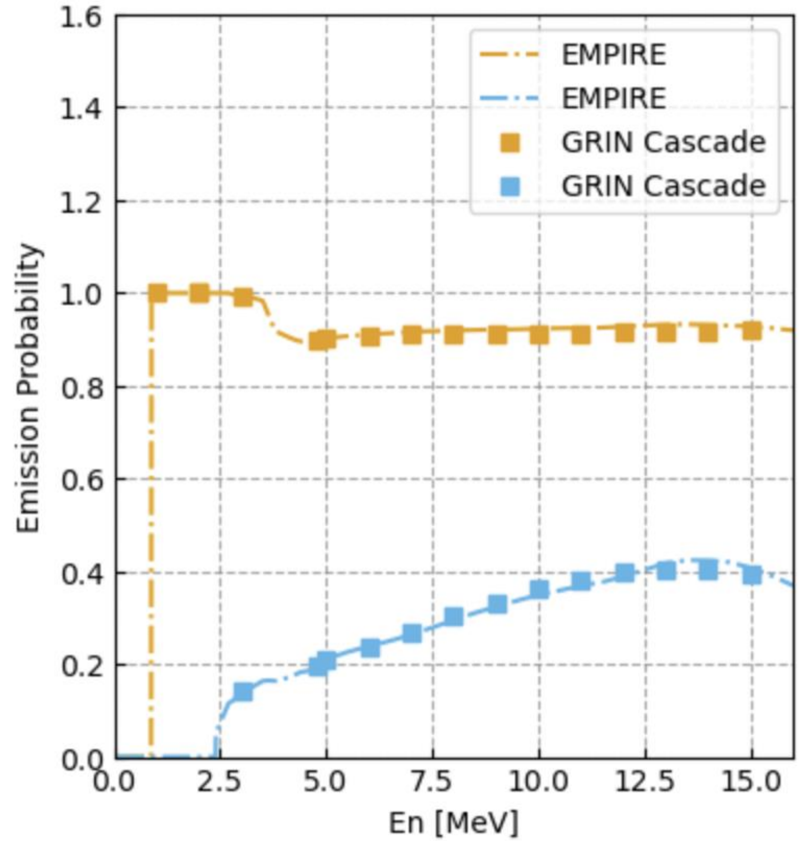


- Reactions inputs from detailed calculation (EMPIRE)
- We are working on extending the GNDS format to accommodate necessary inputs
- Cross sections to each experimental level is already stored in ENDF (mt51-90)



Inelastic cascades: $(n,n'\gamma)^{56}Fe$





- We used the CIELO/EMPIRE evaluation for ^{56}Fe
  All levels, populations and branching ratios (including bins in the continuum) were extracted and compiled in a test file
- By using a simple Monte Carlo sampling we were able to reproduce empire inelastic gamma-ray data results

Capture cascades: $(n,\gamma)^{13}C$

Capture

Gidi+/Mercury

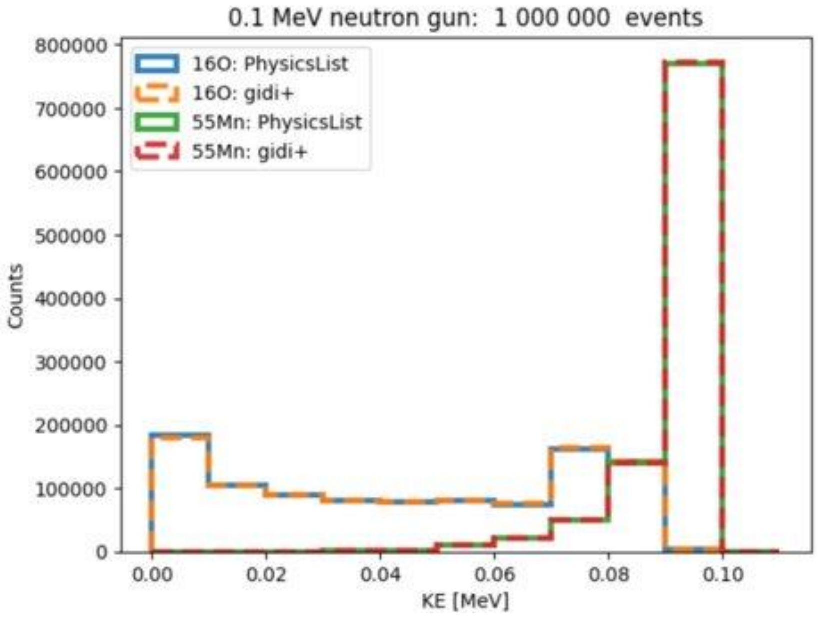
```
47 Neutron   + C13        (C13+n->C14+photon[inclusive])
47 Gamma   8.175020e+00
48 Neutron   + C13        (C13+n->C14+photon[inclusive])
48 Gamma   1.585420e+00
48 Gamma   4.957200e-01
48 Gamma   6.093880e+00
49 Neutron   + C13        (C13+n->C14+photon[inclusive])
49 Gamma   8.175020e+00
50 Neutron   + C13        (C13+n->C14+photon[inclusive])
50 Gamma   1.585420e+00
50 Gamma   4.957200e-01
50 Gamma   6.093880e+00
51 Neutron   + C13        (C13+n->C14+photon[inclusive])
51 Gamma   8.175020e+00
```

Energy conservation on event by event basis

-> the sum of the particle (gammas + residual nucleus) emission energies equals the total CN state energy of 8.17502 MeV (S_n)

GIDI+ as an event generator

https://github.com/LLNL/gidiplus



- GIDI+ uses GNDS rather than legacy ENDF files
- Our **new GNDS files** contain all the inputs needed for **in-line cascade simulation** for both capture and inelastic

GIDI+ has its own broomstick like code but can work in other transport codes (Mercury, Geant4, OpenMC (Hunter + @ RPI))

In our new GNDS

- All new entries are inside "applicationData" section of GNDS
  - do not affect current applications or transport codes
  - later can be officially incorporated
- A pseudo "POPs" data structure for "theory levels":
  - simple table to reduced the size of file
- Capture and inelastic populated states have a new data structure


```xml
<captureLevelProbabilities>
    <captureLevelProbability label="0" probability="1.0" spin="0.5" spinUnit="hbar" parity="1"
                 capturePrimaryToContinua="Fe57_e268">
      <table rows="6" columns="2">
       <columnHeaders>
        <column index="0" name="finalLevel" unit="" types="label"/>
        <column index="1" name="probability" unit=""/></columnHeaders>
       <data>
            Fe57     0.25
           Fe57_e1     0.29
           Fe57_e3     6e-2
           Fe57_e8   0.0111
          Fe57_e10    0.099
          Fe57_e11    0.096
</data></table></captureLevelProbability></captureLevelProbabilities>
```

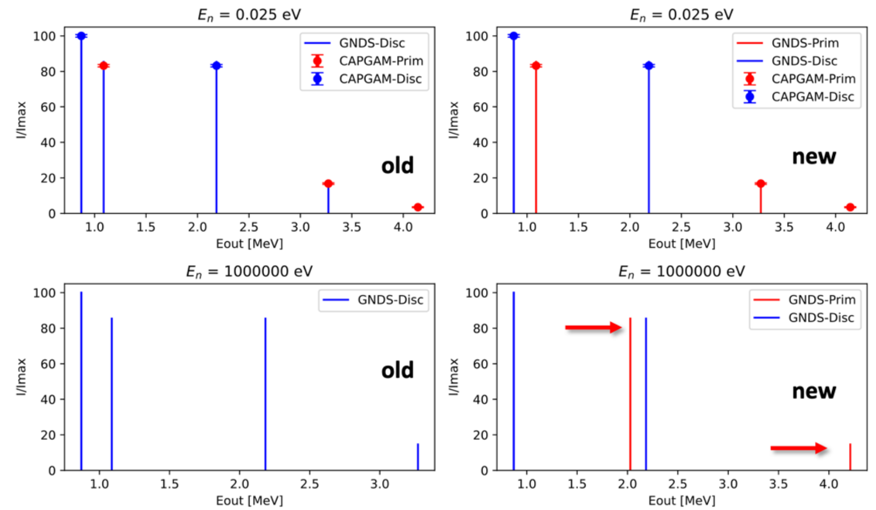
Some other GRIN products also include

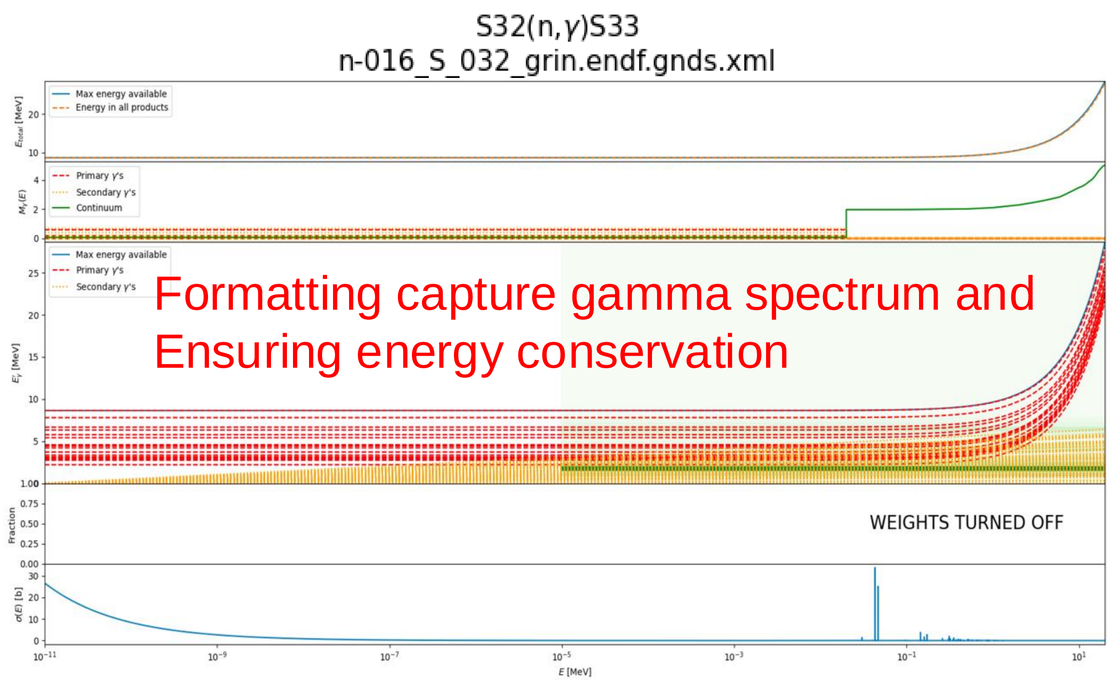
https://git.nndc.bnl.gov/grin/grin-formatter

grin-formatter.py

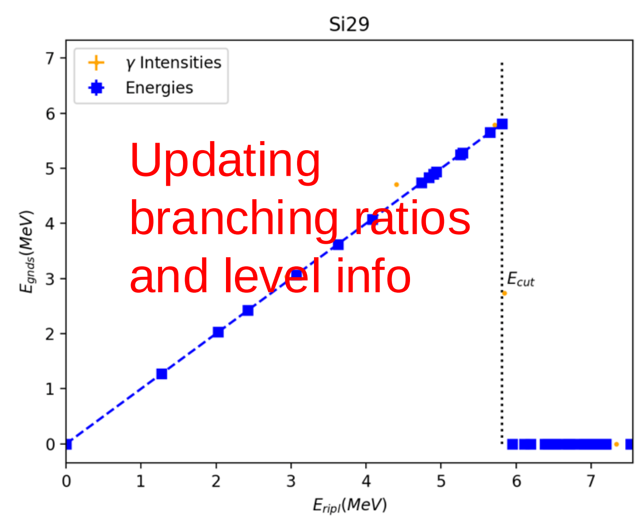
Python package to upgrade and update capture gamma-ray formatting and level and branching ratio fixes in evaluated **ENDF** and **GNDS** files

Properly flagging primary capture gammas

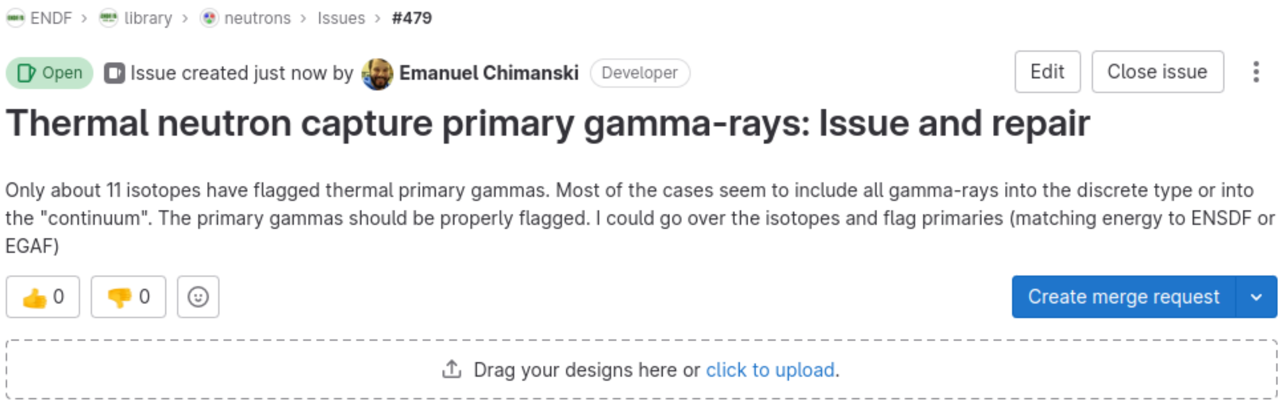




Formatting capture gamma spectrum and Ensuring energy conservation



Updating branching ratios and level info



- We fixed the primary gamma flags of a handful of isotopes for the following up release (more to come for ENDF9)

- Working on validation of our files with inelastic gammas from Baghdad Atlas:
  - Good for low energy but we need more effort on high energies **(where continuum kicks in)**

A Joint Effort: Experiment + Evaluations + Validation

Highlights:

- GIDI+ uses GNDS rather than legacy ENDF files for correlated gamma emissions from capture reaction cascades. Our new GNDS files contain all the inputs needed for in-line cascade simulation.

- Detailed reaction inputs are required: All can be given by reaction codes

- We can **embed discrete levels in the continuum**:
  - a discrete level above E_{cut} and its branching ratios can be incorporated (replacing a “theory” level by the given discrete from RIPL/ENSDF-- under testing)
- I would like to make sure **ICCs** are included in the evaluated files

- We have tested **C, S and Fe** but the list of isotopes of interest is large

- **Benchmarking cases are needed: with coincidence or not; (at different incident energies)**

Reach out if you are interested echimansk@bnl.gov

Thank you

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