Enabling an In-line Gamma-ray Cascade for Neutron Capture and Inelastic Reactions

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+ GRIN collaboration

US Nuclear Data Program Annual Meeting 2024

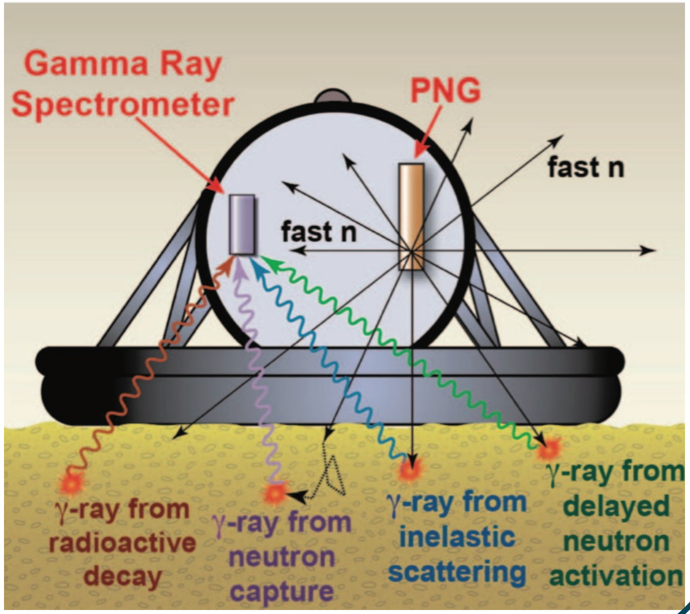
@BrookhavenLab

not export controlled

GRIN- Gamma Rays Induced by Neutrons

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

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



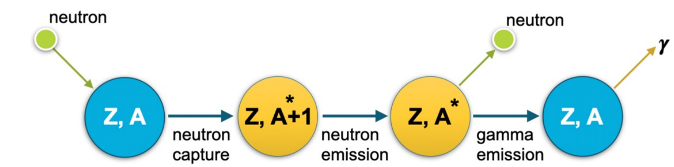
Target users:

- **"Traditional"** users call for a precise particle-γ spectrum to perform material identification.

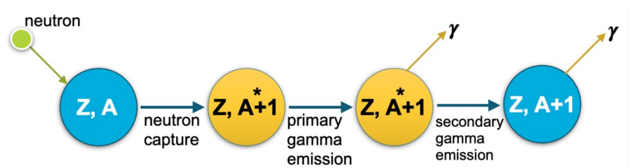
- **"Event-by-event"** users need the **correlations between scattered neutrons, gammas emitted from nuclear de-excitations**. Current evaluated data in ENDF libraries are not sufficient and must be extended.

Neutron Induced Reactions and Gamma-Ray cascades

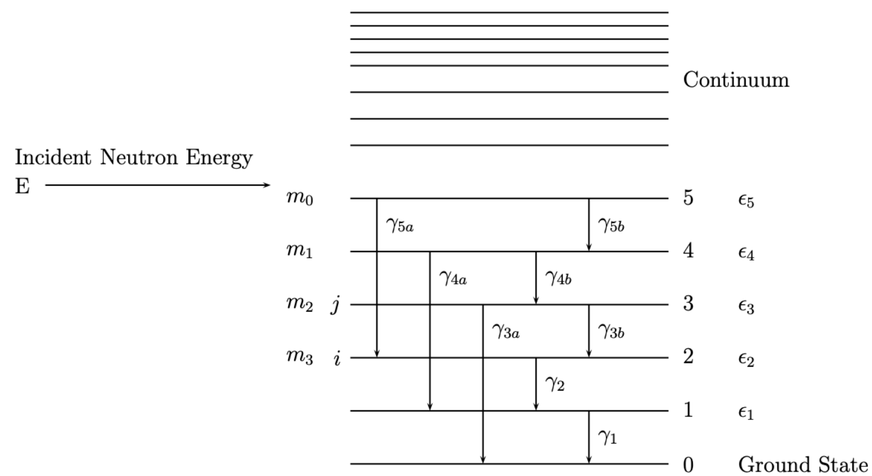
Inelastic reaction gammas



Thermal neutron capture gammas



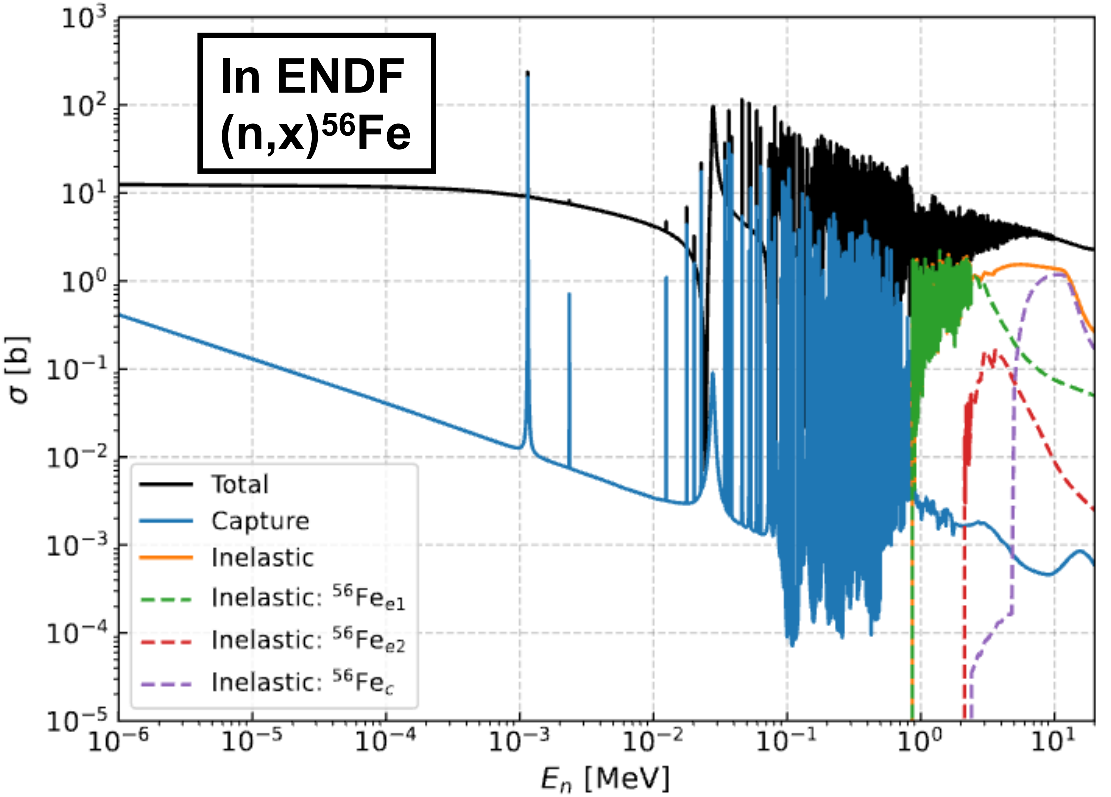
Reactions are different but the decay process is similar



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

Inelastic Reactions

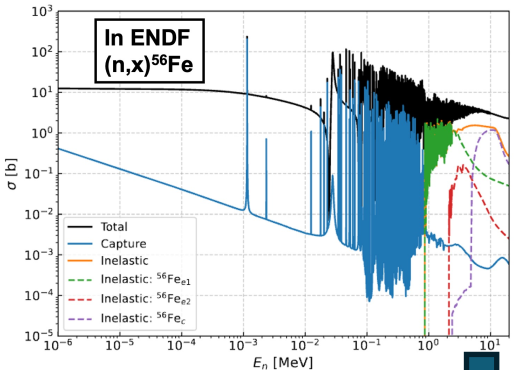
What is in ENDF and what are we missing?



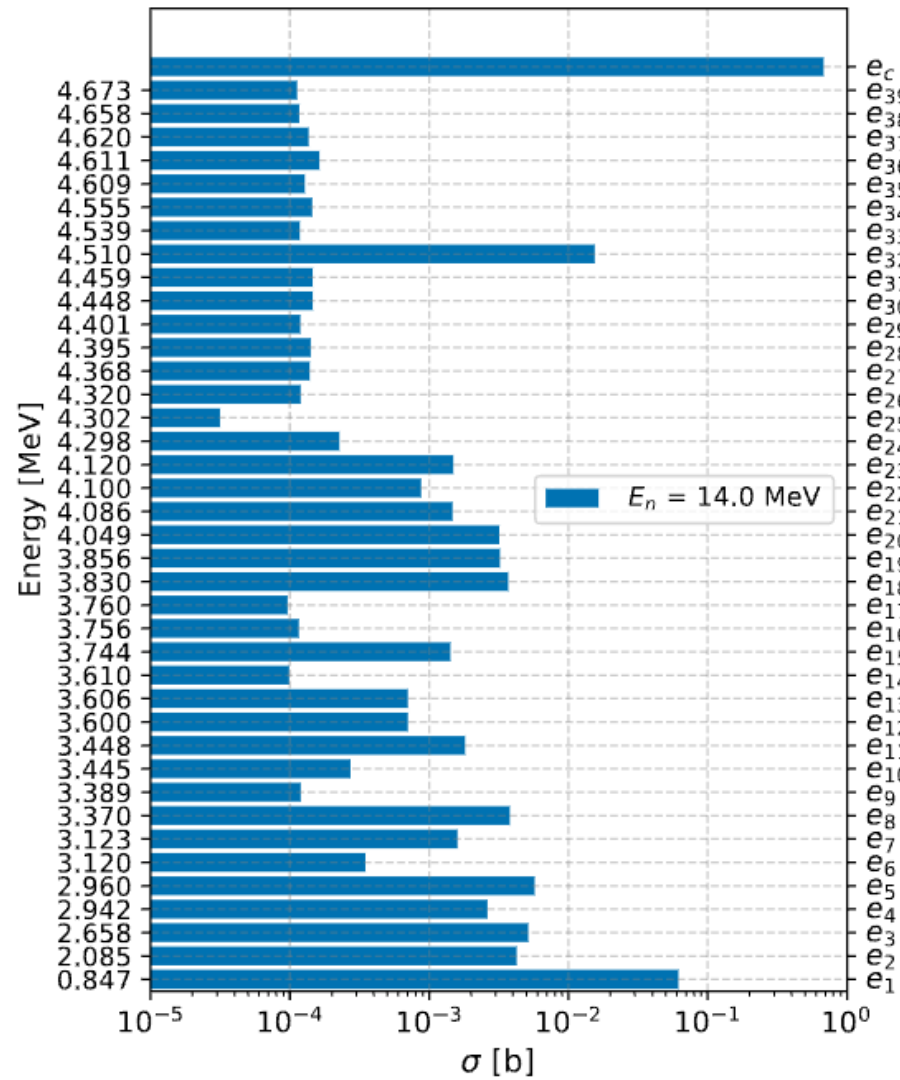
At a given incident Energy En:

- Cross sections
- Outgoing particle spectra (angle (usually isotropic))

What is in ENDF and what are we missing?



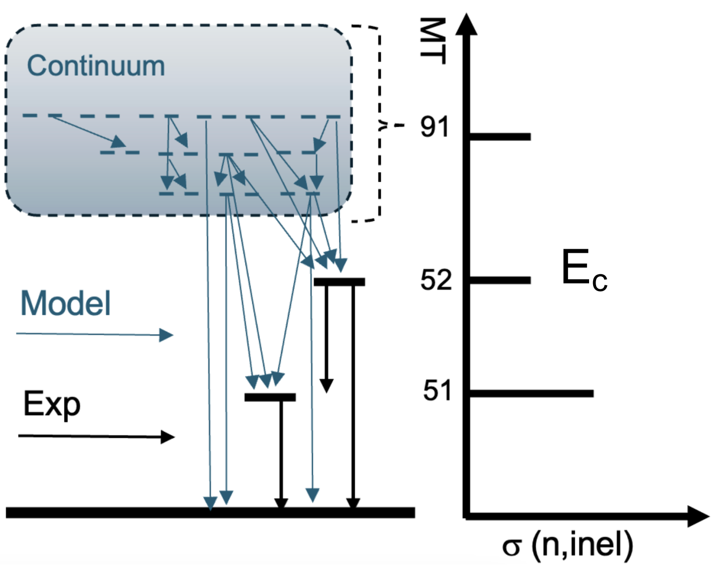
Inelastic at E_n = 14 MeV



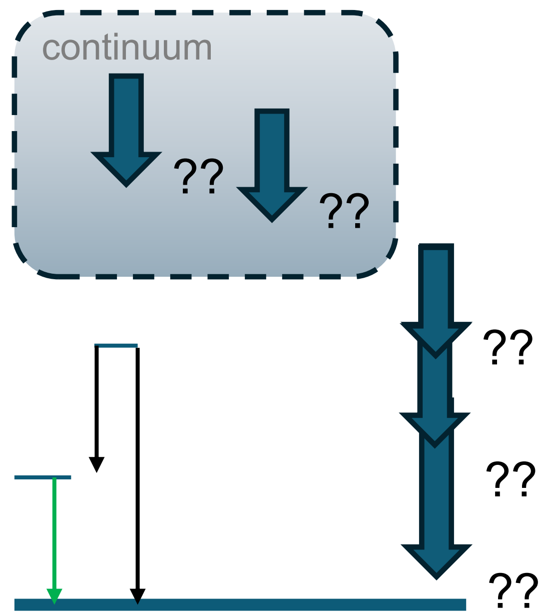
- ENDF can (that does not mean it does) provide everything needed for the cascade up to 39 excited levels;
  - Branching ratios are also stored up to the 39th level
- After 39 discrete states (or above E_c), ENDF uses a continuum (MT91) as “one fake level”.
  - No branching ratio is given for continuum

What is in ENDF and what are we missing?

- In a typical reaction calculation:
  - **Discrete levels** and BR come from **ENSDF/RIPL** (up to E_c)
  - **Pseudo-Continuum is discretized** -> Level Density Models -> PSFs for transitions
- Although calculations are done right, information is left behind when ENDF is compiled



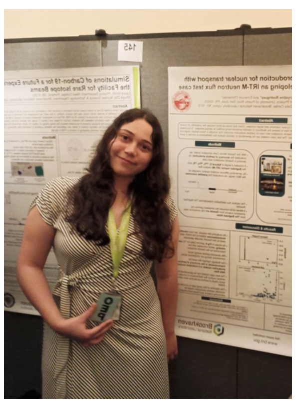
- ENDF does not have a detailed information of level population above E_c
- ENDF does not know how discrete levels are fed from the continuum



How is Geant4 performing ?

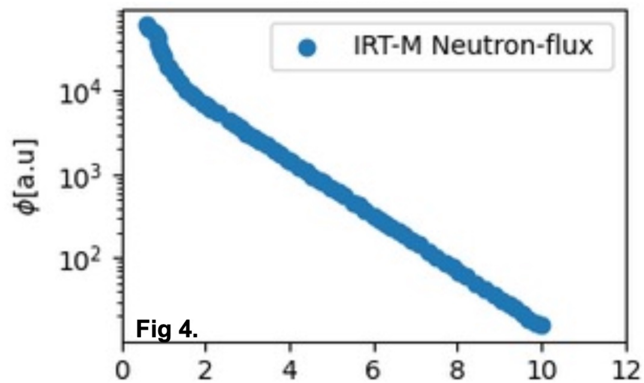
$$^{16}\mathrm{O}(n, n'\gamma) \rightarrow n + {}^{16}\mathrm{O}_{e2}$$

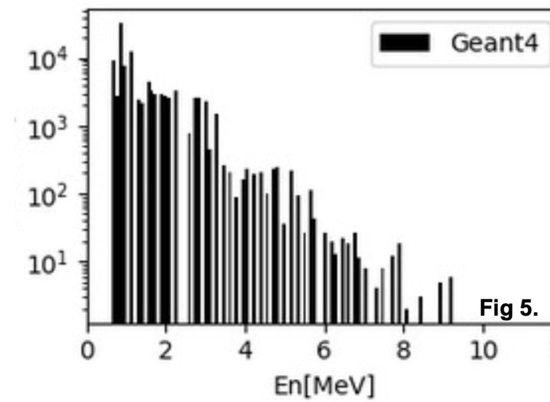
$$^{16}\mathrm{O}_{e2} \rightarrow {}^{16}\mathrm{O} + \gamma.$$

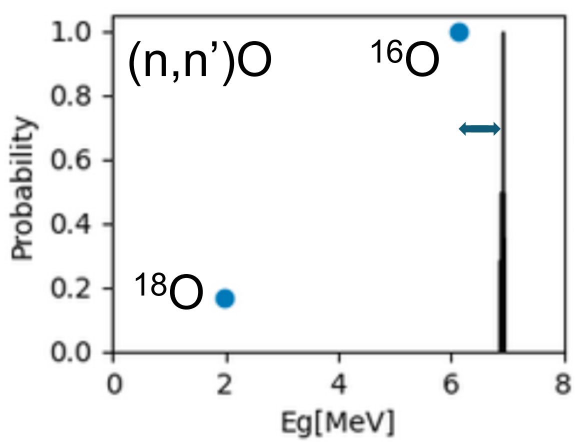


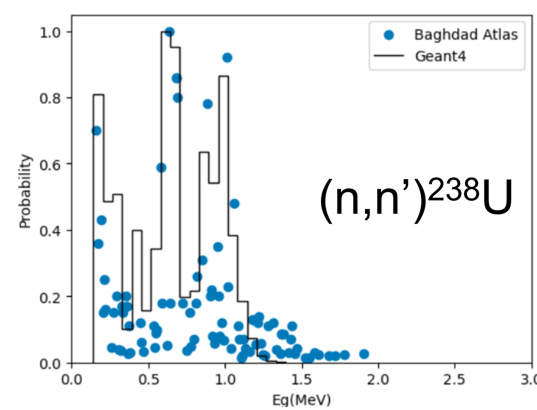
Krystine Rodriguez
(UPR – Puerto Rico)

- Simple monoisotopic target but a neutron flux data from the Baghdad (IRT-M) (^{235}U fission)
- Use Baghdad Atlas: Relational database for (n, n'γ) with elemental samples









*(more during her talk at DNP2024)

We know how to make these calculations: we just need to store some extra info

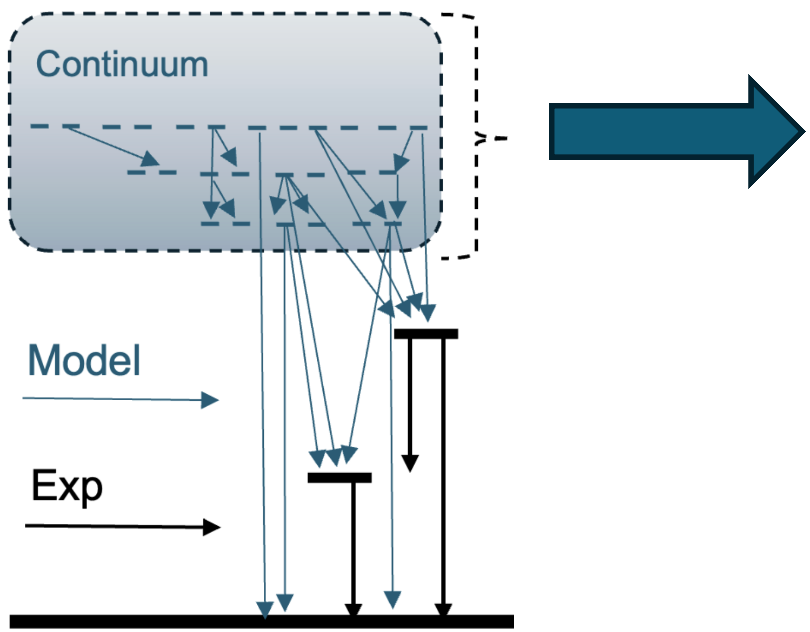
Generalized Nuclear Data Structure (GNDS):

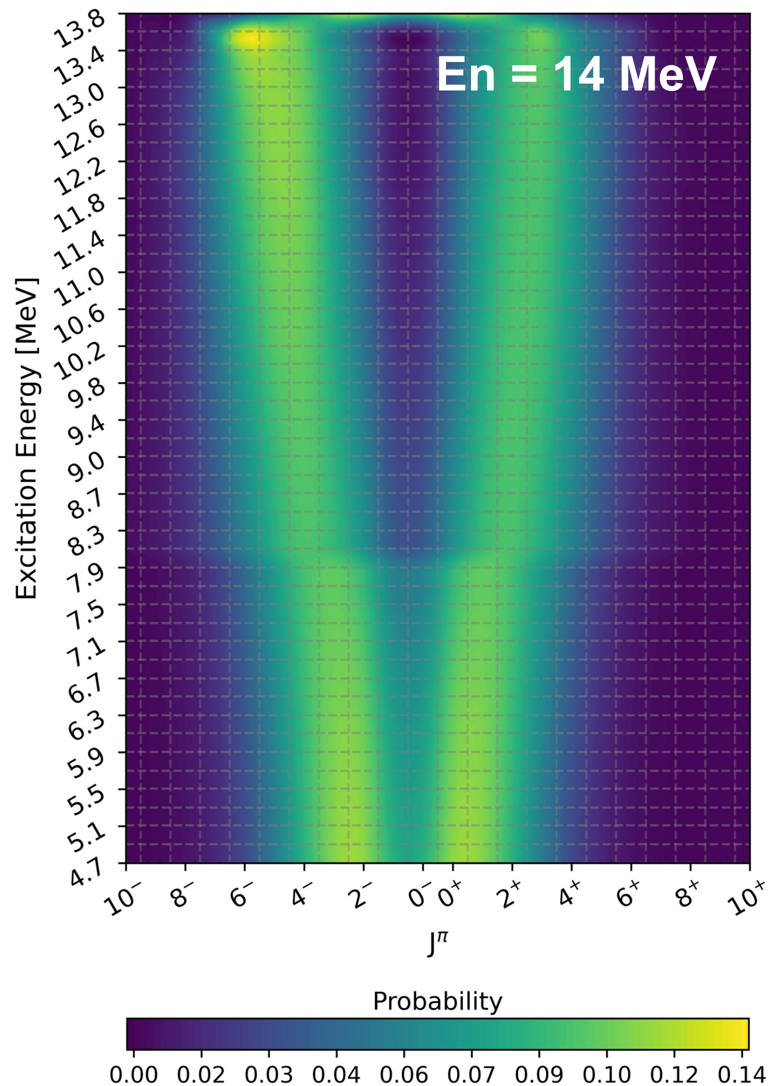
- Less restricted
  – Some formats can be naturally extended to incorporate the “pseudo-continuum” information

GRIN project:
People from different parts of the nuclear data pipeline

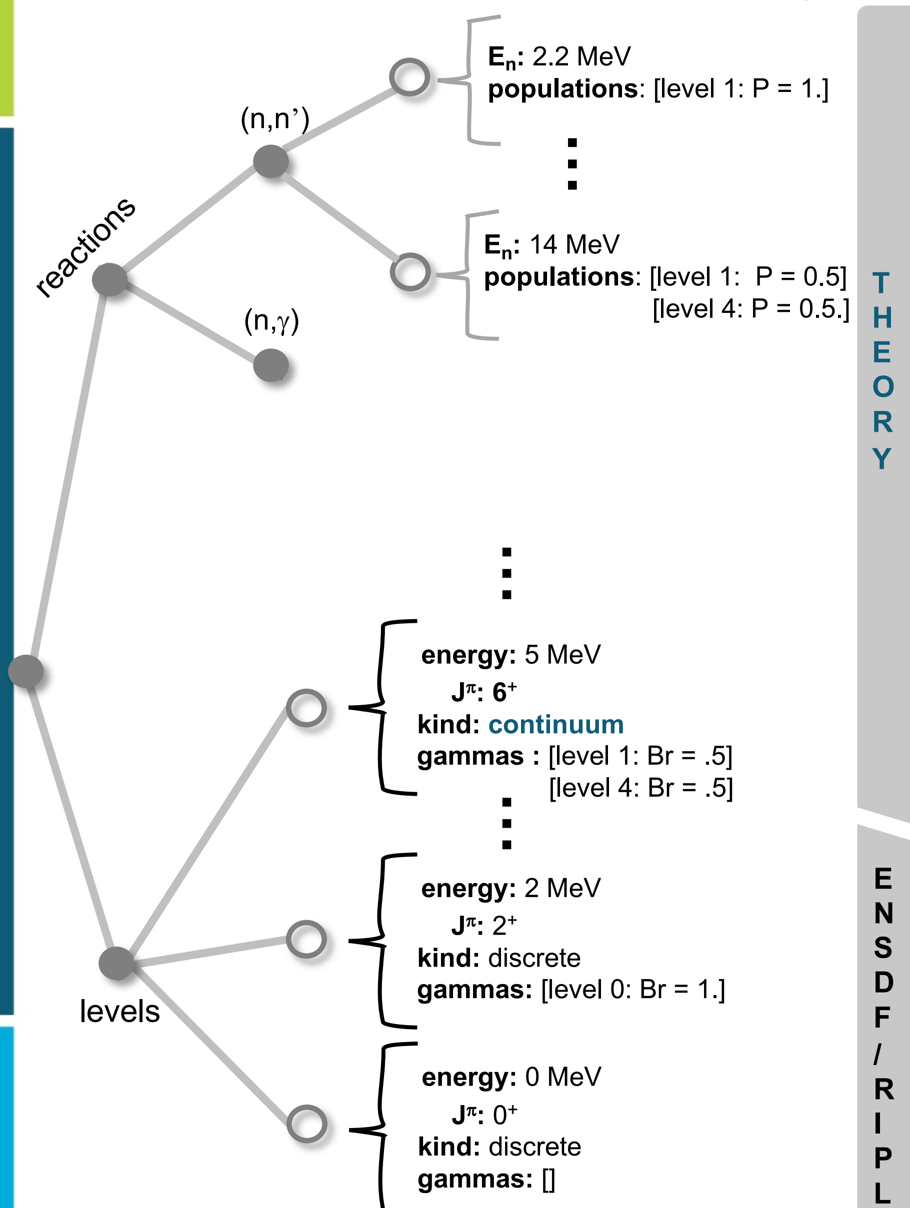
In-line Gamma-Ray cascades

- As test case: We work on top of the ENDF-CIELO (IAEA) evaluation for ^{56}Fe
- Details extracted from calculation (EMPIRE reaction code)



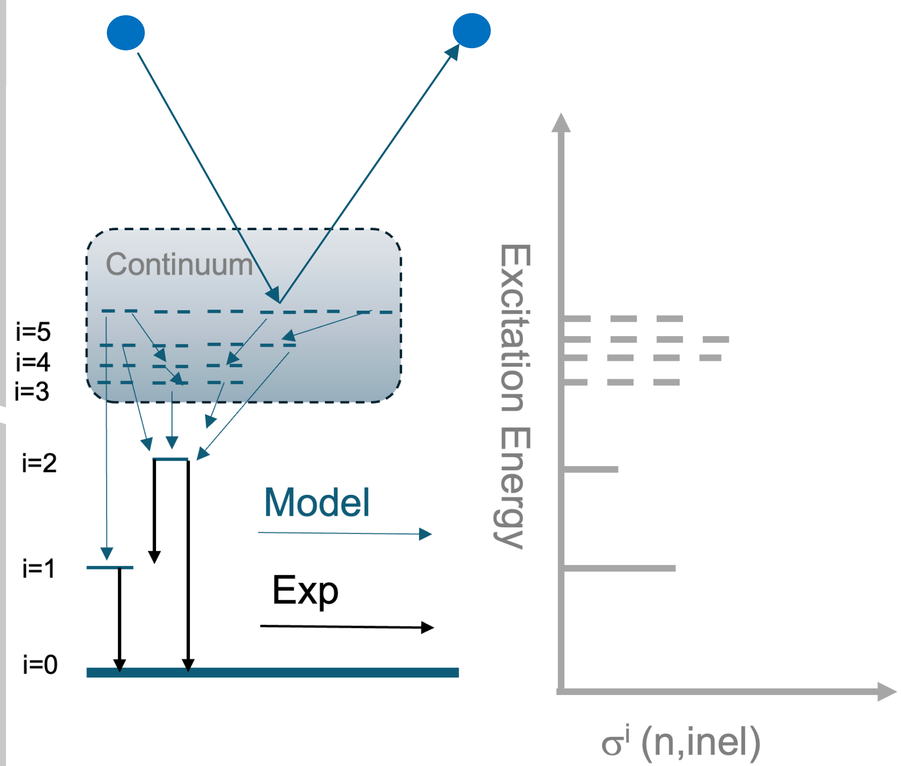


In-line Gamma-Ray cascades

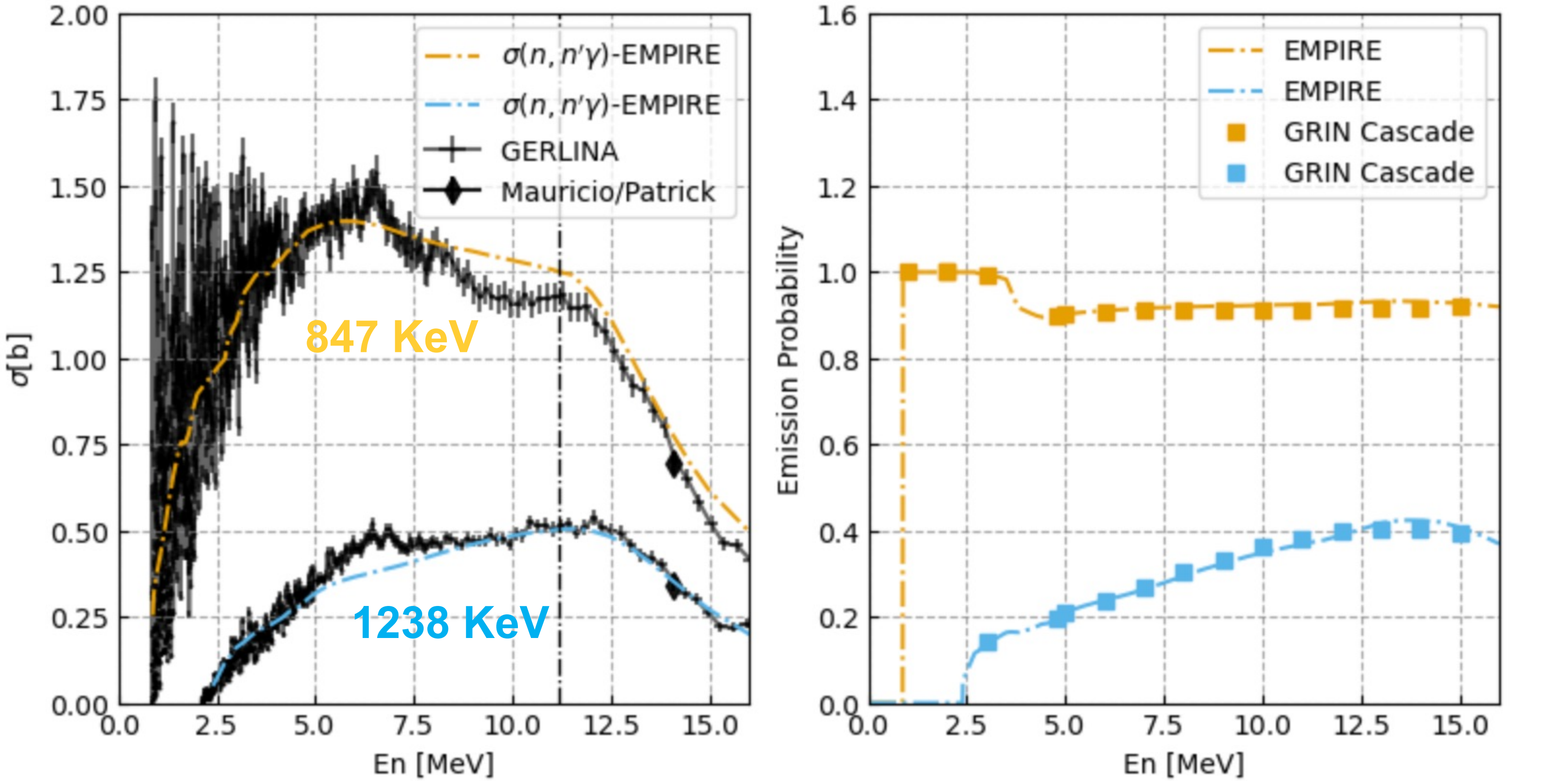


- We are working on extending the GNDS format to accommodate necessary inputs
- **Sample a reaction:**
  - if pseudo-continuum:
    - **sample the initial state**

  - roll dices and just follow branching ratios



Inelastic cascades: (n,n'γ)^{56}Fe



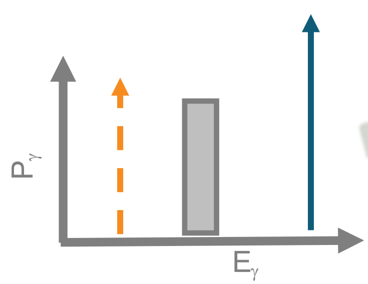
- We used the CIELO/EMPIRE evaluation for ^{56}Fe
  All levels, populations and branching ratios (including bins in the continuum) were extracted and compiled in a test file
- By using a simple python Monte Carlo sampling we were able to reproduce empire inelastic gamma-ray data results

Neutron Capture Cascade

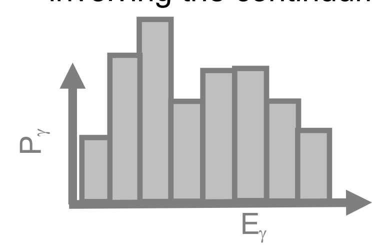
What is in the ENDF and how transport codes handle it?

- **In ENDF, for a given incident energy:**
  - Capture Cross Section
  - List of gammas

Three different types of γ

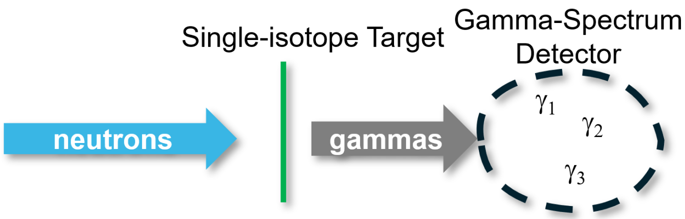


- **Primary**:
  Emissions from the capture state to (known) the discrete levels.
- **Discrete**:
  Emissions from discrete to discrete levels.
- **Continuum**:
  Histogram of $E\gamma$ emissions involving the continuum



* I could list the reasons of how bad sampling this can be (but better if I show …)

GEANT4 Simulations with ENDF/B and the Capture Gamma-rays



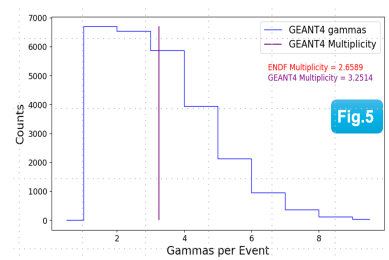
fEvent	primaryParticle	primaryEnergy	scattered Primary Energy	secondary Particle	secondaryEnergy	processName
0	neutron	2.50E-08	0	C13	0.00100	nCapture
0	neutron	2.50E-08	0	gamma	4.94633	nCapture
1	neutron	2.50E-08	0	gamma	4.94651	nCapture
1	neutron	2.50E-08	0	gamma	4.94651	nCapture
1	neutron	2.50E-08	0	C13	0.00255	nCapture

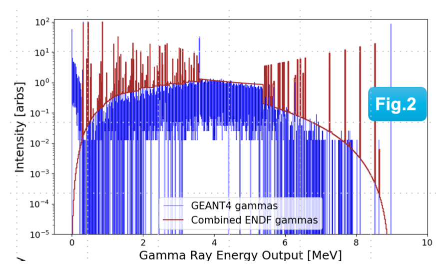
In GEANT4

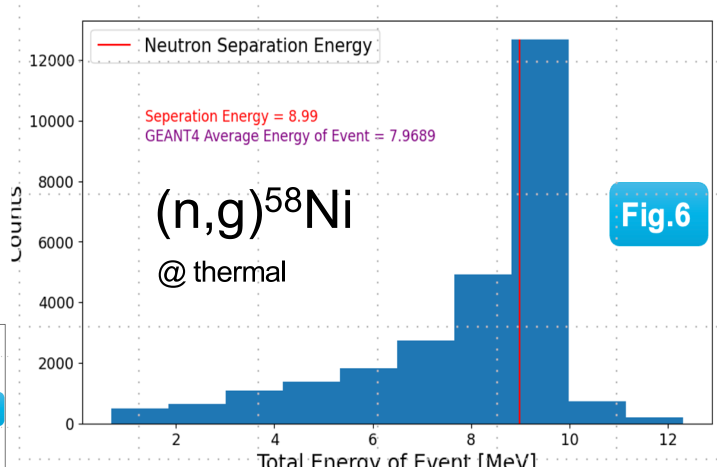
- **Multiple flags to choose and simulate the reaction differently;**
  - some provide better results for a few isotopes

When using ENDF/B inputs only:

- **Geant4 does not distinguish primaries from secondaries even when ENDF/B does**
- **No gamma-ray correlations**
- **Energy is not conserved event-by-event**







Michael Allen (Texas A&M) &
Mauricio Cerda (Texas Tech)
+ Andrea Mattera (NNDC)

Inline Neutron Capture Gamma-ray Cascade

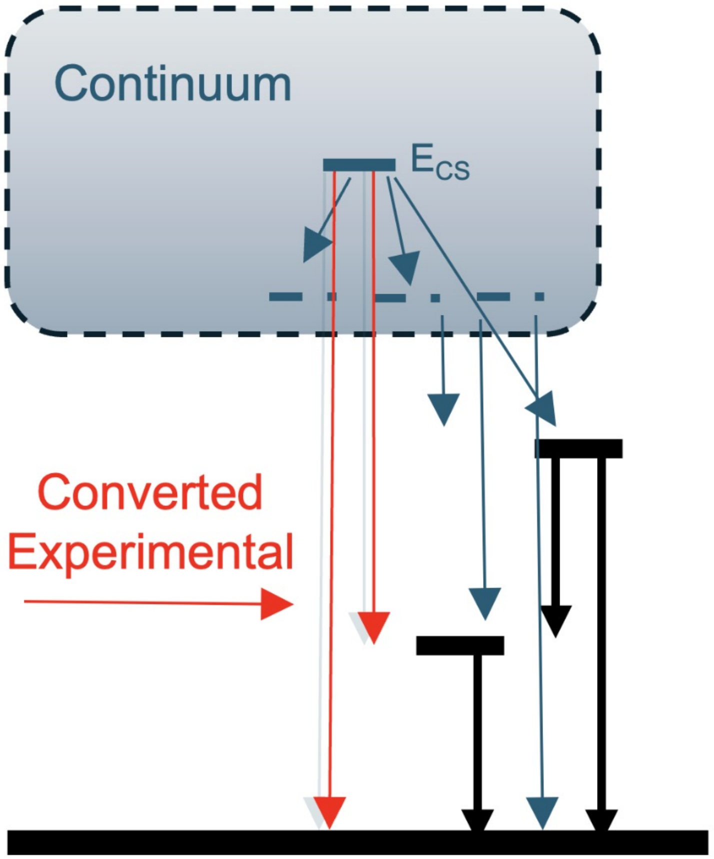
With our new file:

- We already have all levels (including the discretized bins for the pseudo-continuum)

- **Capture State**:
  - Excitation energy: easily computed with $\mathbf{E_{CS} = E_n + S_n}$
  - Spin and Parity: we store them

$$J_{CS} = J_{GS} + l + \tfrac{1}{2}$$
$$\pi_{CS} = \pi_{GS} (-1)^l$$

- Match **Capture State** with a level in the **continuum**:
  - **ENSDF-TH/EGAF for primaries**
    - Models don't do a good job on predicting primaries



In our new GNDS

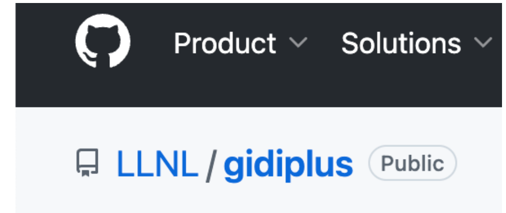
- All levels are included
  - do not affect current applications or transport codes
  - later can be officially incorporated
- A pseudo “POPs” data structure for “theory levels”:
  - simple table to reduced the size of file
- Capture and inelastic populated states have a new data structure

```
<captureLevelProbabilities>
        <captureLevelProbability label="0" probability="1.0" spin="0.5" spinUnit="hbar"
parity="1"
                              <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>
```

Primaries from ENSDF-TH

How can we handle this file that has everything?

GIDI+ with new GNDS



https://github.com/LLNL/gidiplus

- GIDI+ works as a sampler:
  - Produces gamma-ray cascades whenever a neutron capture (inelastic) event is called

Example of a capture cascade event on ^{56}Fe from GIDI+

```
#  •       user id     intid     energy          v_x              v_y              v_z
Event:         0 reaction 72: Fe57 + photon [inclusive]
   product:        6  1000000000  6.01882403e+00  3.88002726e+00  9.35009794e-01  4.50526223e+00
   product:        6  1000000000  1.26049700e+00 -1.24690747e+00 -1.03422628e-01  1.52899315e-01
   product:        6  1000000000  3.52346000e-01 -2.28763952e-01  2.12096093e-01  1.63798674e-01
   product:       -1       26057  0.00000000e+00  0.00000000e+00  0.00000000e+00  0.00000000e+00
   GRIN intermediate residual: Fe57_e10
```

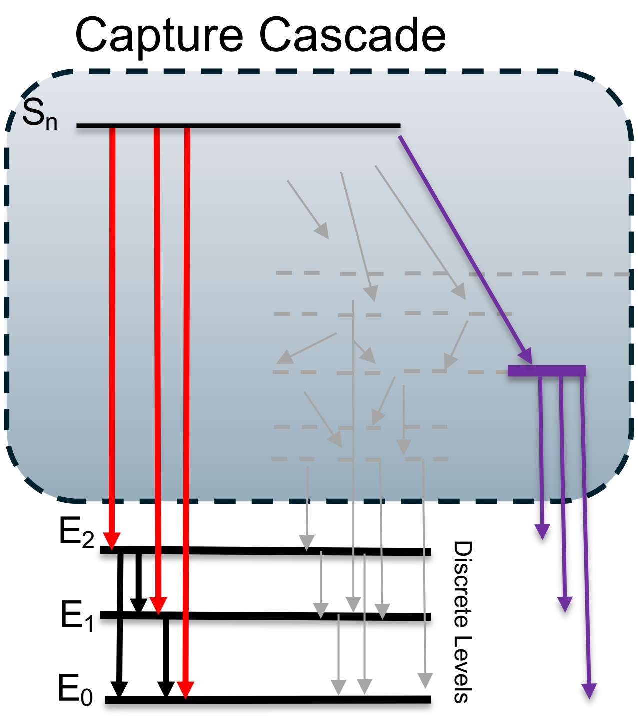
- The sum of each gamma-ray energy in the cascade provides the excitation energy **(energy conservation!)**

- **Users don't need to think about model parameters or experimental primaries**

*** Manuscript in preparation

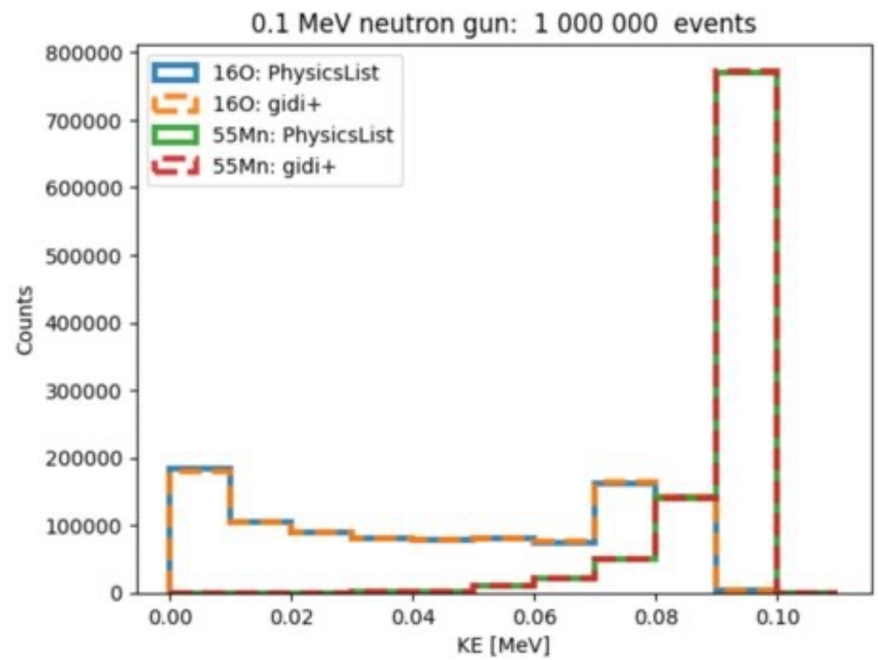
What if there is a high energy level in ENSDF and not in ENDF? We can easily embed levels

A discrete level above E_c can be placed (embedded) In the pseudo-continuum



GIDI+ as an event generator

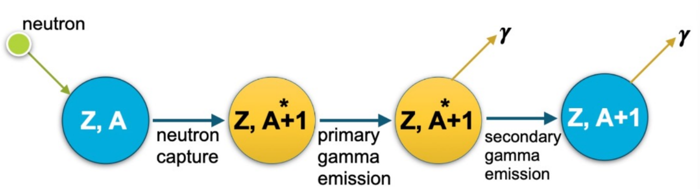
- GIDI+ uses GNDS rather than legacy ENDF files
- Our **new GNDS files** contain all the inputs needed for **in-line cascade simulation** for both capture and inelastic



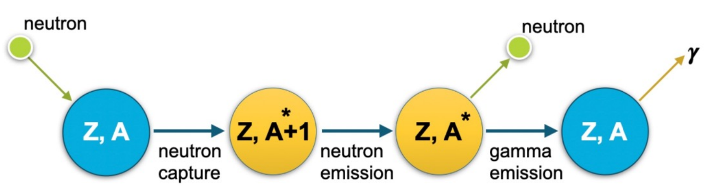
GIDI+ has its own broomstick like code but can work in other transport codes (Mercury, Geant4, OpenMC (Hunter + @ RPI))

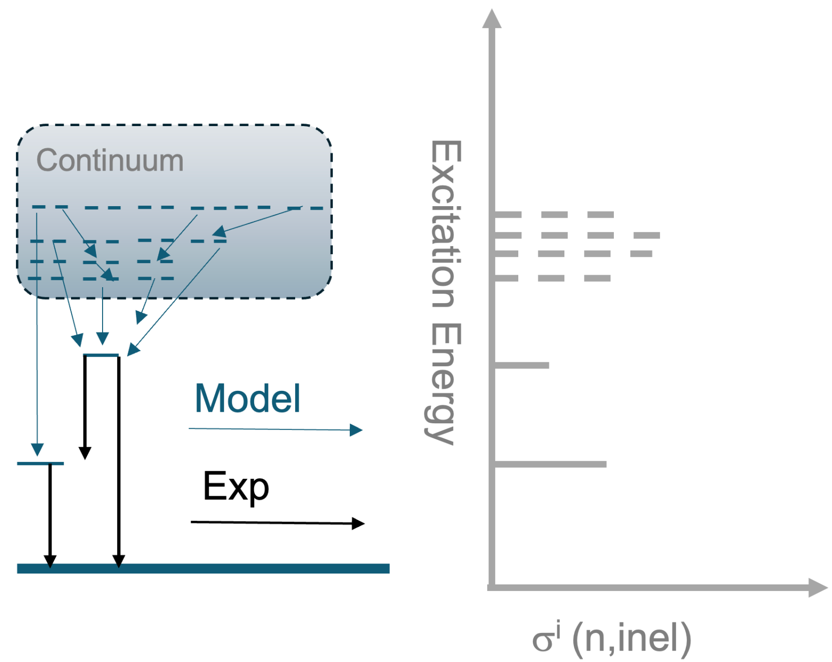
In Summary

Capture Reaction



Inelastic Scattering





- ✓ We need all levels (including "bins" for the continuum)
- ✓ We can have discrete levels above E_c embedded in 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

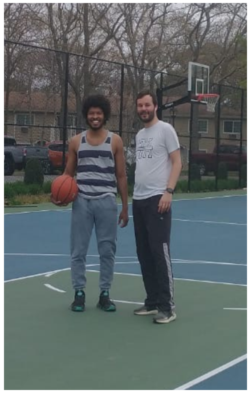
Highlights:

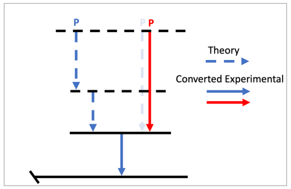
- GIDI+ uses GNDS rather than legacy ENDF files for correlated gamma emissions. Our new GNDS files contain all the inputs needed for in-line cascade simulation.
- GIDI+ has its own “broomstick” like simulation
- We would like to make sure **ICCs** are properly included
- We can **embed discrete levels in the continuum**:
  - a discrete level above E_{cut} and its branching ratios can be incorporated (replacing a kind = “continuum” level by the given discrete from ENSDF)
- As we build these new files, we have spotted a few typos in ENSDF-TH (communicated to ENSDF GRIN people)
- We are showing it works! (project with RPI (Yaron, Ian) on benchmarking (n,g)):
  - Users need this capability for many other isotopes!

Reach out if you are interested echimansk@bnl.gov

Many thanks to

Ayman Abdullah-Smoot (TSU)



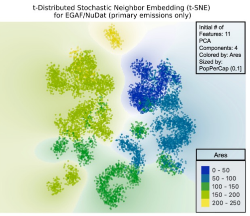


+ Donnie Manson (NNDC)

Ana Pereira (FSU)

*$\hat{f}_{loss}$ can be customized with a **penalty** that increases the loss if model predictions violates our physical constraint:

$0 < \sum_i \sigma_\gamma^i \leq \sigma_0$



NN Hidden Layers (nodes)	Loss (after 20 cycles)
(7, 2)	23147.57
(7, 5, 3)	2363.67
(9, 8, 7, 6, 5, 4, 3, 2)	17.30

Krystine Rodriguez (UPR – Puerto Rico)

Michael Allen (Texas A&M) &
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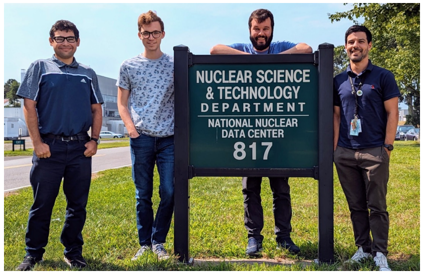

+ Andrea Mattera (NNDC)

Thank you