Measuring and Simulating Capture γ-Ray Spectra using the RPI γ-Multiplicity Detector

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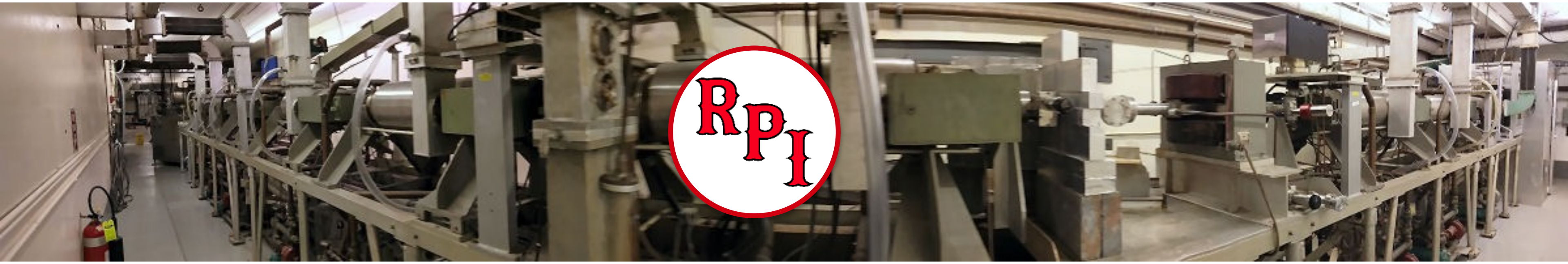

The 17th International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics (CGS17)
MINATEC Innovation Campus in Grenoble, France
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Outline

- Overview of **RPI γ-Multiplicity Detector System**
  - Motivation + Goals
  - Detector System Description + Experimental Validation
- Current status and **updates to models** used to simulate γ-emission spectra
  - MCNP-6.2 with ACE files (ENDF/B-VIII.0), MCNP-6.2 using CGM
  - Modified version of MCNP-6.2 with `DICEBOX`
- **Validating nuclear data** by comparing experimental results to the modified simulation technique
  - Benchmark the system with a well-known isotope (^{56}Fe)

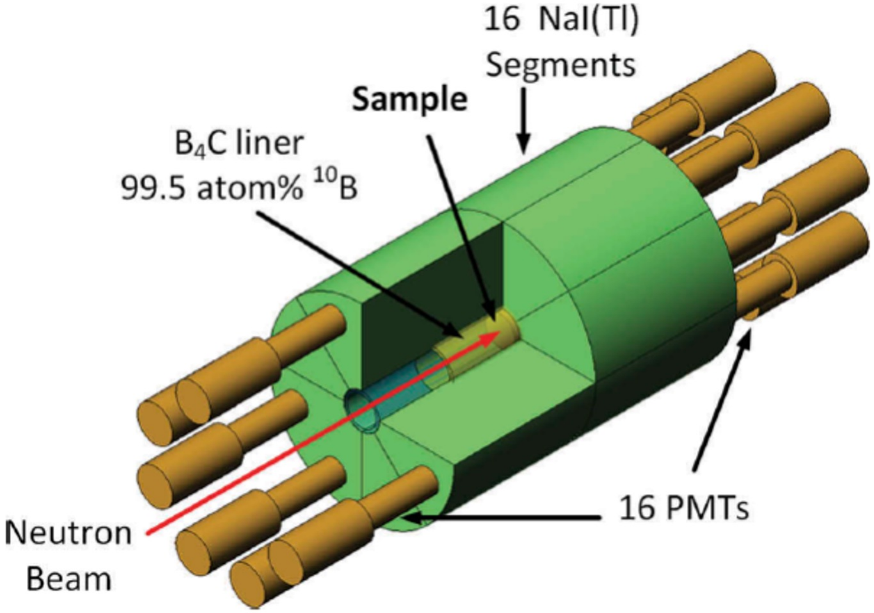
Motivation + Goals

- **Measure neutron capture and fission γ-emission spectra** as a function of energy and multiplicity for important nuclear materials in the RRR
  - Interest includes ^{235}U, ^{238}U, and other structural materials
- **Generate accurate neutron capture γ-cascade data** from experimental results
  - Compare with current simulation tools (using forward modeling methods)
  - Constrain models used for reaction and cascade calculations
  - Characterize for non-proliferation applications
- **Improve the current models** used to simulate γ-emission spectra following neutron capture

RPI γ-Multiplicity Detector

- **16 segment NaI(Tl) γ-multiplicity detector**
  - Total volume: 20 L of NaI(Tl) surrounding the sample
  - Inside the detector is lined (~1 cm) with a B4C ceramic sleeve which is enriched 99.5 atom% in ^{10}B to absorb scattered neutrons from the sample
  - Up to 96% efficiency for detecting γ-cascades

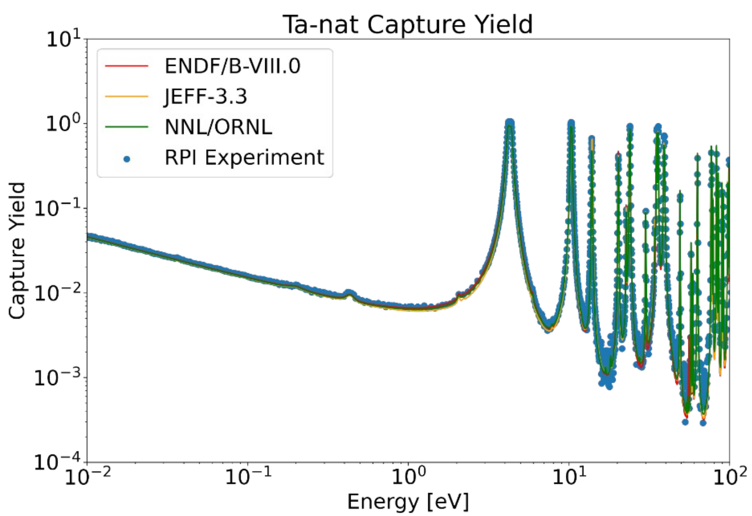
- **Detector is used for capture yield and γ-spectra measurements**
  - Useful neutron energy range: 0.01 eV – 3 keV
- **New SIS3316-DT 16 Channel Digitizer**
  - Digitize pulse wave for all events on all detectors & obtain the energy of each detected event

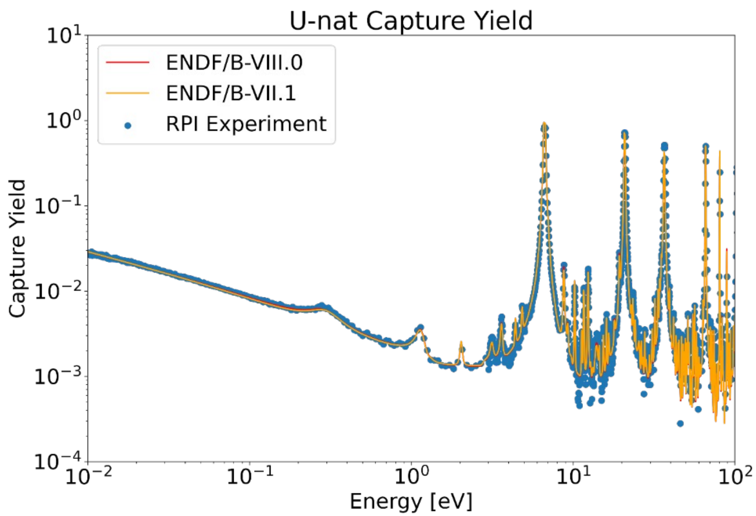


Experimental Validation

Low Energy (0.01 – 100 eV) Capture Yield of ^{nat}Ta and ^{nat}U

- Sample thicknesses:
  - 10 mil ^{nat}Ta (0.012% ^{180m}Ta)
  - 20 mil ^{nat}U (0.7% ^{235}U)
- Validation of the new DAQ system and julia-based processing codes
- Experimental results are compared to first-order theoretical capture yield $\left(Y = [1 - e^{-N\sigma_t}]\frac{\sigma_\gamma}{\sigma_t}\right)$ using the different evaluations





Current MCNP-6.2 Simulation Status

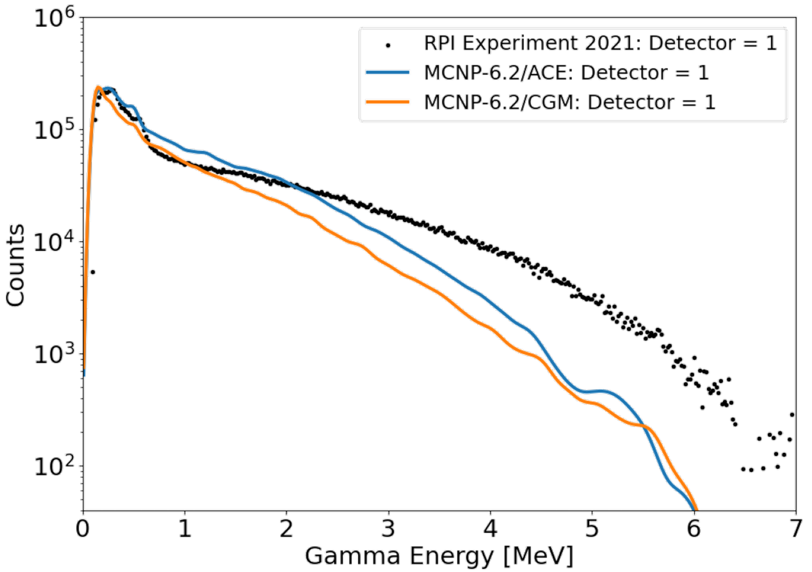
Current tools for modeling γ-emission spectra show a large discrepancy between experimental and simulated γ-spectra for ^{181}Ta(n,γ)

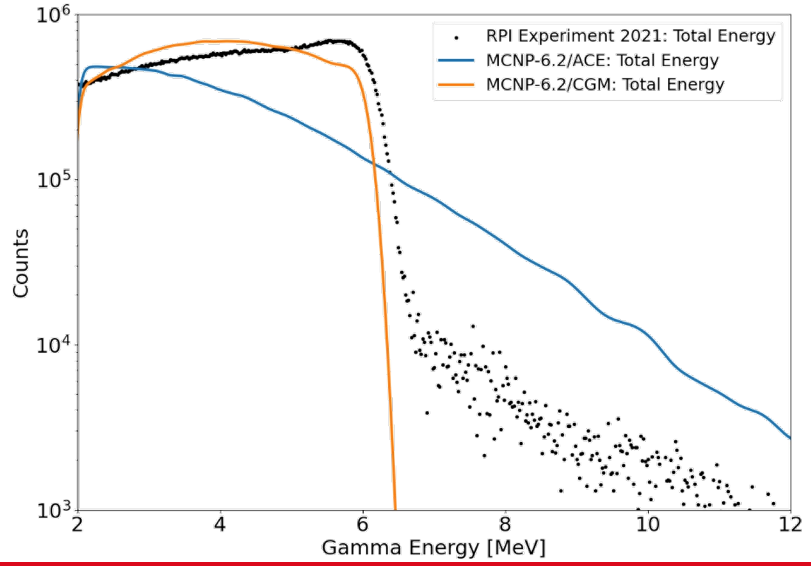
MCNP-6.2/ACE

- Extracts γ-ray data from ACE files (ENDF/B-VIII.0)

MCNP-6.2/CGM

- **C**ascading **G**amma-Ray **M**ultiplicity
- Produces correlated secondary γ-emissions





Updates: Modified `MCNP-6.2`

Step 1: γ-cascades are generated using an external code (i.e., **`DICEBOX`**) and are written to a file

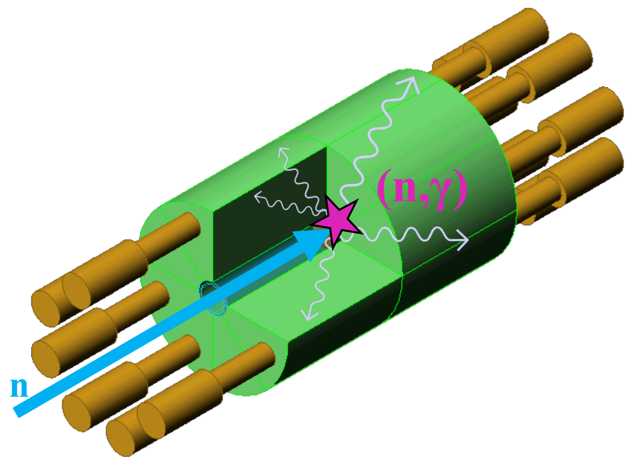
```
6 1.750820 1.641250 2.420890 0.099830 0.133880 0.016270
4 3.739200 1.383080 0.924390 0.016270
5 1.077170 3.693640 0.816570 0.072930 0.402630
4 3.073690 1.329380 1.257240 0.402630
9 3.352750 1.874900 0.095160 0.092480 0.081960 0.074270 0.047810 0.173210 0.270400
5 1.523820 2.843460 1.102700 0.190330 0.402630
7 1.167430 2.036980 1.306060 1.283420 0.118900 0.133880 0.016270
7 2.718790 1.697300 0.732220 0.645580 0.118900 0.133880 0.016270
5 3.656540 2.156420 0.099830 0.133880 0.016270
5 2.228480 2.021640 1.662670 0.133880 0.016270
6 1.127790 1.617990 1.222300 1.115140 0.963450 0.016270
6 3.090780 1.588910 1.133270 0.099830 0.133880 0.016270
6 0.699690 2.839370 2.254830 0.118900 0.133880 0.016270
6 0.788570 1.263900 1.914530 1.346860 0.346450 0.402630
7 0.917810 2.500300 1.769250 0.625600 0.099830 0.133880 0.016270
5 1.480550 2.052000 2.054830 0.072930 0.402630
8 0.917080 2.426180 1.294120 1.061200 0.114380 0.099830 0.133880 0.016270
5 4.761050 1.032840 0.118900 0.133880 0.016270
```

Number of γ-rays in cascade

Energy of each γ-ray in cascade

Step 2: Run **modified `MCNP-6.2`**, for each capture event:

1. Read in γ-cascade from file
2. Transport γ-cascade through the detector geometry
3. Output an event file to tally γ-energy deposition in detector cells



Step 3: Process the output file using event-by-event analysis including coincidence and compare to experimental data

Validating Nuclear Data: Generate γ-cascades

RIPL-3

Discrete Levels

```
182Ta
  number of levels:                              181
  number of gamma-rays:                          359
  number of levels in a complete level scheme:   58
  number of levels with assigned spin and parity: 8
  neutron separation energy:                     6.062939 [MeV]
  proton separation energy:                      6.316698 [MeV]

------------------------------------------------------------------------------
 NL    EL[MeV]     S/P  F    T1/2[s] Ng s unc              s-info  nd m        p      mode
                                        Nf     Eg[MeV]     Pg           Pe          Icc
------------------------------------------------------------------------------
  1   0.000000    3.0 -1  9.914E+06  0 u                     3-   1 =  1.0000E+02 %B-
  2   0.016273    5.0  1  2.830E-01  1 u                     5+   1 =  1.0000E+02 %IT
                                         1     0.0163  2.326E-05  1.000E+00  4.300E+04
  3   0.097830    4.0 -1             1 u                     4-   0
                                         1     0.0978  1.773E-01  1.000E+00  4.640E+00
  4   0.114313    4.0 -1             1 u                     4-   0
                                         1     0.1143  2.519E-01  1.000E+00  2.970E+00
  5   0.150150    4.0  1             2 u                     4+   0
                                         2     0.1339  3.442E-01  9.947E-01  1.890E+00
                                         1     0.1501  4.405E-03  5.348E-03  2.140E-01
```

Model Parameters

Total level density

```
LDP for BSFG Model
------------------------------------------------------------------------------------------------
  Z   A  El  Io     Bn      Do       Derr      Nlow  Ulow  Ntop  Utop    dW      gamma    ainf     aerr   pairing
                  [MeV]   [keV]     [keV]           [MeV]        [MeV]  [MeV]             [1/MeV]  [1/MeV]  [MeV]
------------------------------------------------------------------------------------------------
 73 182 Ta  3.5   6.063  4.200E+00  3.000E-01   5   0.163   17   0.396  1.17603  0.07240  18.47592  0.125  -0.64220
------------------------------------------------------------------------------------------------

LDP for Gilbert-Cameron Model
------------------------------------------------------------------------------------------------
  Z   A  El  Io    Bn       Do        Derr    Nlow  Ulow  Ntop  Utop    dW      gamma    ainf     aerr   pairing  Ematch    Eo       T
                 [MeV]    [keV]      [keV]          [MeV]        [MeV]  [MeV]             [1/MeV]  [1MeV]  [MeV]   [MeV]    [MeV]    [MeV]
------------------------------------------------------------------------------------------------
 73 182 Ta  3.5   6.063  4.200E+00  3.000E-01   5   0.163   17   0.396  1.17603  0.07642  19.95812  0.135  0.00000  3.57017  -1.32509  0.49664
------------------------------------------------------------------------------------------------

LDP for EGSM Model
------------------------------------------------------------------------
  Z   A  El  Io    Bn       Do          dDo           Esh        +da      a      -da
                 [MeV]    [keV]        [keV]         [MeV]    [1/MeV] [1/MeV] [1/MeV]
------------------------------------------------------------------------
 73 182 Ta  3.5  6.063  0.42000E-02  0.30000E-03  0.22500E+00  0.1147 12.4685  0.1056
------------------------------------------------------------------------
```

GSF

```
Experimental GDR Parameters calculated within standard Lorentzian model (SLO)
--------------------------------------------------------------------------------
  Z  A El Reac  E1     CS1     W1    E2    CS2    W2  E_{min}-E{max} Ref.
               Err     Err    Err   Err    Err   Err                 (see
              [MeV]   [mb]  [MeV] [MeV]   [mb] [MeV]      [MeV]      readme)
--------------------------------------------------------------------------------
--------------------------------------------------------------------------------

Experimental GDR Parameters calculated within modified Lorentzian model (MLO)
--------------------------------------------------------------------------------
  Z  A El Reac  E1     CS1     W1    E2    CS2    W2  E_{min}-E{max} Ref.
               Err     Err    Err   Err    Err   Err                 (see
              [MeV]   [mb]  [MeV] [MeV]   [mb] [MeV]      [MeV]      readme)
--------------------------------------------------------------------------------
--------------------------------------------------------------------------------

Theoretical Predictions of GDR Parameters
----------------------------------------------------
  Z   A El    Eta    E1     G1     E2     G2
                   [MeV]  [MeV]  [MeV]  [MeV]
----------------------------------------------------
 73 182 Ta  1.230  12.28   2.96  14.85   4.81
----------------------------------------------------
```

ENSDF

Thermal Capture Primary Intensities

^{181}Ta(n,γ) E=thermal 1979Va10,1971He13,1974An12 (continued)

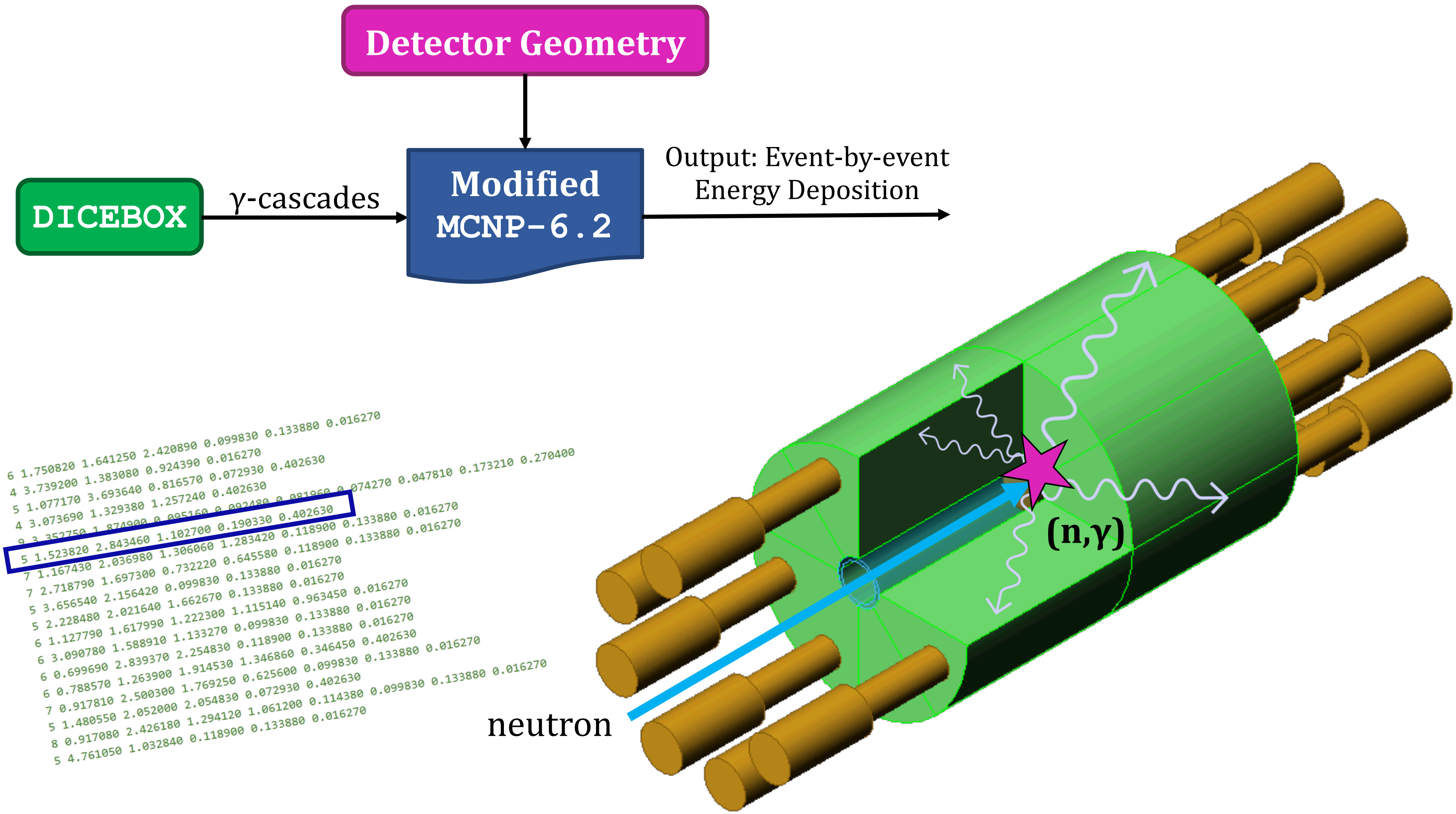
γ(^{182}Ta) (continued)

E_γ†	I_γ‡h	E_i(level)	J_i^π	E_f	J_f^π	E_γ†	I_γ‡h	E_i(level)	J_i^π	E_f	J_f^π	Mult.[b]
5123.0 5	0.56 19	(6062.92)	$3^+,4^+$	939.634	5^-	5515.7 5	1.13 11	(6062.92)	$3^+,4^+$	547.1030	$(3)^-$	
5147.4 4	0.56 19	(6062.92)	$3^+,4^+$	915.4		5557.4 5	0.50 10	(6062.92)	$3^+,4^+$	505.613	5^+	
5153.0 6	0.69 19	(6062.92)	$3^+,4^+$	909.8		5583.8 6	0.63 13	(6062.92)	$3^+,4^+$	480.036	4^-	
5165.4 5	0.44 13	(6062.92)	$3^+,4^+$	897.5		5665.5 8	0.16 6	(6062.92)	$3^+,4^+$	396.335	(6^-)	[M2,E3]
5181.4 5	0.31 9	(6062.92)	$3^+,4^+$	881.4		5702.1 6	0.25 5	(6062.92)	$3^+,4^+$	360.518	$(3)^-$	
5206.8 5	1.88 19	(6062.92)	$3^+,4^+$	856.052	$(4)^-$	5769.9 5	0.75 8	(6062.92)	$3^+,4^+$	292.9352	5^-	
5227.7 6	0.44 13	(6062.92)	$3^+,4^+$	835.289	3^-	5792.5 5	1.25 13	(6062.92)	$3^+,4^+$	270.4027	2^-	
5245.8 5	2.38 25	(6062.92)	$3^+,4^+$	817.021	$(4)^-$	5812.6 8	0.19 6	(6062.92)	$3^+,4^+$	249.982	$(3)^+$	
5280.6 5	0.56 11	(6062.92)	$3^+,4^+$	782.538	(5^-)	5825.0 8	0.11 5	(6062.92)	$3^+,4^+$	237.2860	5^-	
5343.3 5	2.19 25	(6062.92)	$3^+,4^+$	719.552	$(3)^-$	5889.6 7	0.41 8	(6062.92)	$3^+,4^+$	173.2370	5^-	
5396.6 5	0.44 25	(6062.92)	$3^+,4^+$	666.149	2^-	5912.1 6	0.19 8	(6062.92)	$3^+,4^+$	150.150	4^+	
5402.7 5	0.26 13	(6062.92)	$3^+,4^+$	659.862	$(4)^-$	5948.7 5	0.88 9	(6062.92)	$3^+,4^+$	114.3126	4^-	
5411.9 5	0.44 19	(6062.92)	$3^+,4^+$	651.215	$(4)^-$	5965.0 5	6.3	(6062.92)	$3^+,4^+$	97.8304	4^-	
5434.6 5	0.44 19	(6062.92)	$3^+,4^+$	628.425	5^-	6062.9 5	3.8 2	(6062.92)	$3^+,4^+$	0.0	3^-	
5497.0 5	0.63 13	(6062.92)	$3^+,4^+$	565.693	$(3)^-$							

DICEBOX

γ-cascades

Validating Nuclear Data: Run Modified MCNP-6.2



Comparing Experimental Data to Simulated γ-Spectra

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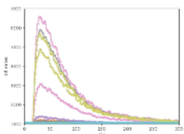
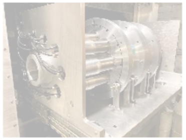
Experiment

Digitize pulse wave for all events on all detectors & obtain the energy of each detected event

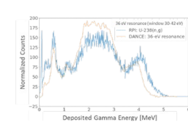
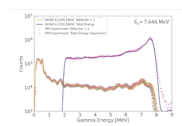
Incident neutron energy
Detector geometry
Sample material composition
NaI γ-energy Resolution

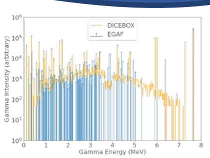
Modified MCNP-6.2

Event-by-event Energy Deposition in detector cells

julia
Processing Code

Compare various results:
- Neutron capture γ-spectra
- γ-multiplicity spectra
- Angular distributions
- Total energy deposition

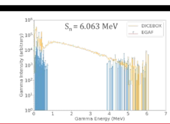
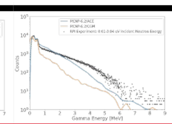


γ-cascades, Probability Distributions, etc…

Nuclear Data Evaluation from ENDF/B-VIII.0, DICEBOX (which uses ENSDF + RIPL) or other source

Identify where there are deficiencies in the nuclear data and suggest where improvements can be made

Evaluate the accuracy of the nuclear data input

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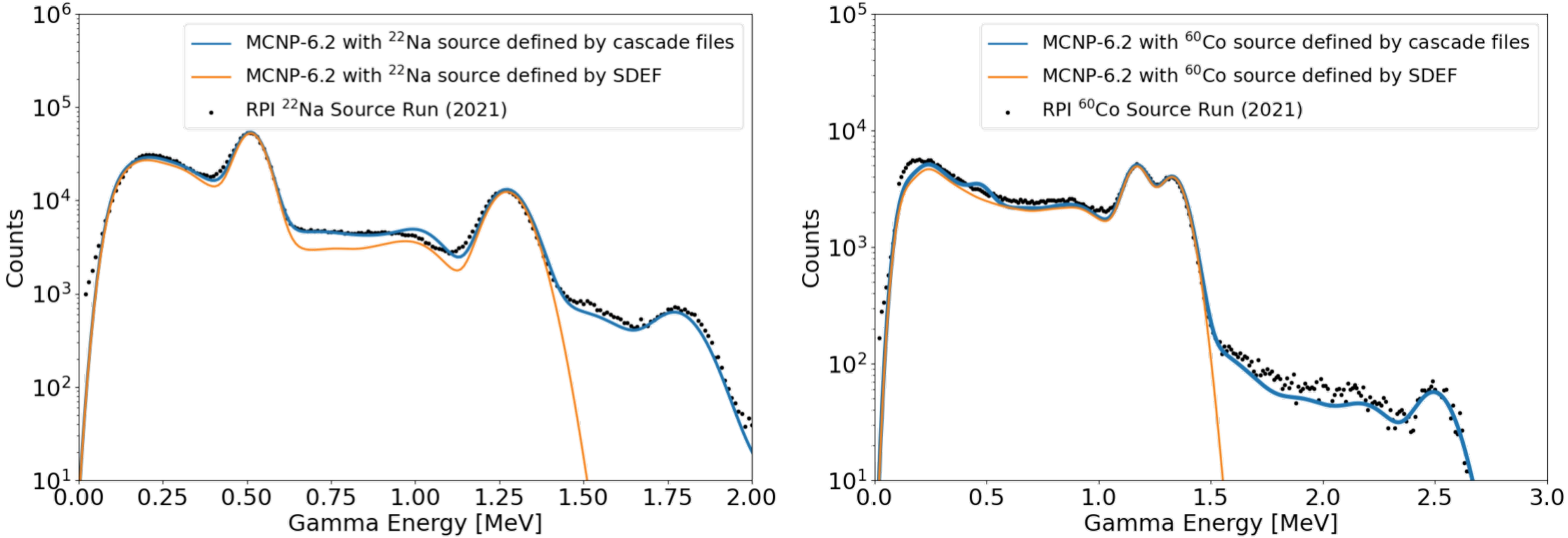
Simulation Validation: Modified `MCNP-6.2`

- Test Cases: ^{22}Na & ^{60}Co coincidence γ-sources
- Modified `MCNP-6.2` reproduces the high energy sum peak resulting from coincidence



Validating Nuclear Data: Benchmark Experimental System

To measure capture γ-spectra accurately, **the detector system needs to be benchmarked by isotopes with well-known capture γ-ray data (like ^{56}Fe)**

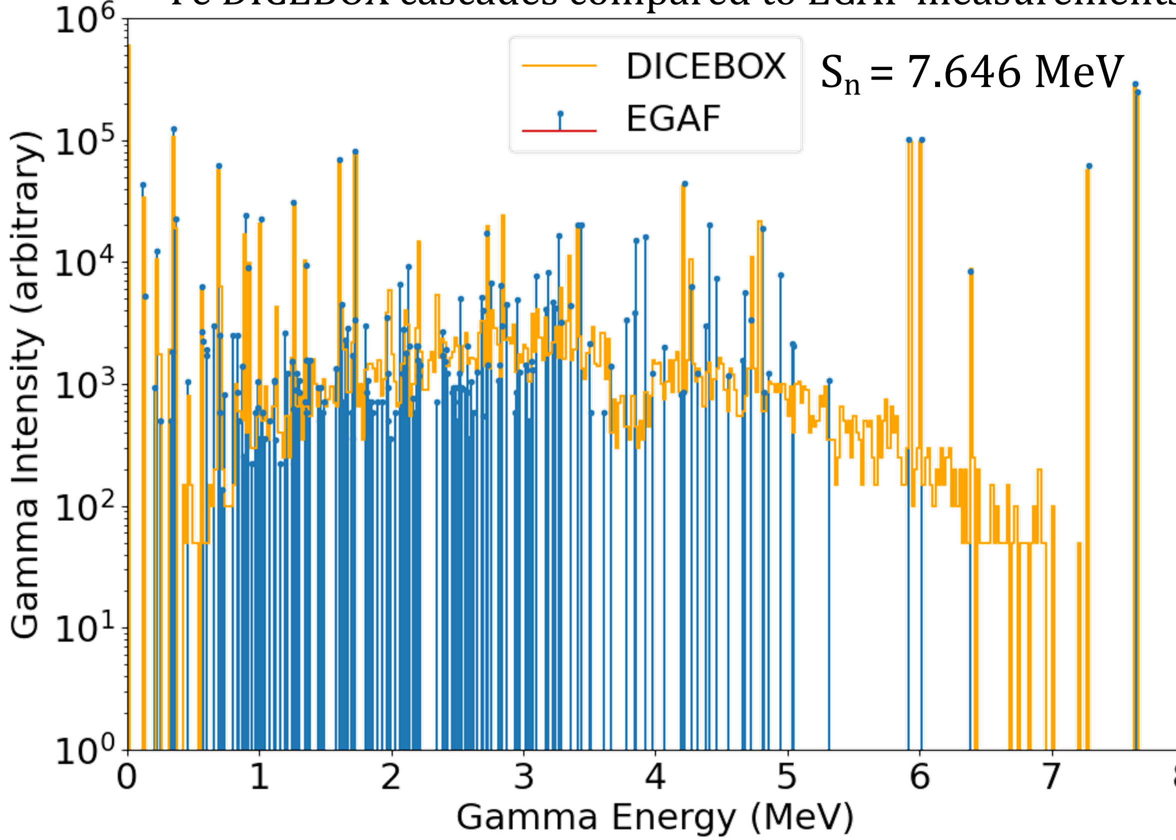
DICEBOX

- Models full γ-cascades using evaluated nuclear data

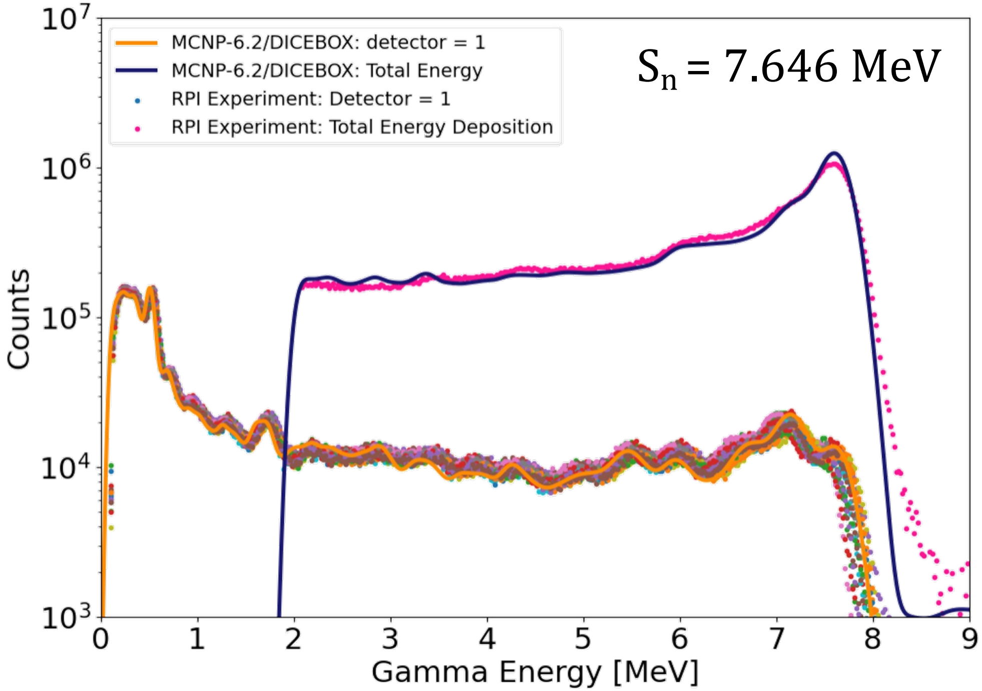
EGAF

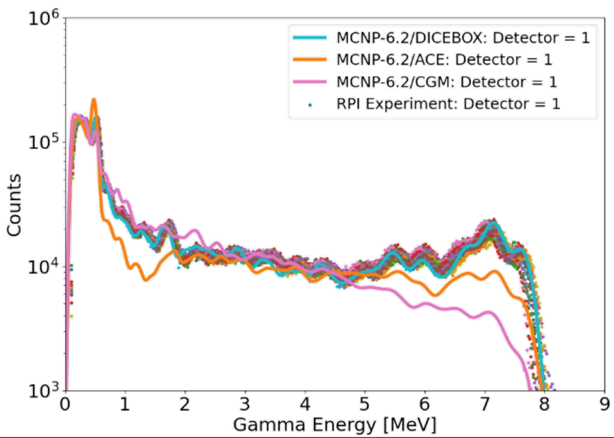
- Shows experimentally measured γ-ray lines (does not necessarily represent the full spectrum)

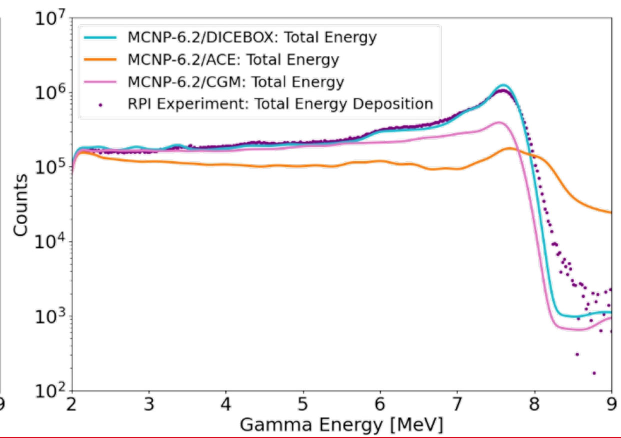
^{56}Fe DICEBOX cascades compared to EGAF measurements



Validating Nuclear Data: ^{56}Fe(n,γ) Benchmark Results





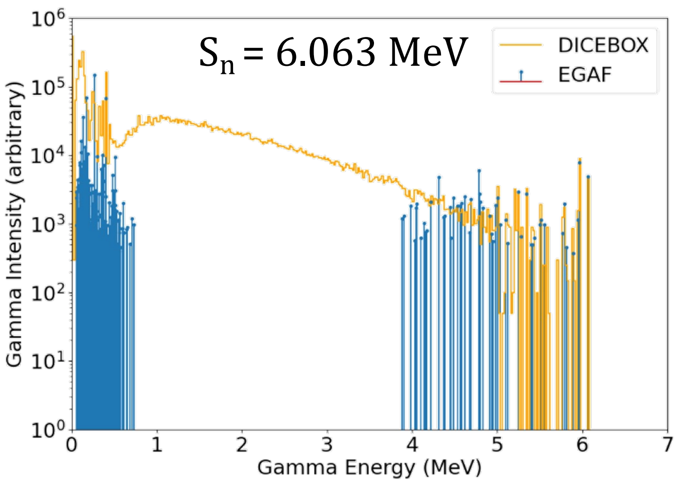


- **Conclusion**: experimental γ-spectra agree with modified `MCNP-6.2/DICEBOX` calculations for isotopes with well-known capture γ-ray data

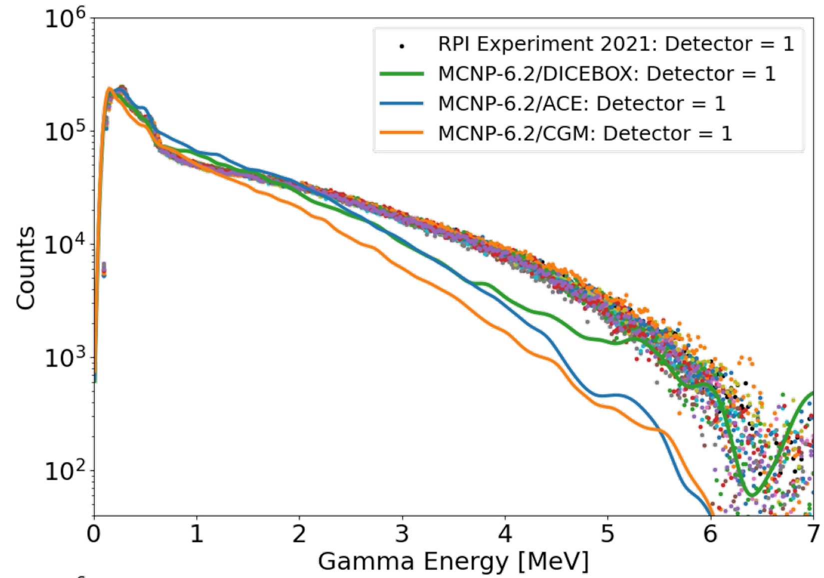
- Results show modified `MCNP-6.2/DICEBOX` calculations perform better than ENDF/CGM

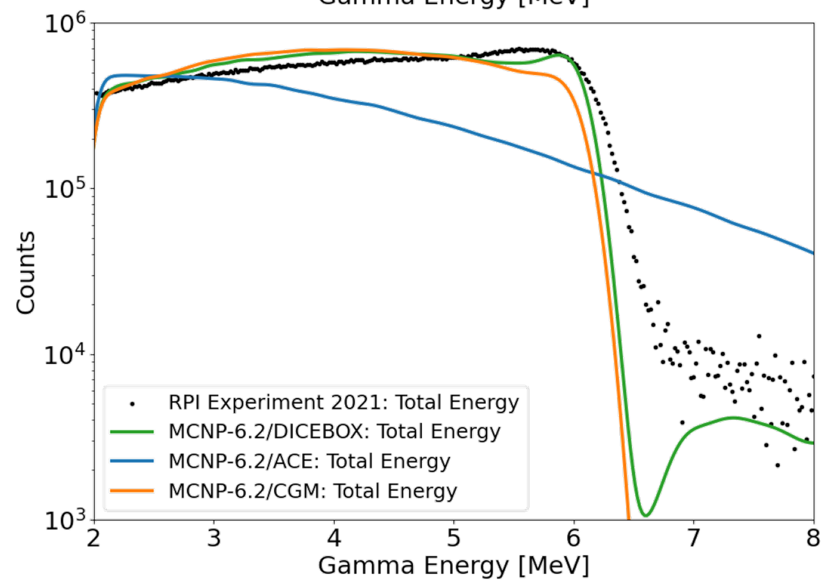
Applications: Deficiencies in evaluated γ-ray data

- ^{181}Ta(n,γ) spectra compared to modified `MCNP-6.2/DICEBOX` simulation



- **Conclusion**: modified `MCNP-6.2/DICEBOX` calculations for isotopes with gaps in capture γ-ray data agree better than ACE/CGM; however, improvements still need to be made

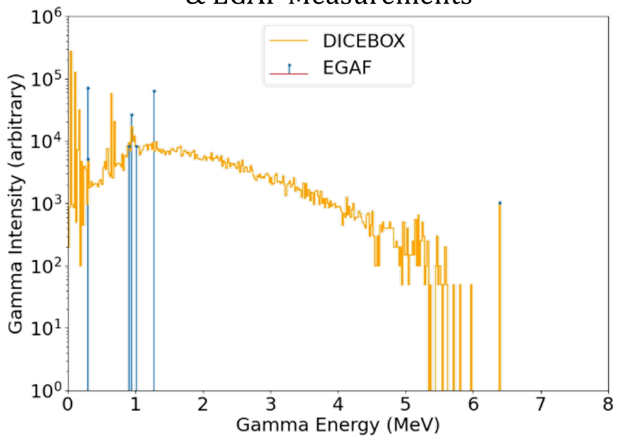




Conclusions + Future Work

- Experimental, simulation and nuclear data methods were validated for the RPI γ-Multiplicity Detector
- When neutron capture γ-cascade data is well-known, the γ-emission spectra can be accurately calculated using the modified `MCNP-6.2/DICEBOX` simulation method.
- RPI γ-Multiplicity Detector system is now ready to analyze neutron capture γ-ray data and provide recommendations for isotopes with deficiencies in γ-ray data (like ^{181}Ta and isotopes of U)

^{235}U **DICEBOX** Capture γ-Cascades & EGAF Measurements



- Looking forward…
  - Determine the accuracy of capture γ-spectra data for several isotopes including ^{55}Mn, ^{59}Co, ^{181}Ta, and ^{238}U
  - Validate any new evaluations using the modified **MCNP-6.2/DICEBOX** forward modeling method and experimental results