

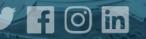


## Overview of the Gamma Rays Induced by Neutrons (GRIN) Project

David Brown, for the GRIN project

October 12, 2023

WINS Workshop, RPI, Troy NY, 10-12 October 2023





## Active interrogation with neutrons is common technique in many applications

- Inelastic (14 MeV) gammas are an obvious need
- Less obvious needs:
  - Capture gammas neutrons moderate in surrounding material
  - Decay gammas these are often background (but could be signal too)

The gamma data in ENDF is woefully deficient



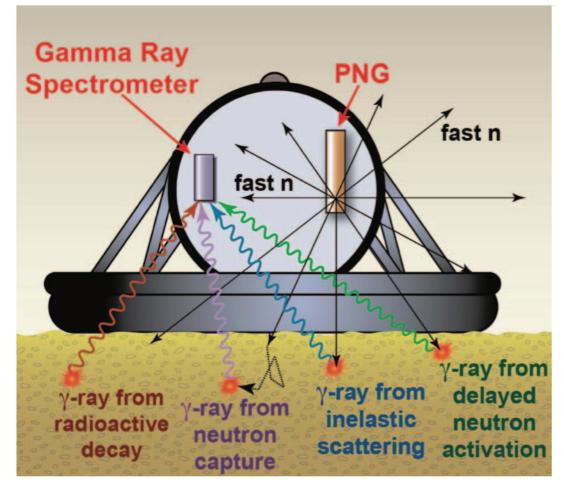


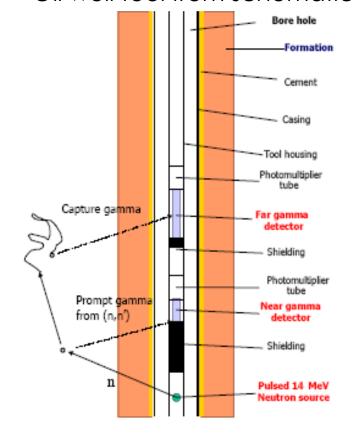
Figure 1: The Bulk Elemental Compositional Analyzer (BECA) instrument proposed for a future NASA mission to Venus. From Fig 1. of [Parsons 2016].

## Material Identification with Neutron-induced Gamma Spectrometry









Oil well tool from schematic



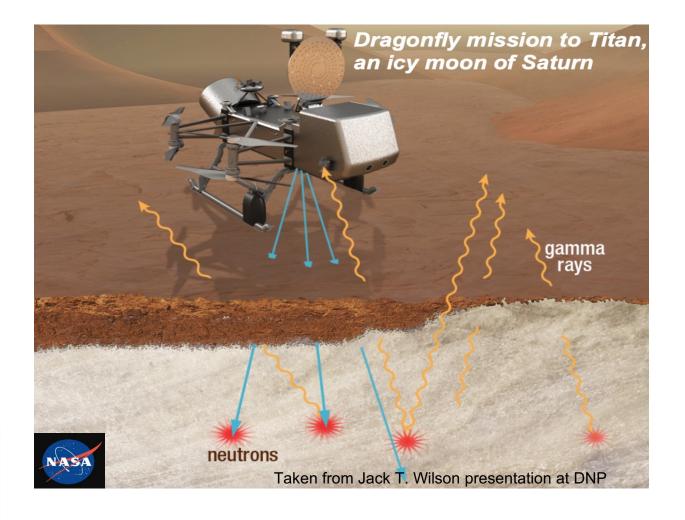




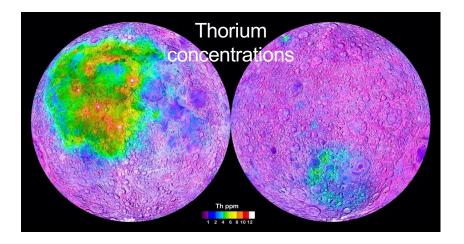
- Developers of these technologies are User Group #1 in this study
- These users need the number of absorption or scattering reactions and the number and energies of emitted gammas to be correct on average over many source neutrons



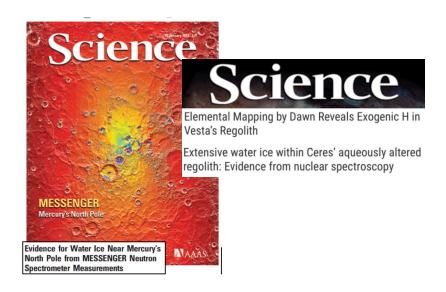
## More cool applications



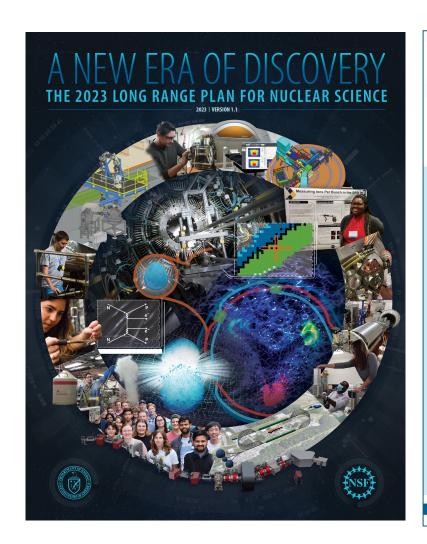
### Lunar Prospector (1998) - gamma rays



### **High Impact Science!!**



## Active Interrogation even got a full page spread in the DOE/NSF Long Range Nuclear Science Plan!



#### 11 | NUCLEAR SCIENCE APPLICATIONS

routinely use PIXE and PIGE to screen for contamiinants. For example, PIGE tests of firefighters' gear revealed that significant quantities of fluorochemicals are being shed from the textiles used in the personal protective equipment during the in-service lifetime of the garment. These measurements help to assess the magnitude of PFAS absorption through the skin and to recommend safety measures to reduce exposure for fire service personnel. In another environmental pollution project, researchers used PIXE to scan soil samples from the area of the George Washington Bridge on the Hudson River in Manhattan for heavy metals. Considerable amounts of lead were found in the soil at the base of the bridge, with decreasing concentration as the distance from the bridge increased. PIXE has been also used to quantify airborne pollutants, such as sulfur, in aerosol samples, helping to assess the effects of acid rain. These valuable data help identify the sources and elucidate the transport, transformation, and effects of airborne and soil pollutants.

#### Sidebar 11.4 Nuclear Physics in Oil Well Logging

Nuclear physics principles are used in gamma-ray logging of oil wells, water wells, and mineral mines. Gamma-ray logging is a method of measuring naturally occurring gamma-ray radiation in rocks or sediment in a borehole or drill hole. Different types of rock emit different amounts and different spectra of natural gamma-ray radiation. For example, shales usually emit more gamma rays than other sedimentary rocks, such as sandstone, gypsum, salt, coal, dolomite, or limestone, because radioactive potassium is a common component in their clay content, and because they absorb uranium and thorium. This difference in radioactivity between shales and sandstones/ carbonate rocks allows the gamma-ray tool to distinguish between shales and non-shales. Non-shales point to potentially hydrocarbon-rich areas. An advantage of the gamma-ray loggers over some other types (nonnuclear) of well loggers is that they work through the steel and cement walls of cased boreholes.

Using the most sophisticated, spectroscopic detectors with good energy resolution allows for spectral logging of gamma rays emitted from natural radioactivity in the rock formation. A spectroscopic logger can be used to map the fraction of elements (e.g., potassium [%], thorium [ppm], and uranium [ppm]) as a function of depth. Furthermore, spectral gamma-ray logs help identify specific clay types, such as kaolinite or illite, and are also useful for calculating the effective porosity of reservoir rock (Figure 1).

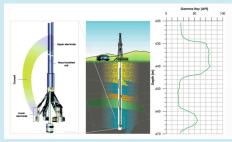


Figure 1. Aloging tool (left), demonstration of a wireline logging operation (middle), and example of a recorded gamma ray log display (right))-bensity logging uses a source of gamma-ray relation from a radiostope, such as cessum-137, and gamma-ray detectors. The detectors are placed away from the source and measure the signal after attenuation by the rocks. Neutrons are also used in oil logging; they have different interaction mechanisms than gamma rays and can provide different information about the formation. Several types of stands which are used in community various ground test of the formation such as the possible SSP jamma-ray stands, which are used to community various ground test of the formation such as the possible SSP jamma-ray.

#### A NEW ERA OF DISCOVERY THE 2023 LONG RANGE PLAN FOR NUCLEAR SCIENCE

#### 11.6 ENERGY-NUCLEAR FISSION AND FUSION TOWARD A CARBON-FREE FUTURE

Continued US economic prosperity requires access to energy resources in sufficient quantities and at low enough cost to sustain an economic growth rate that is globally competitive. Since 2006, the top three energy consumers have been China, the United States, and Russia. The accumulated damage to the planet caused by burning fossil fuels for massive energy production is now clear. Industrialized nations are leading the global campaign to reduce earbon emis-

sions while maintaining economic growth. Their early efforts are based on technological innovations, including energy efficient smart appliances, improved
building and window insulation by engineering and
developing new materials, electrification of vehicles,
and investments in renewable energy sources such
as wind, solar, and hydroelectric. For electrical energy generation, many nations are replacing coal with
natural gas, which is a much cleaner fossil fuel in
terms of heat production per ton of emitted carbon.
In the United States, 38% of the current annual ener-

Neutron-induced gamma-ray radiation measurements (spectroscopy) directly identify chemical elements, allowing precise determination of hydrocarbon content. These advanced systems use active neutron sources and several gamma-ray spectroscopy detectors, both designed by nuclear physicists. The physicists conduct advanced modeling studies and produce algorithms to compute properties of the rock formation, the quantity of hydrocarbons, and how easily they can be extracted.

Current developments of oil well and mineral mine logging systems aim to advance efficiency and precision of spectral gamma-ray identification (Figure 2), including efforts to validate Monte-Carlo simulations using standard nuclear physics software packages such as Geant4. This improved capability translates into measurement speed and accuracy. Higher flux neutron sources and high-efficiency radiation detectors are being developed.

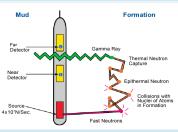


Figure 2. A generalized representation of a neutron logging tool for oil well logging [S88].

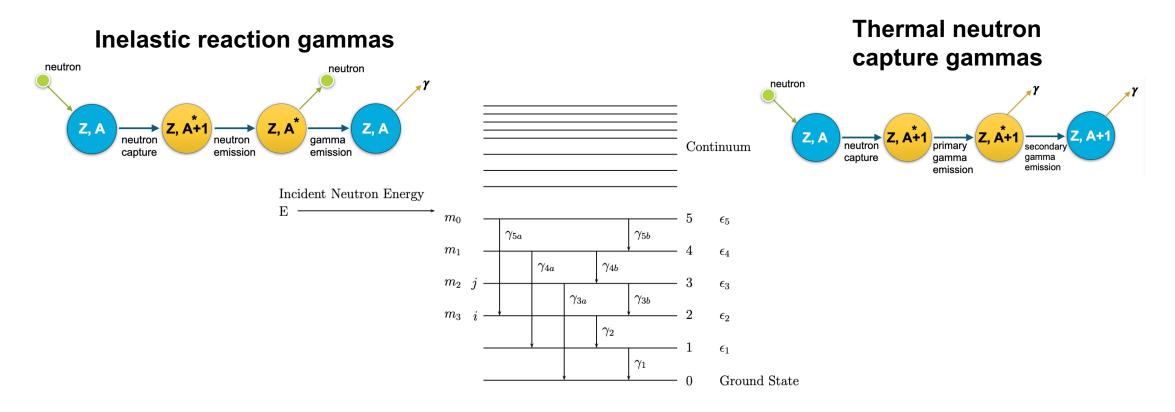
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# Although we are "supposed" to do only inelastic, we really need to consider capture

(neutrons moderate after all!)



## Capture and inelastic reactions start differently, but end in a gamma cascade



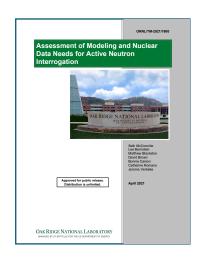
- Inelastic reactions involve target (A) state resonances
- Capture populates compound system (A+1) resonances;
- The **nuclear structure should agree** for the same isotope

### **Materials of interest**

Category	Materials	Elements
Planetary spectroscopy	Soils, Rocks, vehicle housing	C, N, O, Na, Mg, Al, Si, S, Cl, K, Ca, Sc, Ti, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Pb
Controlled Substances	Explosives, Drugs, Chemical agents, Special Nuclear Materials	H, C, N, O, F, P, S, Cl, As, U, Np, Pu
Structural	Aluminum, Steel, 3D printing materials	H, C, N, O, Al, Si, Ti, Cr, Mn, Fe, Ni, Mo, Sn
Intervening, Shielding, Surrounding	Polyethylene, Water, Thermal-neutron absorbers, Lead, Tungsten, Concrete	H, Li, Be, B, C, O, Na, Mg, Si, K, Ca, Fe, Cd, Sb, W, Pb, Bi
Detectors	Organic scintillators, Inorganic scintillators, Semiconductors, Detector housing, Photomultiplier tubes (PMTs)	H, He, C, O, Na, Al, Si, Cl, Ar, Ni, Ge, Br, Kr, I, Xe, Cs, La, Gd, Bi
Sources	Housing, Source reaction elements	Li, Be, Al, Cr, Fe, Ni, Cu, Pu, Am



## Two (general) use cases as articulated by S. McConchie, et al.



### **Traditional**

- One detector
- Coarse binned spectrum or high resolution spectrum with specific lines

### **Event by event**

- Multiple detectors
- Coincident events
- Gate on one gamma given observation of another in a time window

Users may be analyzing data or simulating experiment with transport code



## However...

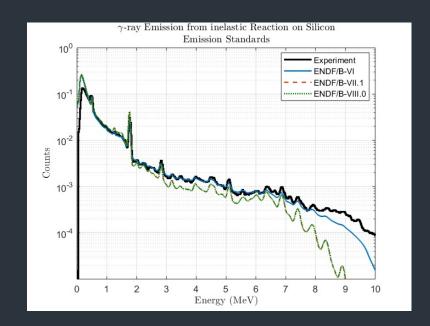


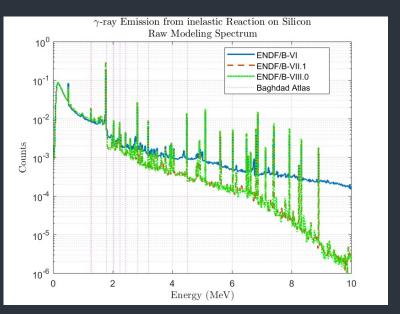
### Silicon Inelastic

Use of natural compound in ENDF/B-VI, Si-28 afterward

Totally different response between ENDF/B-VI and newer releases

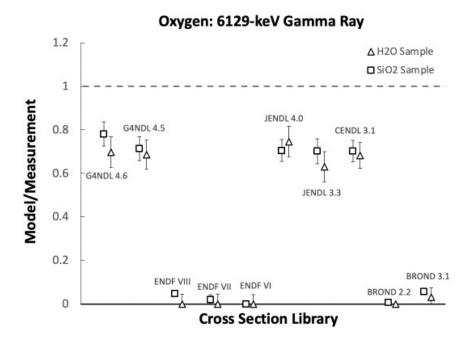
ENDF/B-VI in better agreement with our experimental results above 2 MeV







### This is just the tip of iceberg



No acceptable cross section library (agreement for two separate measurements)

**Summary Results** 

IIIai '	y I`	762	uit								
•		Gamma			Sir	nulation/	Measure	ment Rati	0		
		Ray (keV)	G4NDL 4.6	G4NDL 4.5	ENDF VIII	ENDF VII	ENDF VI	JENDL 4.0	JENDL 3.3	CENDL 3.1	BROND 3.1
	С	4438	1.40±0.03	1.36±0.03	1.34±0.03	1.37±0.03	1.30±0.03	1.47±0.03	1.38±0.03	1.41±0.03	1.38±0.03
	0	6129	0.78±0.06	0.71±0.05	0.05±0.01			0.71±0.05	0.70±0.05	0.70±0.70	0.06±0.01
	Na	440	1.13±0.03	0.45±0.01	0.25±0.01	0.25±0.01	0.25±0.01	1.26±0.03	1.26±0.03		1.17±0.03
		1634	1.92±0.03	1.73±0.17				1.66±0.02	1.69±0.02		2.06±0.03
	Mg	1369	1.42±0.02	1.42±0.02	1.41±0.02	1.41±0.02		1.40±0.02	1.40±0.02	0.86±0.02	1.42±0.02
		843	1.22±0.01	1.07±0.01	1.09±0.01	1.10±0.01	1.11±0.01	1.09±0.06	1.05±0.01	1.05±0.01	1.11±0.01
	Al	1014	1.47±0.01	1.32±0.01	1.31±0.01	1.31±0.01	1.30±0.01	1.22±0.08	1.22±0.00	1.20±0.00	1.31±0.01
Library		2211	1.21±0.01	1.18±0.01	1.18±0.01	1.12±0.01	1.12±0.01	1.01±0.01	0.98±0.01	0.94±0.01	1.14±0.01
Accuracy	Si	1779	1.05±0.02	1.12±0.02	1.13±0.02	1.13±0.02	1.13±0.02	0.07±0.00	1.07±0.02	1.13±0.02	1.13±0.02
Within 5%	S	2232	1.31±0.01	0.78±0.01		0.78±0.01	0.80±0.01	0.79±0.01	0.79±0.01		0.80±0.01
Within 5-10%	Cl	1763	0.99±0.01	1.02±0.01	1.03±0.01	1.02±0.01	1.02±0.01				1.10±0.02
Within 10-20%	Ca	3736	1.00±0.04				0.06±0.01		1.12±0.04	0.04±0.01	
Diff. >20%	Ti	983	1.07±0.03	1.06±0.03	1.06±0.03	1.05±0.03		1.07±0.03	1.08±0.03	1.09±0.03	1.05±0.03
"" = No Peak		846	0.88±0.01	0.94±0.01	0.99±0.01	0.94±0.01	0.94±0.01	0.95±0.01	0.95±0.01	0.90±0.01	1.06±0.02
in Model	Fe	1238	0.71±0.03	0.80±0.03	0.83±0.03	0.81±0.03	0.77±0.03	0.85±0.03	0.87±0.02	0.67±0.03	0.75±0.09
		1408	1.14±0.07	0.91±0.06	0.89±0.06	0.83±0.06	0.78±0.06	0.94±0.06	0.92±0.05	0.88±0.06	1.27±0.19
		1099	1.28±0.04	1.30±0.04	0.93±0.04				0.88±0.04		0.84±0.05
		1190	1.13±0.02	1.15±0.02	1.08±0.02				0.85±0.02		0.86±0.02
	Co	1292	1.31±0.06	1.32±0.05	1.93±0.05				1.40±0.06		1.37±0.07
		1459	1.71±0.04	1.67±0.04	0.86±0.03				0.67±0.03		0.65±0.03
		1481	1.24±0.06	1.20±0.05	1.02±0.05				0.89±0.05		0.95±0.07
	Ni	1332	1.02±0.01	1.11±0.02	1.03±0.01	1.10±0.02	1.09±0.01	0.91±0.01	0.90±0.01	1.05±0.01	1.00±0.01
	141	1454	0.84±0.02	0.87±0.02	0.93±0.02	0.89±0.02	0.87±0.02	0.73±0.02	0.72±0.01	0.99±0.02	0.86±0.01

GEANT4 simulations of Cf source irradiating slugs of materials. Plot & table from P. Peplowski, et al.



### **Intended Goals**

For traditional user: just fix the ^%#@\$ evaluations

For event-by-event user: need to rethink the API & what data we store in an evaluation

## Either way, need to correctly model the reaction, incorporating all experimental knowledge

- Levels and gamma branchings in ENSDF
- Thermal gammas in ENSDF and/or EGAF
- Thermal capture cross sections in the Atlas of Neutron Resonances

Start with a gap analysis to help us focus our efforts!



### Gap analysis

- Compared level schemes between ENDF, RIPL and ENSDF
  - In most cases ENDF needs minor tweaks
  - Cannot fix cross sections, so cannot fix big problems
  - 170, for example, is a BIG PROBLEM
- Compared primary gammas in ENDF, ENSDF & EGAF
  - Also have thermal capture cross section from the Atlas of Neutron Resonances
- No easy way to check capture spectrum above thermal



BNL-224447-2023-INRE

The current status of inelastic and capture Gamma-ray production evaluations in translated ENDF-VIII.0 GNDS files and recommended remediation actions

E Chimanski

May 2023

Nuclear Science and Technology Department

Brookhaven National Laboratory

#### U.S. Department of Energy

USDOE Office of Science (SC), Nuclear Physics (NP) (SC-26)

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https://www.osti.gov/biblio/1983773/

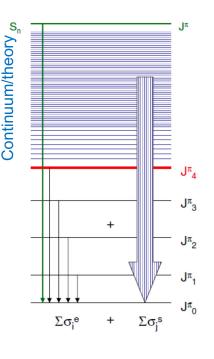


## Thermal gammas

Total (n,  $\gamma$ ) cross section is :

$$\sigma_0 = \sum_{k=1}^P \sigma_{\gamma_k}^{\mathsf{primary}} = \sum_{i=1}^N \sigma_{\gamma_{i0}}^{\mathsf{expt}} (1 + lpha_{i0}) + \sum_{j=1}^M \sigma_{\gamma_{j0}}^{\mathsf{sim}},$$

- $P_0$  is the population per neutron capture of the GS with  $\sum \sigma_{\gamma_j}^{sin}$  obtained from the simulation (continuum);
- with  $\sum \sigma_{\gamma_{j0}}^{\mathsf{sim}} = P_0 \sigma_0$ ;



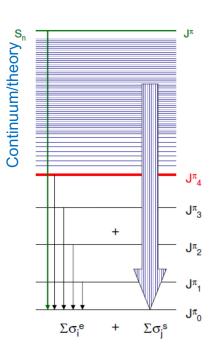
- Exp (from EGAF)  $^{28}$ Si(n,  $\gamma$ ): 0.1852(23)b;
- From ATLAS:  $\sigma_0 = 0.177(5)$  b.
- This means data is complete.
   Good test for theory?

## Thermal gammas

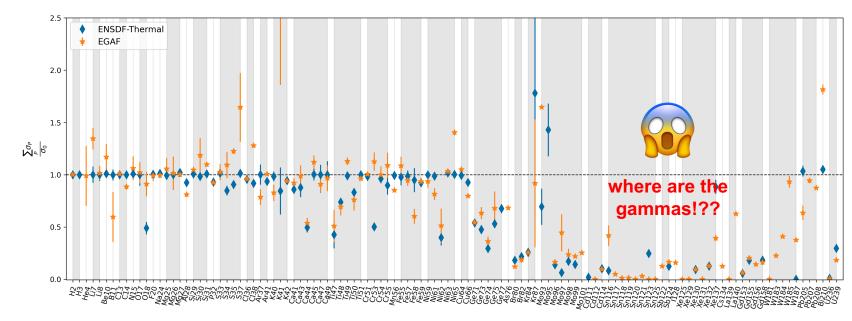
Total (n,  $\gamma$ ) cross section is :

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with  $\sum \sigma_{\gamma_{i0}}^{\rm sim} = P_0 \sigma_0$ ;



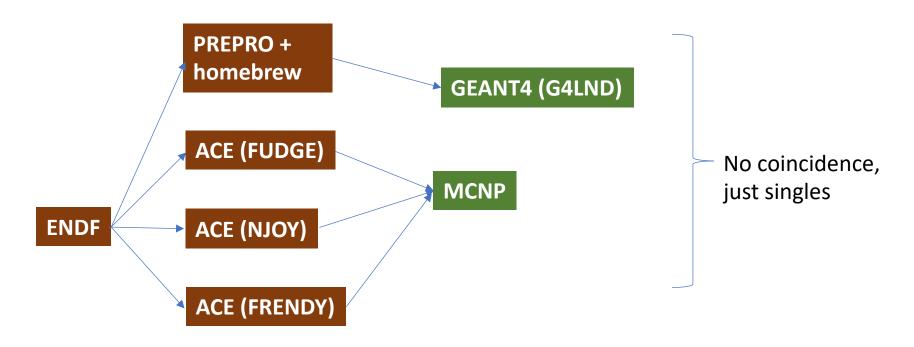
- P<sub>0</sub> is the population per neutron capture of the GS obtained from the simulation (continuum);
- Exp (from EGAF) <sup>28</sup>Si(n, γ): 0.1852(23)b;
- From ATLAS:  $\sigma_0 = 0.177(5)$  b.
- This means data is complete.
   Good test for theory?



## Fixing evaluations



## To understand our strategy to fix, it is useful to understand whole processing chain



### ENDF's myriad of ways to store gammas

#### MF12/MF13/MF14/MF15

- "old way"
- Multiplicity in MF12, angular dists in MF14, energy dists in MF15
- Cannot correlate energy/angle (but no one uses them anyway)
- Primary gammas flagged in MF12
- Has branching ratio table!

#### MF6

- "new way"
- All in MF6
- Energy-angle can be correlated
- Primary gammas flagged in MF6 (but interpolation painful for processing codes)
- No branching ratios

We will embrace the branching ratio!

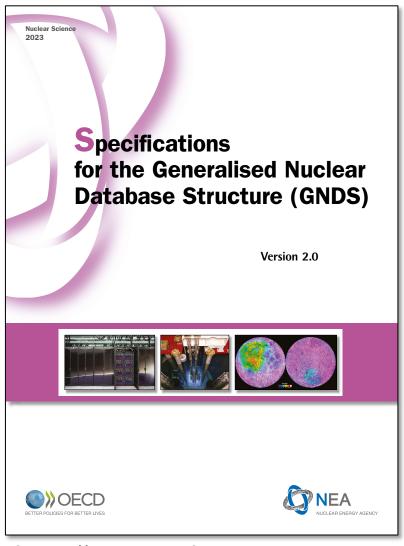


## **GNDS-2.0** has feature that allows us to treat primary gammas using two-boy kinematics

```
oduct pid="photon" label="photon__a">
 <multiplicity>
   <XYs1d label="eval">
       <axis index="1" label="energy_in" unit="eV"/>
       <axis index="0" label="multiplicity" unit=""/></axes>
     <values>1e-5 0.072811 1.5e8 0.072811/\text{values}/\text{XYs1d}/\text{multiplicity}
   <uncorrelated label="eval" productFrame="lab">
     <angular>
       <isotropic2d/></angular>
            .maryGamma value="7199355.51208" domainMin="1e-5" domainMax="1.5e8" finalState="Si29 e1"
```

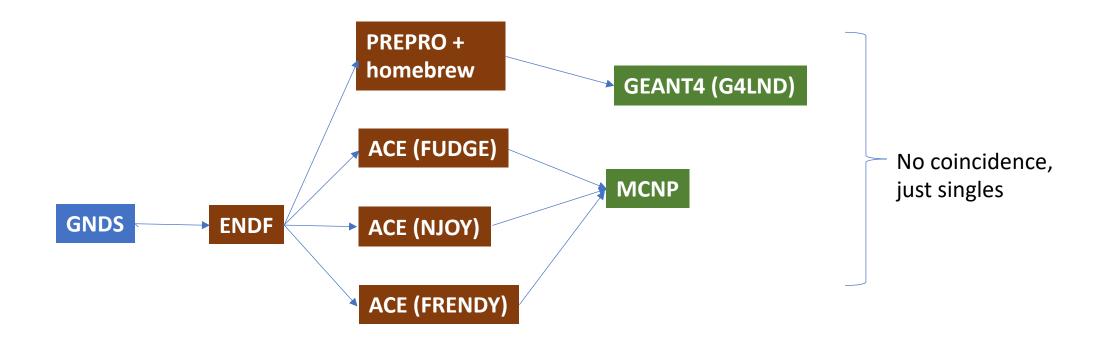
GNDS also has a spot for the levels & branching ratio information for any nucleus





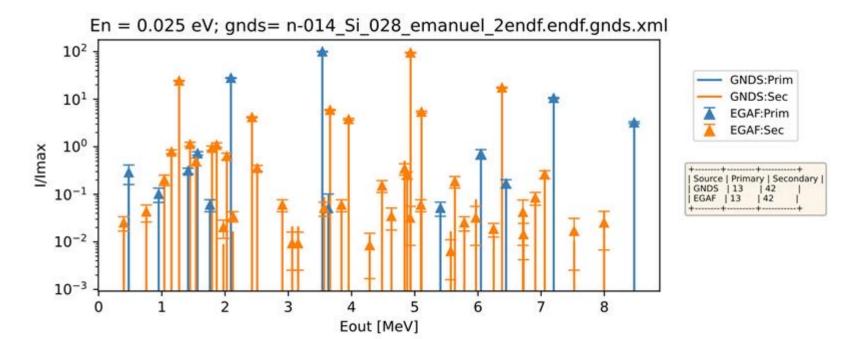
https://www.oecdnea.org/jcms/pl\_85822/specificatio ns-for-the-generalised-nucleardatabase-structure-version-2-0 20

### This suggests we should do this



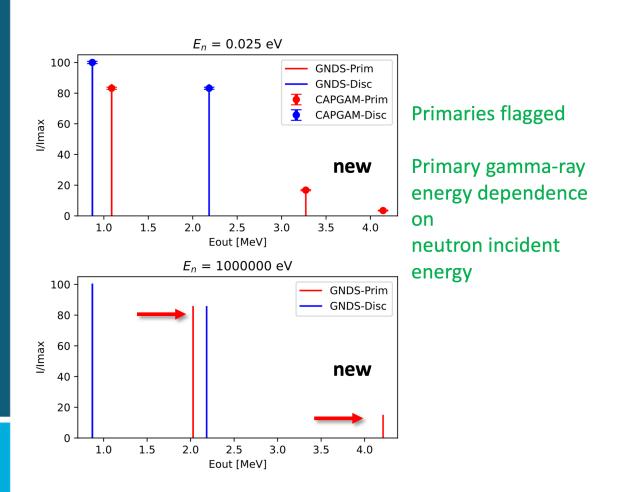
### Developed a formatting code

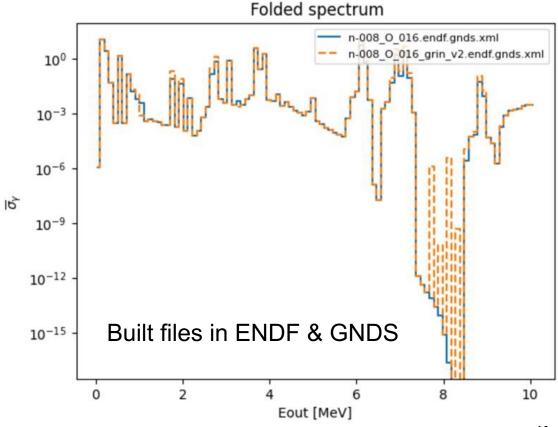
- Reads RIPL and ENSDF-JSON data
- Formats level & gamma data in GNDS-2.0 "properties of particles" (PoPs) data structure
  - Can do this for all residuals in (n, n')-like reactions
  - Can do this for residual in (n, g) reactions too
- Formats capture gamma spectra
  - Formats primary (& secondary if needed) gamma data
  - Working on proper merger to epi-thermal and higher capture spectra





## <sup>16</sup>O: primary gammas now fixed in ENDF/B-VIII.1Beta2 (approved by Mark & Gerry)





## 16O: Working on fixes(not yet Mark & Gerry approved)

#### Problem gammas in 16O evaluation (Peplowski et al. FIXME)

$^{16}O(n,n'\gamma)^{16}O$	6128.6	2 <sup>nd</sup> (3-) → G.S. (0+)	100% E3
<sup>16</sup> O(n,p) <sup>16</sup> N	6128.6	2 <sup>nd</sup> (3-) → G.S. (0+)	100% E3
<sup>16</sup> O(n,n'pγ) <sup>15</sup> N	5269.2	1 <sup>st</sup> (5/2+) → G.S. (1/2-)	100% (M2 + E3)
<sup>16</sup> O(n,n'αγ) <sup>12</sup> C	4438.0	1 <sup>st</sup> (2+) → G.S. (0+)	100% E2

"Missing" from ENDF/B-VIII.0 & VIII.1Beta2. Currently they are in MT22 so coincidences are impossible. Should be coded as breakup reactions in MT51-90. This is straightforward in GNDS.

### Other materials

<sup>12</sup>C – flagged primaries, submitted to ENDF phase1, also GNDS files we can use for testing coincidence modeling

<sup>28</sup>Si – flagged primaries, submitted to ENDF phase1

Other Si – "done"

<sup>32</sup>S – "close"

<sup>207</sup>Pb – experimental ENDF file that uses MT900-999 (n, gamma[i]) format (Thank you Amanda!)



# Rethinking formats and API for e-by-e: discrete levels

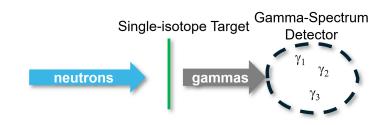


## GEANT4's implementation of gamma emission is so so wrong

Michael Allen & Mauricio Cerda



Emanuel & Andrea (BNL-Staff)



Gamma-ray multiplicity





#### Simple idea:

- Verify how Geant4 uses ENDF/B to simulate neutron capture.
- How that affects the capture gamma-ray simulation



## GEANT4's implementation of gamma emission is so so wrong

Michael Allen & Mauricio Cerda



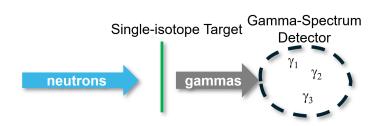
Emanuel & Andrea (BNL-Staff)

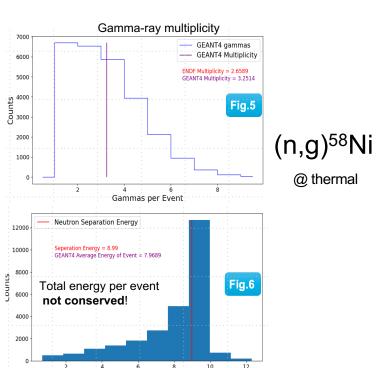
Multiple flags to choose and simulate the reaction differently;
 some provide better results for a few isotopes

#### 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 on event-by-event
- · Gamma-ray multiplicity is affected by the problems above





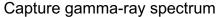


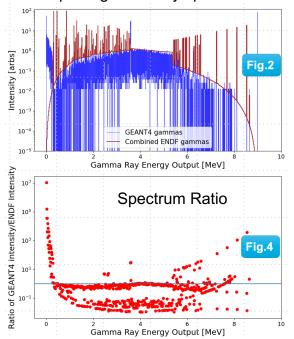
Total Energy of Event [MeV]

### Simple idea:

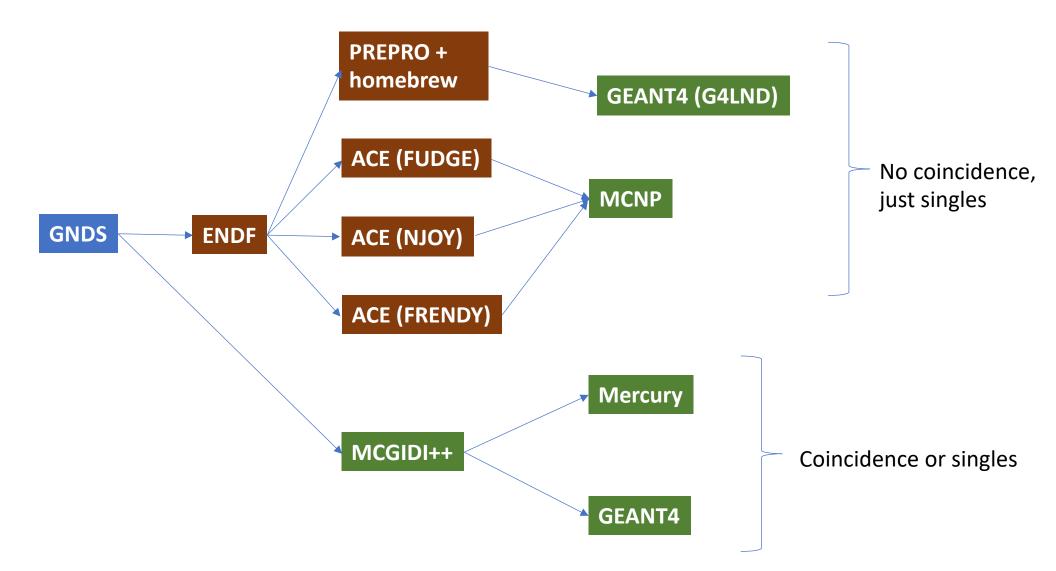
- Verify how Geant4 uses ENDF/B to simulate neutron capture.
- How that affects the capture gamma-ray simulation

GEANT4





## To understand our strategy to fix, it is useful to understand whole processing chain

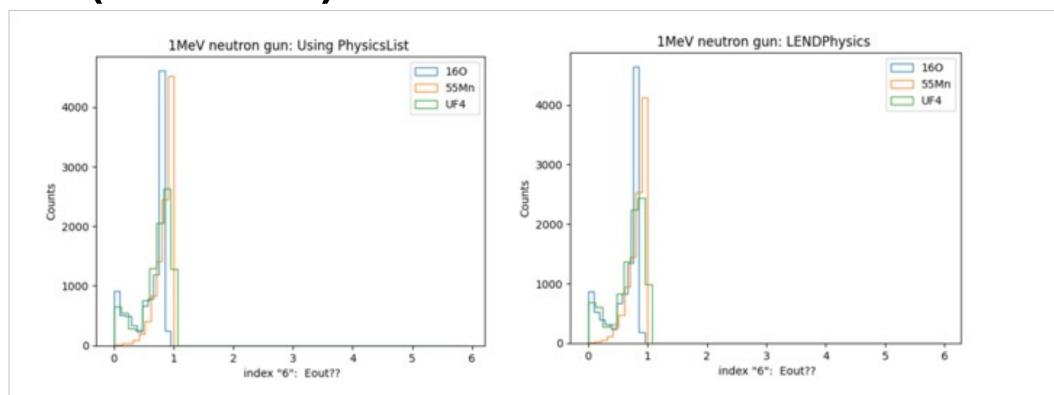


## MCGIDI++ is an open source GNDS-flavored collision kernel

- Part of GIDI+: <a href="https://github.com/LLNL/gidiplus">https://github.com/LLNL/gidiplus</a>
- Open source (MIT license)
- Used in LLNL's unclassified transport codes Mercury (MC) and ARDRA (Sn)
- Data tables in GNDS-2.0
  - XML
  - JSON+HDF5 (for speed!)
- Knows about OpenMP, MPI
- GPU ready (or will be very soon)



# MCGIDI++ is now working as an event generator in GEANT4 using vanilla ENDF data (in GNDS)



We have not tested the event-by-event capability of GIDI yet.

# Rethinking formats and API for e-by-e: pseudo-continuum

(Note, we don't want to re-invent GCM. We want something fast that integrates into existing ENDF evaluations)



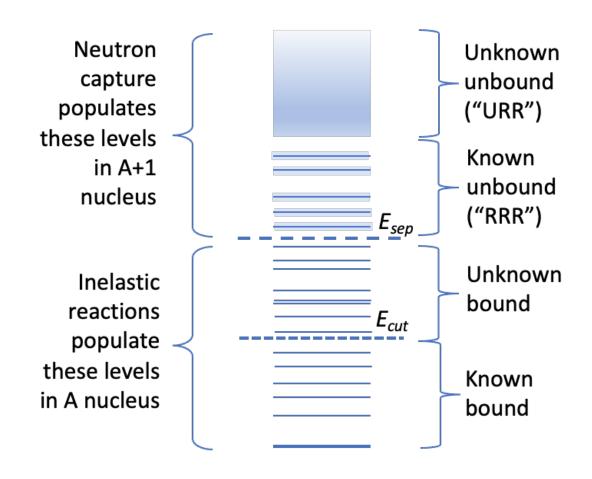
## Reactions are different, but cascades more or less same, differ only in levels

#### Inelastic:

- Cascade from states below separation energy
- We may not know high lying states

#### Capture:

- Direct (primary) gammas first, land below separation energy
- Compound gammas come from states with width
- We do not know high lying resonances
- Cascade like inelastic





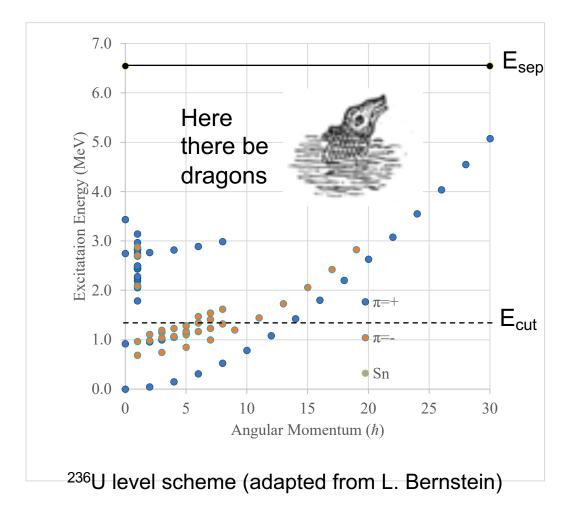
### The essential problem when modeling

The level scheme above a certain energy E<sub>cut</sub> is not well known (if at all)

Above the neutron separation energy E<sub>sep</sub> we have resonance data

We do have information about what happens between E<sub>sep</sub> and E<sub>cut</sub>:

- Some levels & gammas (whatever basic science thought was interesting)
- Thermal capture cross section
- Primary (+secondary) gammas
- Lots of systematics
- Oslo method results





### Pros and Cons of some competing codes

#### **DICEBOX** y decay simulation tool

The FORTRAN tool for simulation of gamma decay from well-defined highly excited nuclear states

- Statistical gamma-decay cascade code:
- FORTRAN:
- Very complex input file:
- Possibility to treat expected fluctuations:
  - transition intensities
  - actual number of levels



Development repo for the nuclear decay code







- Statistical gamma-decay cascade code:
- C++/ROOT library;
- Simple input file:
- Possibility to treat expected fluctuations;
  - transition intensities
  - actual number of levels
- Not developed anymore
- Somewhat easy to handle and modify



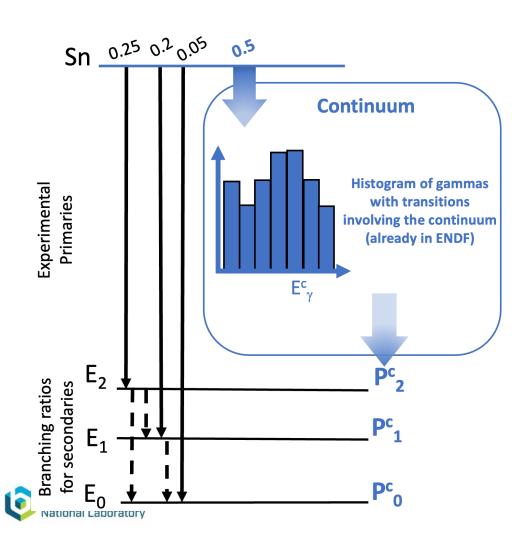
- Reaction code:
- FORTRAN:
- "Simple" input file;
- Modeling of various nuclear reactions including y-cascade
- No treatment of expected fluctuations ("deterministic");
- Fast and widely used
- Can provide a consistent capture cross section with other reaction modes
- Active developers

Single generation of level scheme and transition probabilities

Monte Carlo method to simulate level and width fluctuations but is restricted to y-ray decay

Each of these are too heavy handed for use as an event generator

## Approach #1: Two emissions in Continuum



#### Need:

- Transition probabilities continuum to discrete states
- Histogram of continuum gamma rays

#### • Pros:

- Very little space
- Evaluator has a lot of control

#### Cons:

 Is wrong: not enough gammas can be made

# Approach #2: All levels, all branching ratios

- Needs (i.e. evaluator provides):
  - Simulated level scheme (can be fixed width/spacing bins)
  - Population of all simulated levels
  - Simulated branching ratios out of simulated levels

#### Pros:

- Enables the user to easily reproduce the entire cascade.
- Evaluator makes the choice of best theoretical models and parameterizations to create inputs
- Embedded levels can be incorporated ensure that known discrete and continuum transitions are simulated correctly.

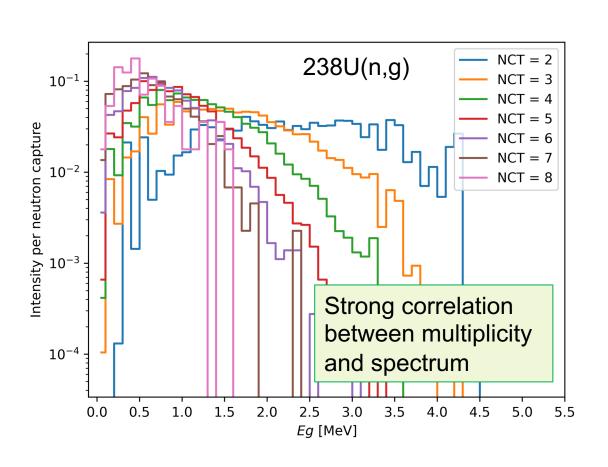
#### Cons:

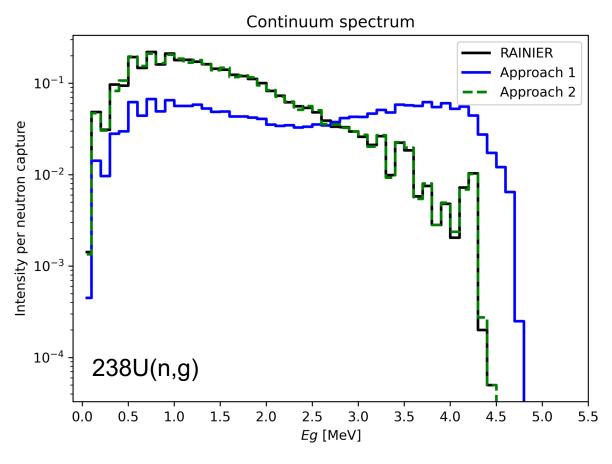
- Lots more data needed
- Transport codes will need to implement cascade (but MCGIDI already does!)



EMPIRE, RAINIER & CoH provide this

### Approach #1 fails for most nuclei





**NCT=Number Continuum Transitions** 

## Validation



Lining up folks to validate tools & evaluations



Lab	POC	Code	Needs coincidence	Details
ORNL	Seth McConchie	GEANT4	Yes	unknown
UTK	Jason Haywood	MCNP	Must check	DT generator
Schlumberger	Marie-Laure Mauborgne*	MCNP	No	DT generator, many materials (proprietary)
JHAPL	Patrick Peplowski*	GEANT4 & MCNP	Yes and No	<sup>252</sup> Cf source, many materials
RPI	Yaron Danon*	MCNP	Yes, event list	RPI ToF, segmented Nal detector: <sup>56</sup> Fe, <sup>55</sup> Mn, <sup>59</sup> Co, <sup>181</sup> Ta, and <sup>238</sup> U
LBNL	Aaron Hurst**	Baghdad Atlas Code	No	Bagdhad Atlas (Fast reactor but soft spectrum)
PNNL	Brian Archambault	GEANT4	YES YES YES	unknown
U. Mass Lowell	Marian Jandel*	N/A (experiment)	Yes	Ge detector, neutrons come from reactor. Cu, Cr, Ni
LLNL	Jo Ressler/Marie- Anne Descalle/Ali Dreyfuss**	Mercury	Yes and No	Computation tests of everything, broomstick, any energy
"GRIN"	"Us"**	MCGIDI++	Yes	Computational broomsticks
LANL	Matt Devlin	N/A (experiment), GEANT?	Yes	unknown
Rež	Roberto Capote*	MCNP	No	MnSO <sub>4</sub> bath, <sup>252</sup> Cf source, gamma spectrum

## Where we are now



### In last year of the project\*

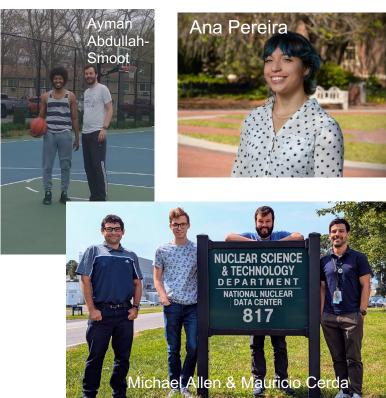
#### To do:

- Pump out evaluations
- NIM article demonstrating how GEANT4/G4LEND stinks and GEANT4/MCGIDI works great
- Develop light weight cascade widget for quasi-continuum/RRR
- Ramp up validation projects
- Continue experimenting with using ML to predict primary gammas (that's another talk)

\*But we are part of 3 follow-on validation projects



#### **Our Interns**



Rest of the GRIN team: E. Chimanski, D. Brown, C. Morse, S. Ota (BNL), A. Hurst (LBNL), B. Beck, C. Mattoon, G. Gert (LLNL), A.Lewis (NNL)

### Publications/Reports/Codes

- E. V. Chimanski, B. Beck, G. Nobre, E. A. McCutchan, G. Gert, C. Morse, L. A. Bernstein, A. M. Hurst, A. M. Lewis, C. M. Mattoon, S. Ota and D. Brown, "A Precise Evaluation of Neutron Induced Gamma Ray Production: Upgrading ENDF, Formatting and Reaction Models", IEEE NSS-MIC-RTSD Conference, 5-12 Nov. 2022, Milan, Italy (2022).
- Aaron M. Hurst, for the GRIN collaboration, "Level density and photon strength function models and their adopted parametrizations for GRIN", LBNL Report LBNL-2001455 (2022)
- GIDIplus v3.25, LLNL Report LLNL-Code-778320 (2022)
- pyEGAF, <a href="https://pypi.org/project/pyEGAF/">https://pypi.org/project/pyEGAF/</a> (2023)
- Aaron M. Hurst et al., pyEGAF: An open-source Python library for the Evaluated Gamma-ray Activation File . Submitted to NIMA (2023)
- E. V. Chimanski, B. R. Beck, L. A. Bernstein, G. Gert, A. M. Hurst, A. M. Lewis, C. M. Mattoon, E. A. McCutchan, C. Morse, G. Nobre, S. Ota, D. Brown, The current status of inelastic and capture gamma-ray production eval-uations in translated endf-viii.0 gnds files and recommended remediation actions, Tech. Rep. BNL-224447-2023-INRE (2023). doi:10.2172/1983773. URL https://www.osti.gov/biblio/1983773



## **Backup Slides**



### **CEA work: Cordero Ramirez & Jouanne**

https://indico.frib.msu.edu/event/52/contributions/981/attachments/597/2268/ND2022\_CORDERO.pdf

#### Inelastic

- Found a mix of MF12 and MF6 data (depending on the MT)
- Very strange
- Is apparently allowed in ENDF format
- Uncommon in JEFF-3.3
- TK (LANL) does this in CoH/Dece

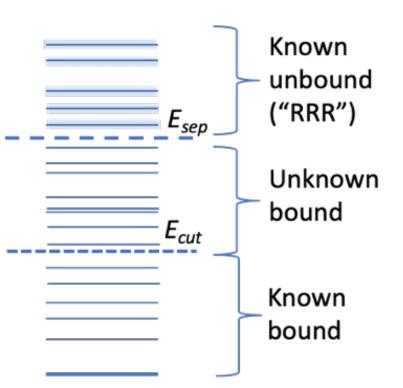
#### Capture

- Use EGAF/Capgam for primaries
- Use RIPL for cascade
- Rescale continuum to get energy balance
- Strangeness with PHITS

Done completely in API, so not in sync with rest of evaluation



# For cascades starting above Ecut, need simulated level scheme



- The evaluator can generate the levels scheme, but need to denote which levels are partly or completely simulated – a simple flag can do the trick in GNDS
- API (GIDI+) can generate the levels. Need:
  - Mean spacing/level density for each J<sup>π</sup>
  - Short range spacing rule (GOE, fixed, ...)
  - Multipolarity of gammas (including mixing)
  - Rule for width sampling
  - Gamma ray strength function



levels

BR's

# Generating levels requires algorithm & GNDS format for parameters

#### Mean spacing/level density

- Constant spacing/temperature
- Gilbert Cameron
- Back Shifted Fermi Gas
- User-specified interpolation table in spacing
- Either specify for each Jpi or give spin & parity distributions

Each require simple GNDS data structure

Parameters given in RIPL

Some are implemented in DICEBOX or RAINIER, all in EMPIRE, TALYS, CoH

#### Short range spacing rule

- Full GOE (realistic)
- Wigner distribution ala AMPX
- Constant (picket fence)
- Random (Poisson, not realistic)

Specify scheme with a flag

Algorithms implemented in Python in FUDGE, some are implemented in DICEBOX or RAINIER



# Generating BR's also requires algorithm & GNDS format for parameters

#### Gamma ray strength function

- Many options in RIPL
- More options in LBNL-2001455
- User-specified interpolation table

## Multipolarity of gammas (including mixing)

#### Rule for width sampling

- Sample from Porter Thomas (realistic, but large fluctuations), needs DOF parameter too
- Just take mean (converges faster)

Each require simple GNDS data structure

Parameters given in RIPL

Some are implemented in DICEBOX or RAINIER, all in EMPIRE, TALYS, CoH

Specify scheme with a flag

Algorithms implemented in Python in FUDGE, some are implemented in DICEBOX or RAINIER

