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

Emanuel Chimanski, for the GRIN project

November 15, 2023

Nuclear Data Week 2023 (CSEWG-USNDP-NDAG)

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

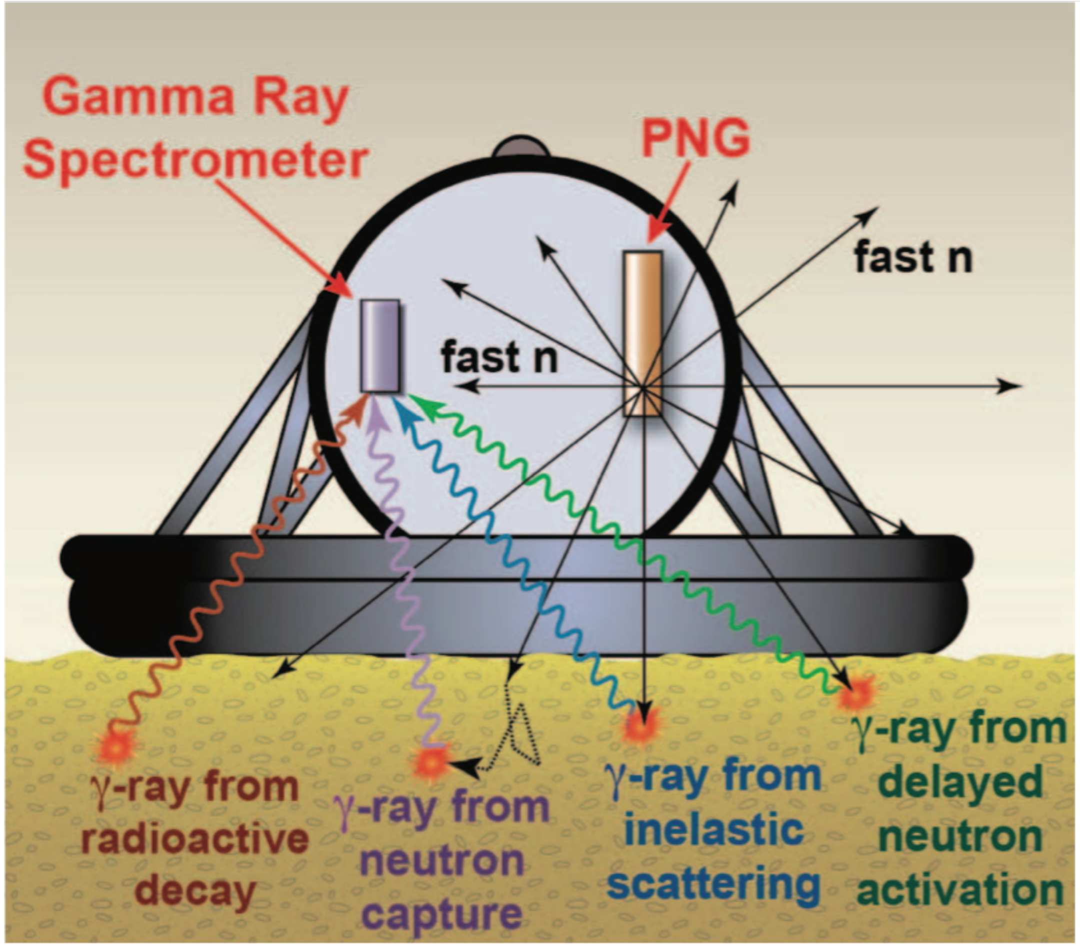

Figure 1: The Bulk Elemental Compositional Analyzer (BECA) instrument proposed for a future NASA mission to Venus. From Fig 1. of [Parsons 2016].

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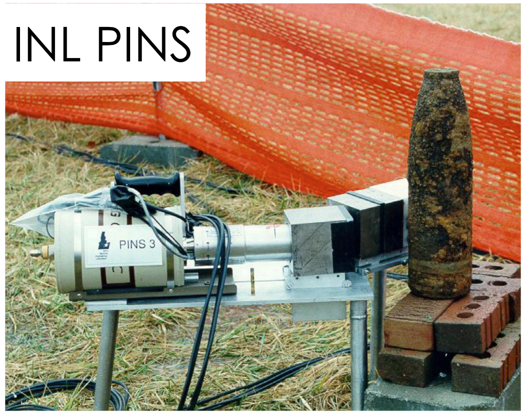
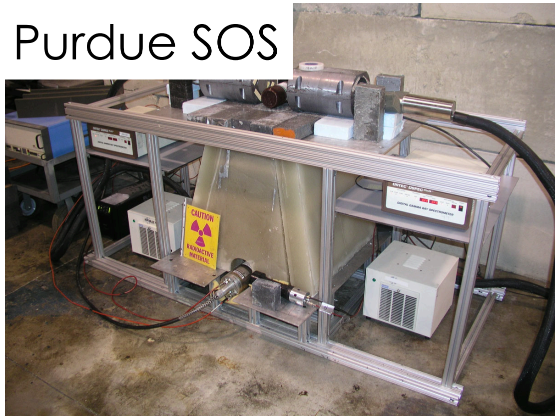
Material Identification with Neutron-induced Gamma Spectrometry

INL PINS



Purdue SOS



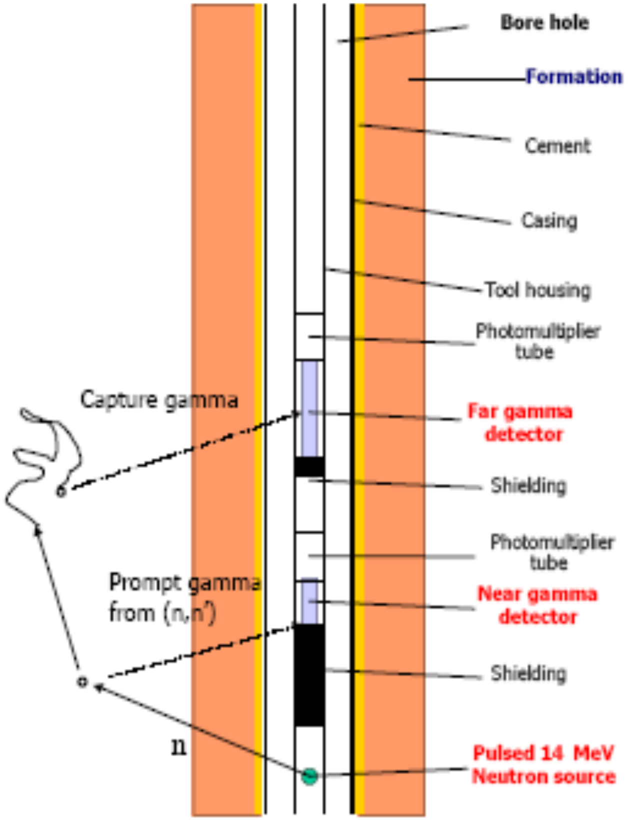
EURITRACK

WKU PELAN

A.C.T.d.o.o. Surveyor

CSIRO NITA

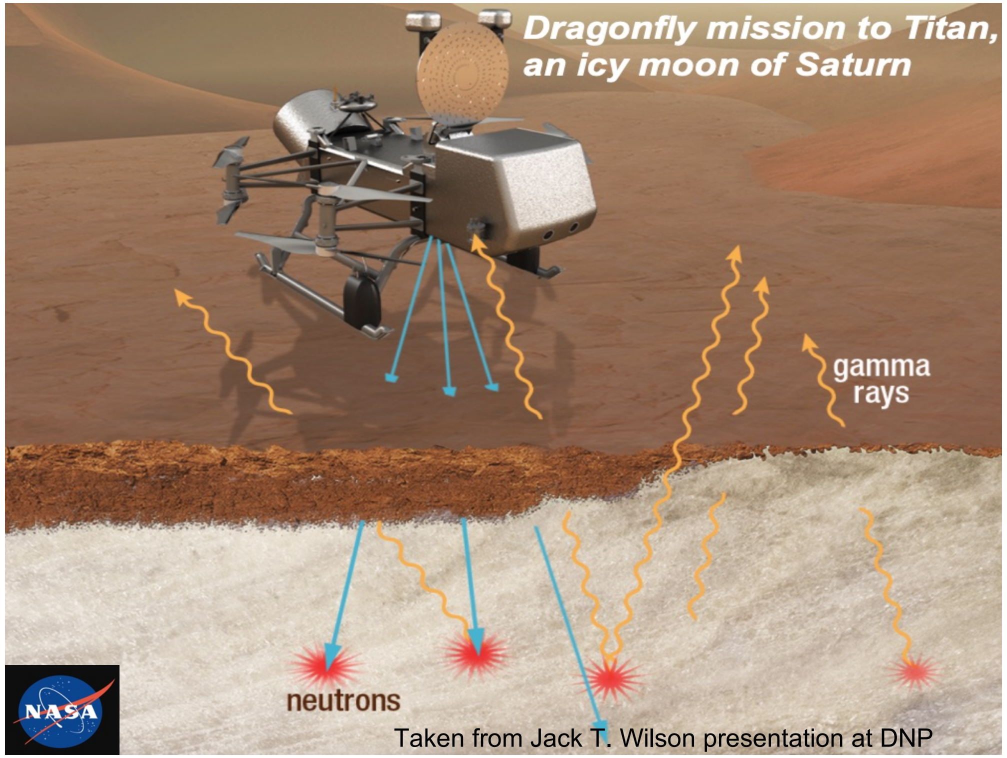
Oil well tool from schematic



- 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

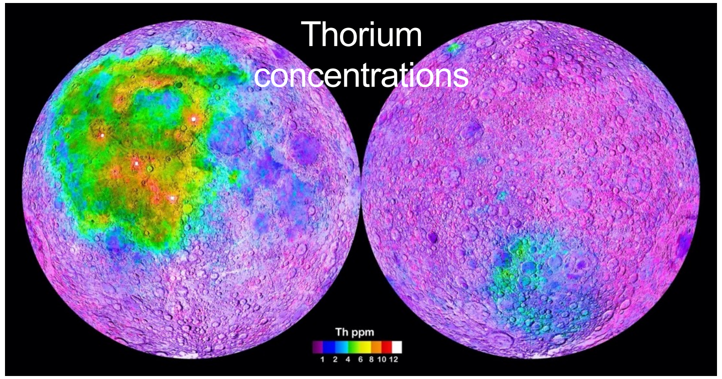
Slide from S. McConchie (ORNL)

More cool applications

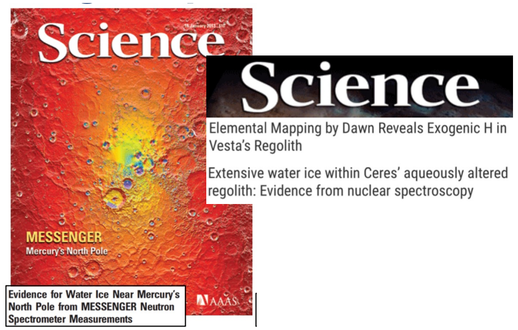


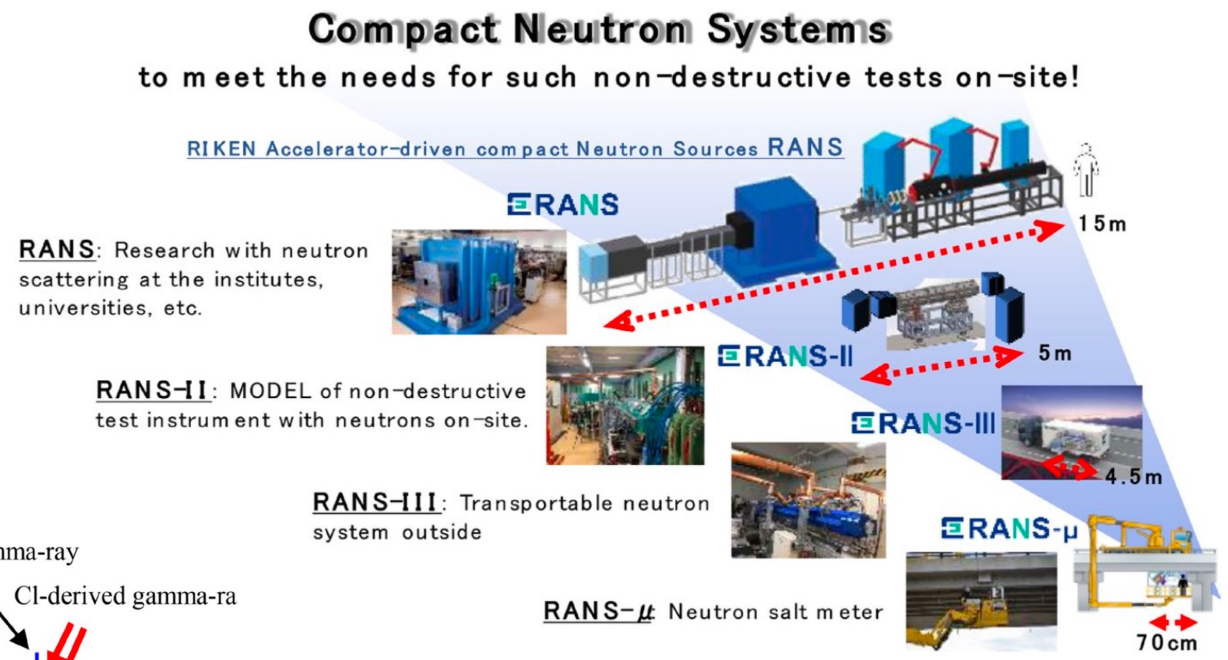
Taken from Jack T. Wilson presentation at DNP

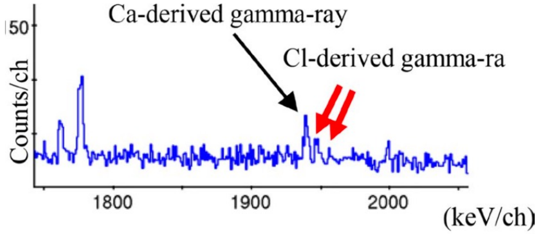
Lunar Prospector (1998) - gamma rays



High Impact Science!!

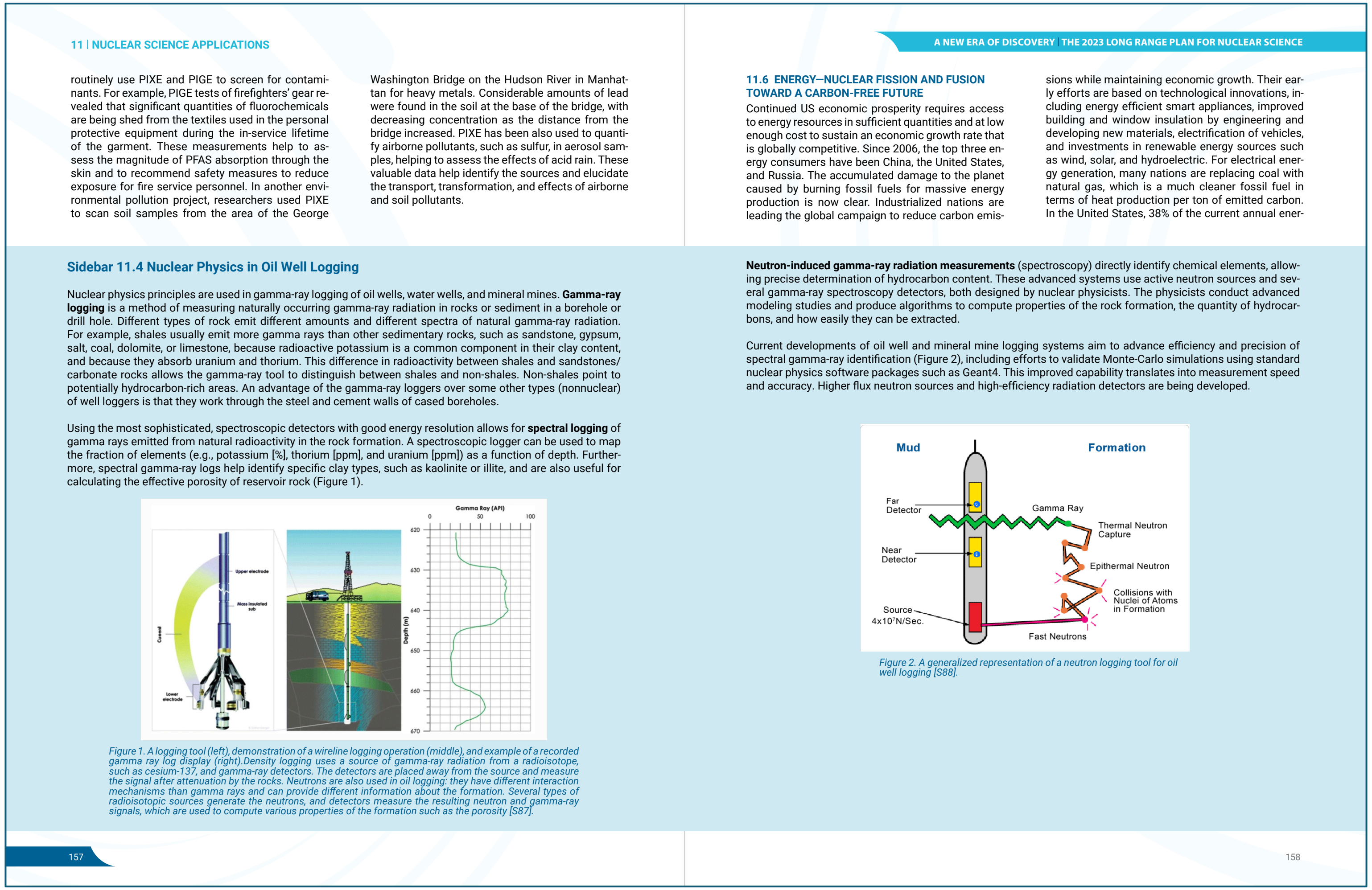






2023 Nuclear Physics News Volume 33/No. 2

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



routinely use PIXE and PIGE to screen for contaminants. 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. A logging tool (left), demonstration of a wireline logging operation (middle), and example of a recorded gamma ray log display (right).Density logging uses a source of gamma-ray radiation from a radioisotope, such as cesium-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 radioisotopic sources generate the neutrons, and detectors measure the resulting neutron and gamma-ray signals, which are used to compute various properties of the formation such as the porosity [S87].

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 carbon emissions 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.

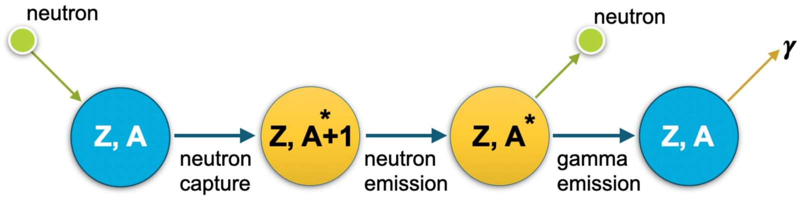
Figure 2. A generalized representation of a neutron logging tool for oil well logging [S88].

Although we are “supposed” to do only inelastic, we really need to consider capture

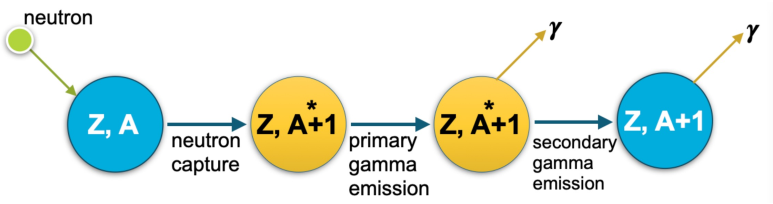
(neutrons moderate after all!)

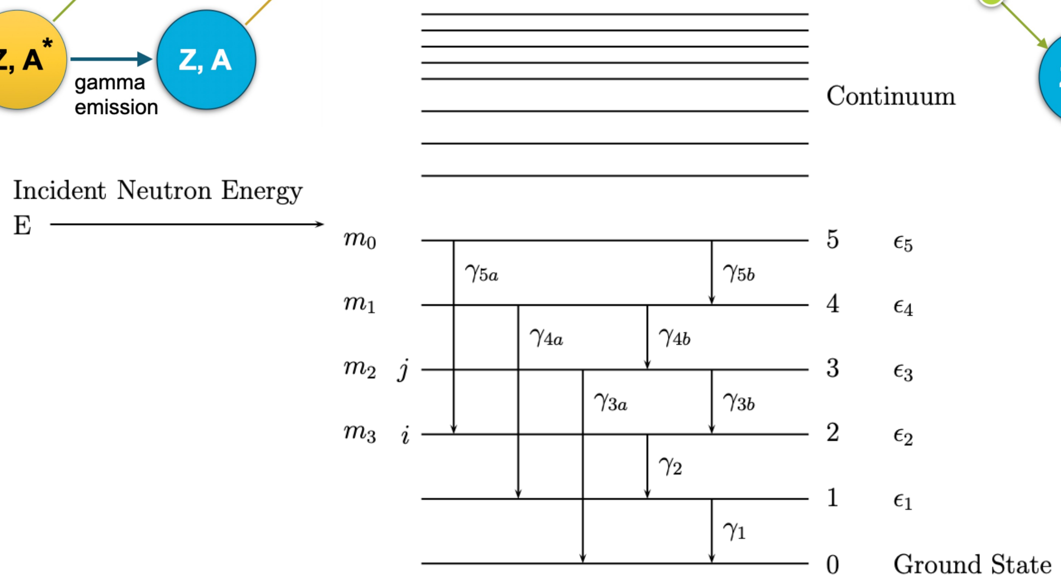
Capture and inelastic reactions start differently, but end in a gamma cascade

Inelastic reaction gammas



Thermal neutron capture gammas



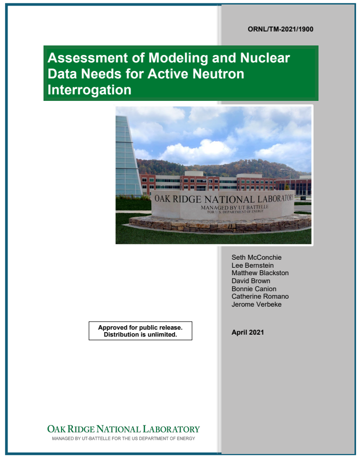


- Inelastic reactions involve target **(A)** state resonances
- Capture populates compound system **(A+1)** resonances;
- The **nuclear structure should agree** for the same isotope

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.*


ORNL/TM-2021/1900

Assessment of Modeling and Nuclear Data Needs for Active Neutron Interrogation

Seth McConchie
Lee Bernstein
Matthew Blackston
David Brown
Bonnie Canion
Catherine Romano
Jerome Verbeke

Approved for public release. Distribution is unlimited.

April 2021

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

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

Brookhaven National Laboratory

However…

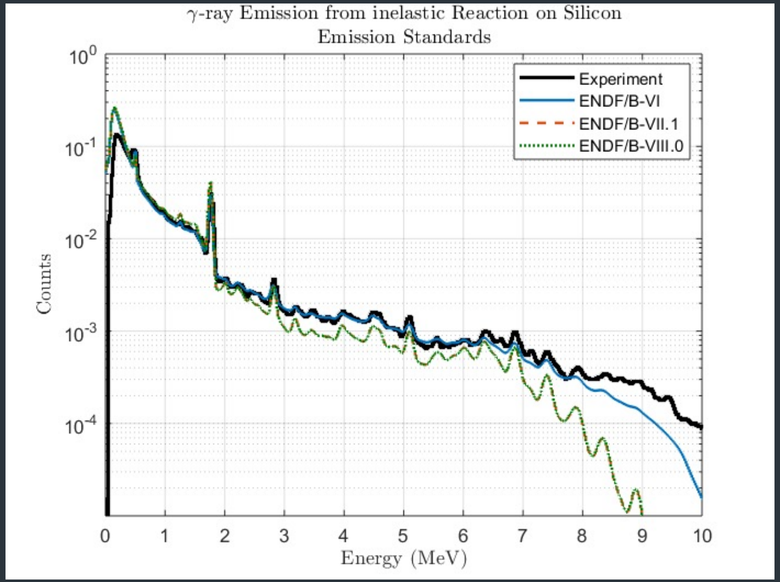
we know ENDF is not perfect
for gamma ray productions

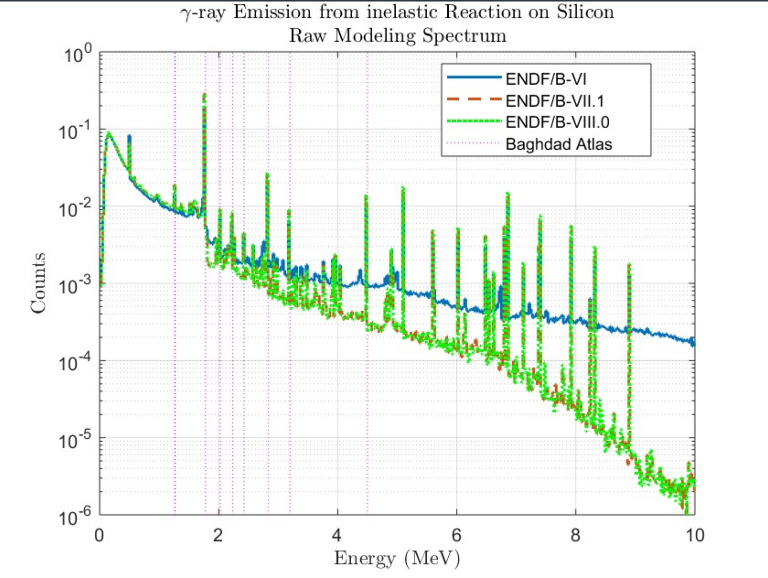
Silicon Inelastic

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

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

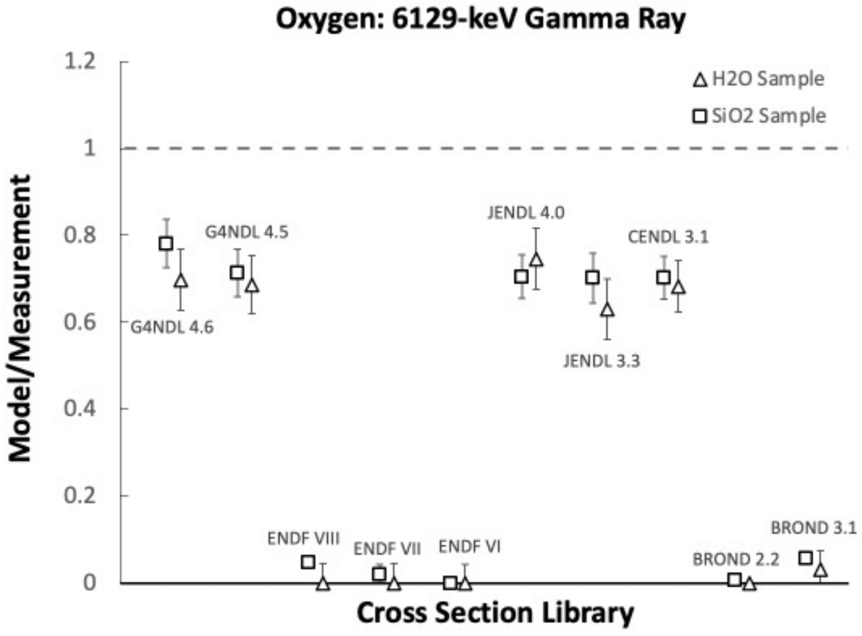
ENDF/B-VI in better agreement with our experimental results above 2 MeV





Marie-Laure Mauborgne et al., WANDA2021

This is just the tip of iceberg



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

Summary Results

Library Accuracy
Within 5%
Within 5-10%
Within 10-20%
Diff. >20%
"--" = No Peak in Model

Simulation/Measurement Ratio

	Gamma 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
C	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
O	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
Al	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
	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
	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
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
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
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
Ca	3736	1.00±0.04	--	--	--	0.06±0.01	--	1.12±0.04	0.04±0.01	--
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
Fe	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
	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
Co	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
	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
	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: fix the evaluations (capture spectrum, include missing gammas and branching ratios for inelastics)

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

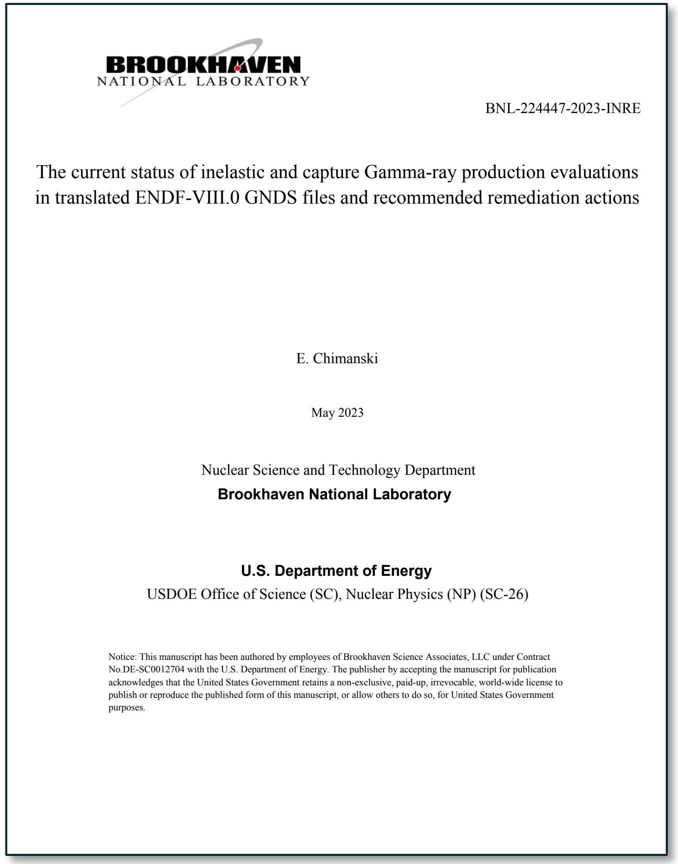
Either way, need to correctly model the reaction, incorporating all experimental knowledge

- 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
  - 17O, 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**



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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/

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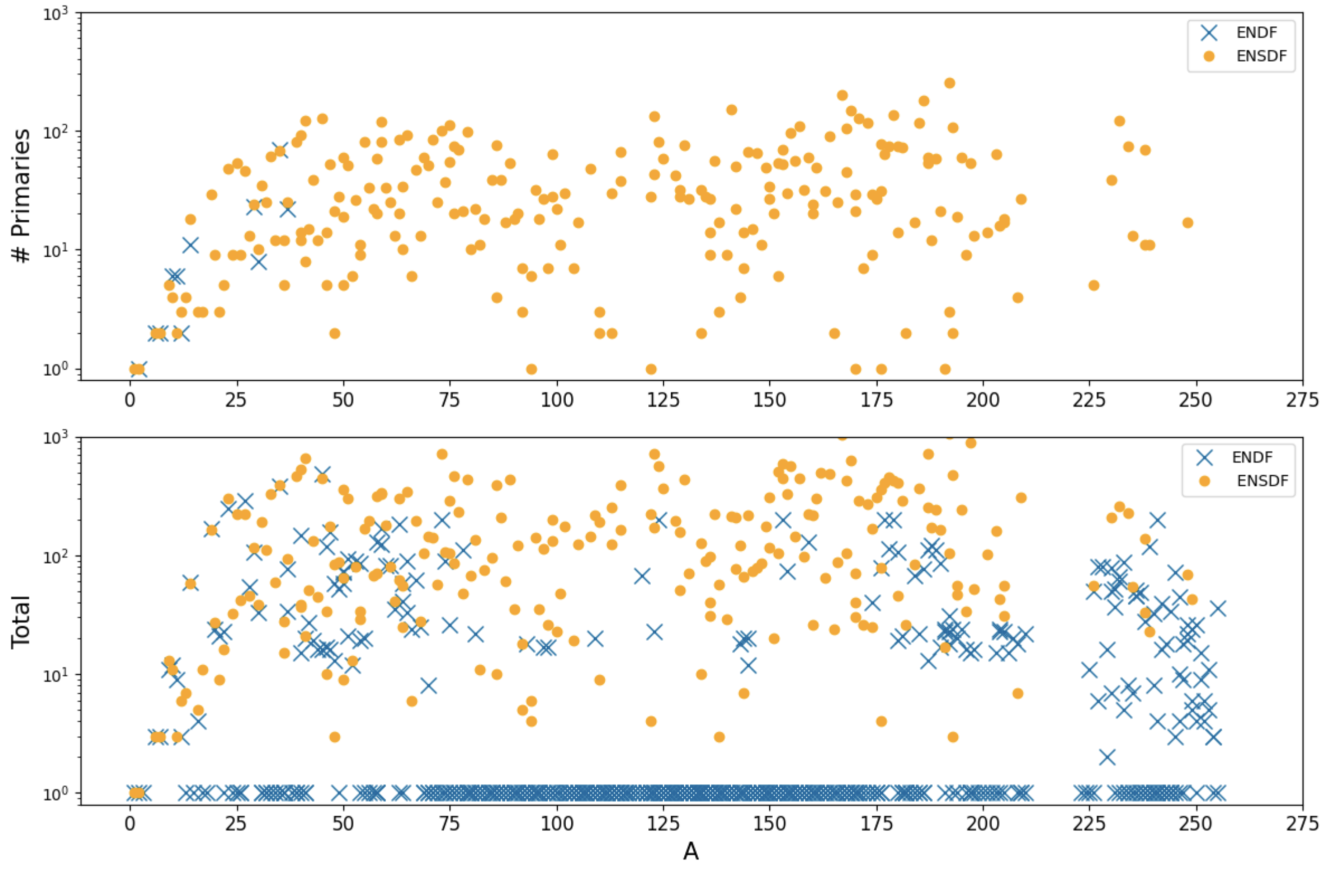
Thermal photons (gammas): a triage

ENDF/VIII.0

- 144 targets with no photon data for capture in ENDF;
- 11 with primary + discrete photons;
- 161 with only discrete photons;
- Most isotopes in ENDF do not have flagged primary transitions separately but seem to include them all into the discrete type (or in the “continuum”).



The number of photons is in overall good agreement with ENSDF up to A= 80 and 150 < A < 210
Not every isotope present in ENSDF is included in ENDF (ENDF prioritize applications and near stability).

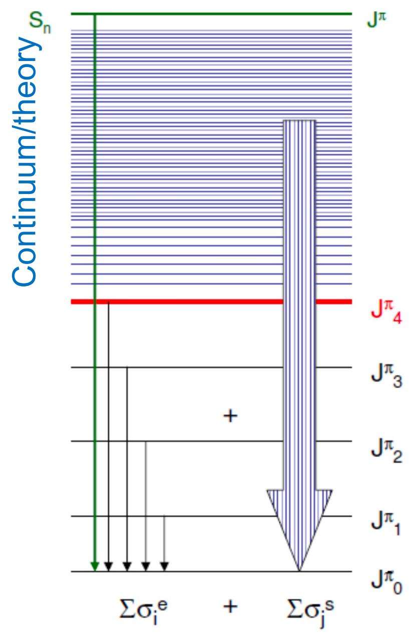
Thermal gammas

Total (n, γ) cross section is :

$$\sigma_0 = \sum_{k=1}^{P} \sigma_{\gamma k}^{\text{primary}} = \sum_{i=1}^{N} \sigma_{\gamma i0}^{\text{expt}}(1+\alpha_{i0}) + \sum_{j=1}^{M} \sigma_{\gamma j0}^{\text{sim}},$$

with $$\sum \sigma_{\gamma j0}^{\text{sim}} = P_0\sigma_0;$$

- P_0 is the population per neutron capture of the GS obtained from the simulation (continuum);



IAEA is working on EGAF II
-- more gammas
-- we can help: training op

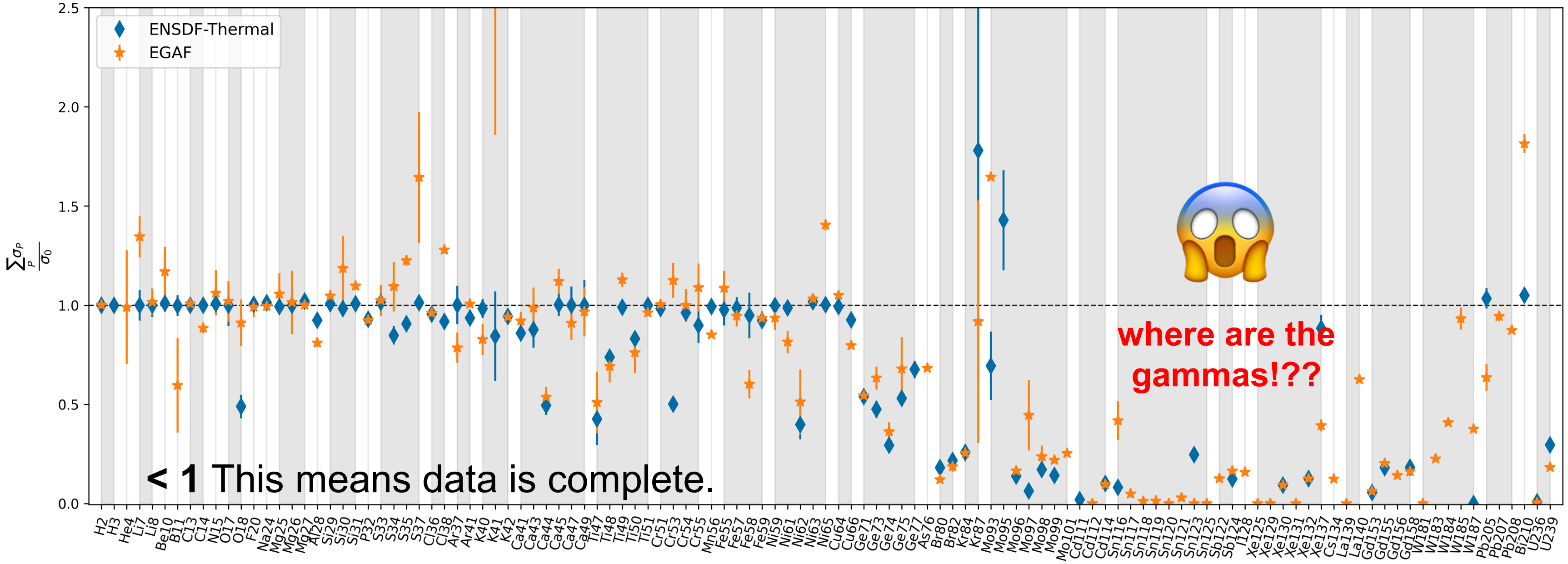
Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment

Volume 1057, December 2023, 168715

Full Length Article

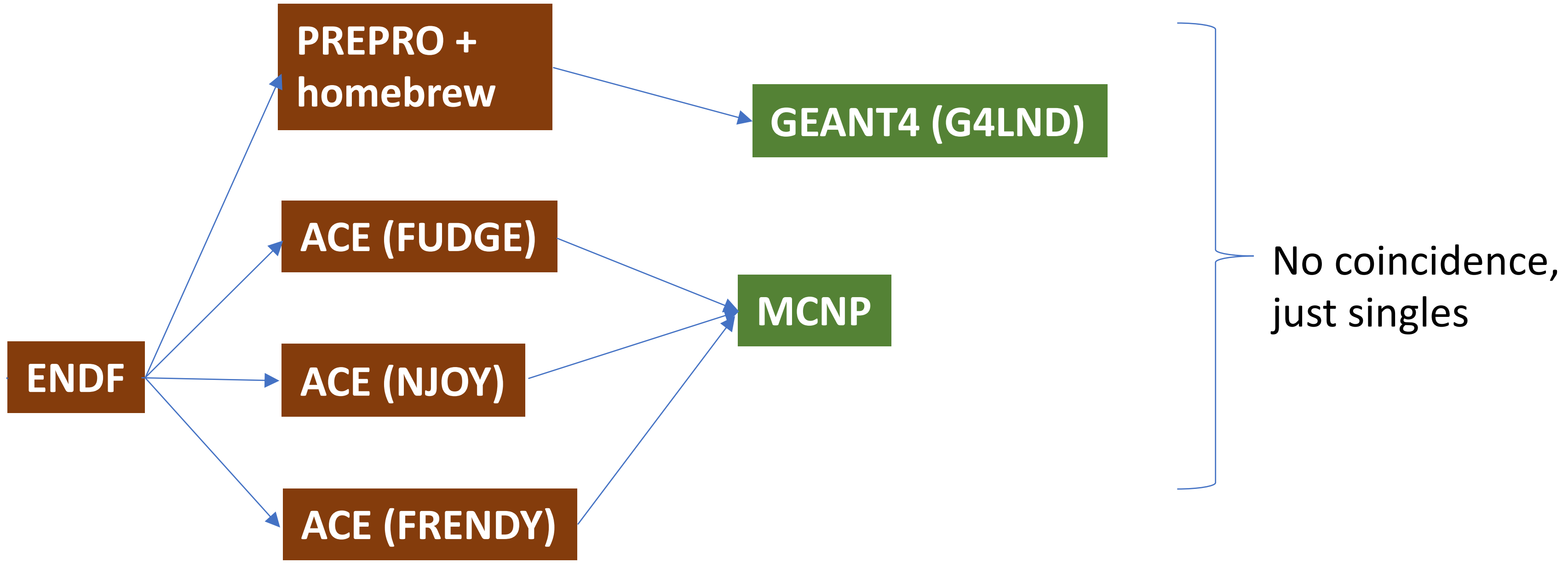
pyEGAF: An open-source Python library for the Evaluated Gamma-ray Activation File

https://github.com/AaronMHurst/python_egaf



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

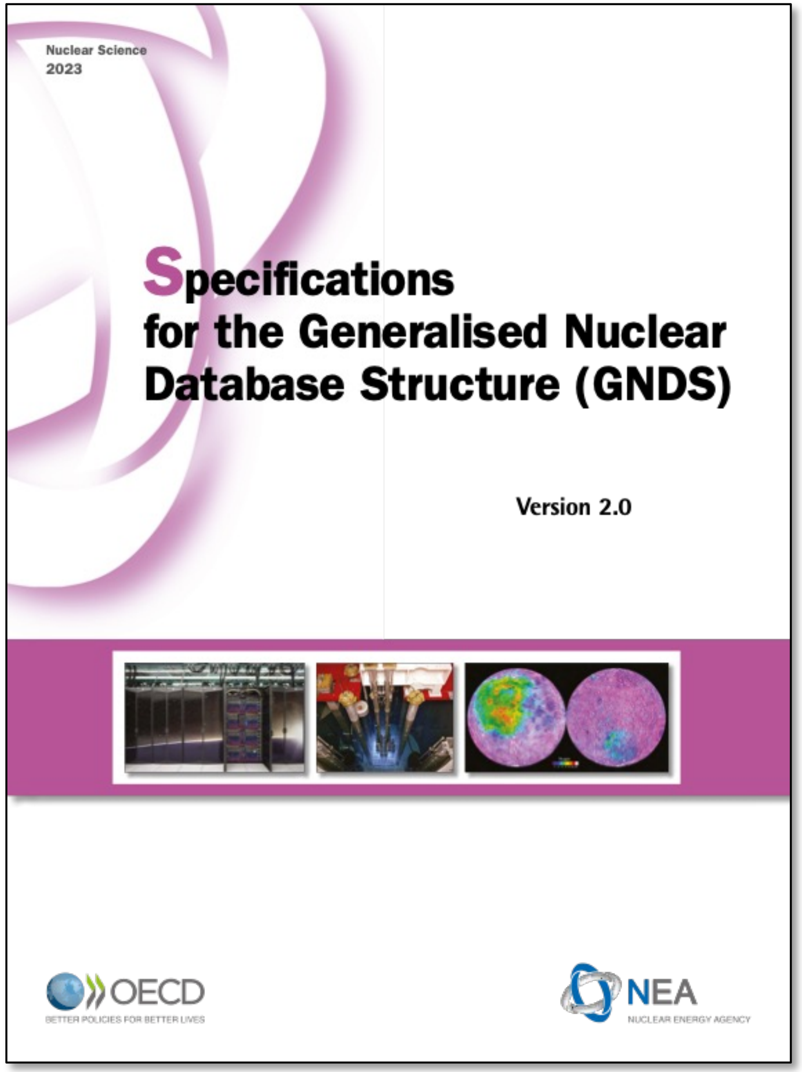
- “new way”
- All in MF6
- Energy-angle can be correlated
- Primary gammas flagged in MF6 (but interpolation painful for processing codes)
- No branching ratios

We will embrace the branching ratio!

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

```
<product pid="photon" label="photon__a">
  <multiplicity>
    <XYs1d label="eval">
      <axes>
        <axis index="1" label="energy_in" unit="eV"/>
        <axis index="0" label="multiplicity" unit=""/></axes>
      <values>1e-5 0.072811 1.5e8 0.072811</values></XYs1d></multiplicity>
  <distribution>
    <uncorrelated label="eval" productFrame="lab">
      <angular>
        <isotropic2d/></angular>
      <energy>
        <primaryGamma 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.oecd-nea.org/jcms/pl_85822/specifications-for-the-generalised-nuclear-database-structure-version-2-0

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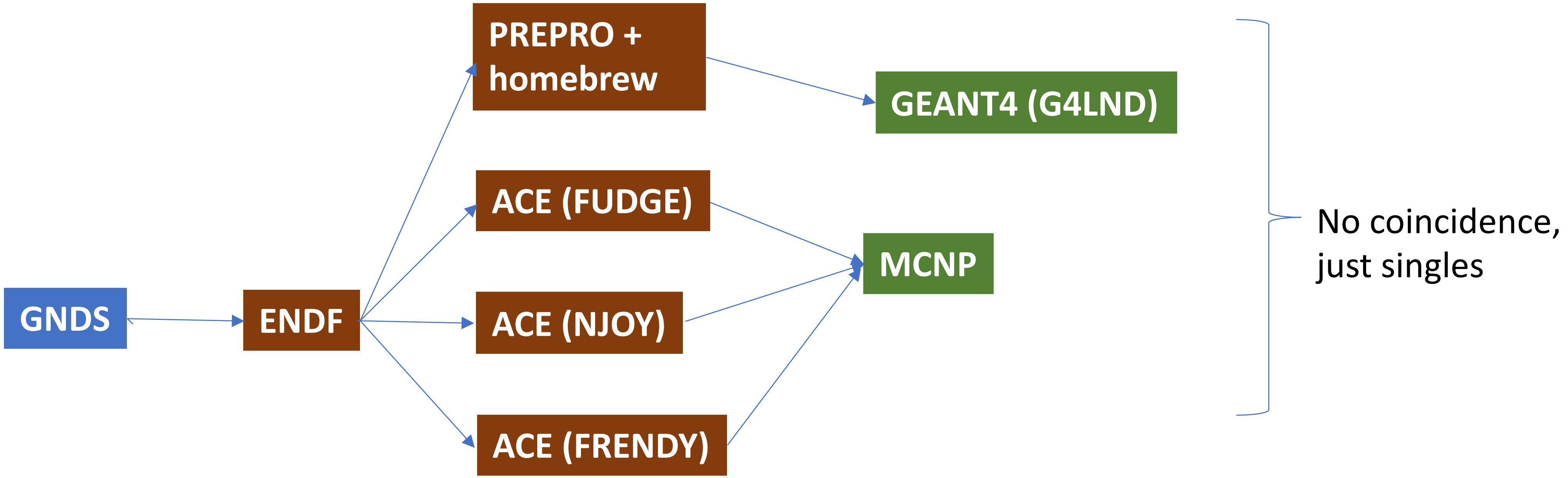
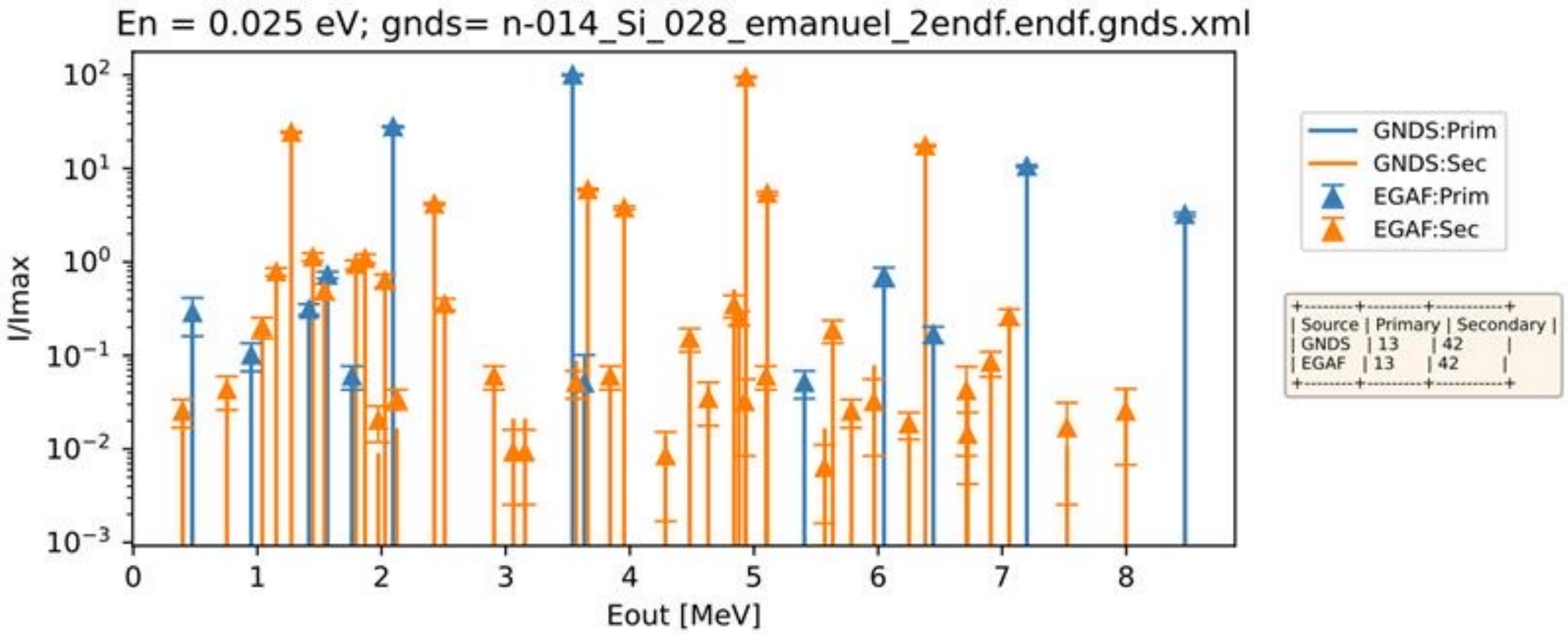
This suggests we should do this



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



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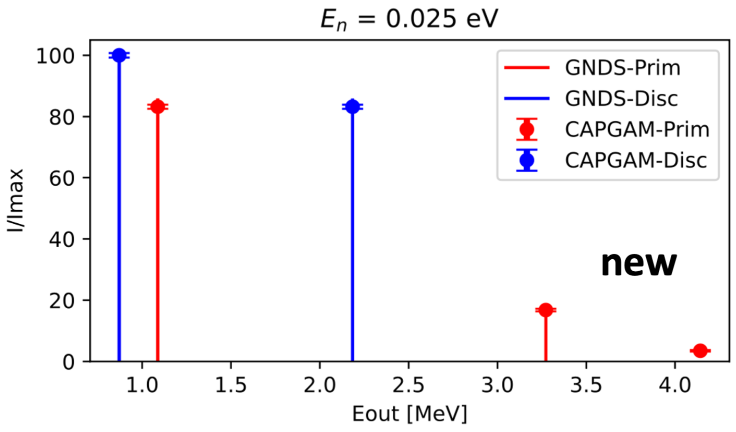
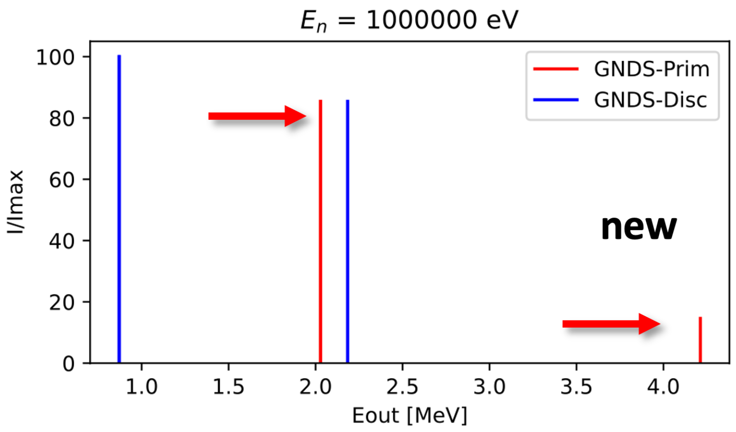
^{16}O: primary gammas now fixed in ENDF/B-VIII.1Beta2 (approved by Mark & Gerry)

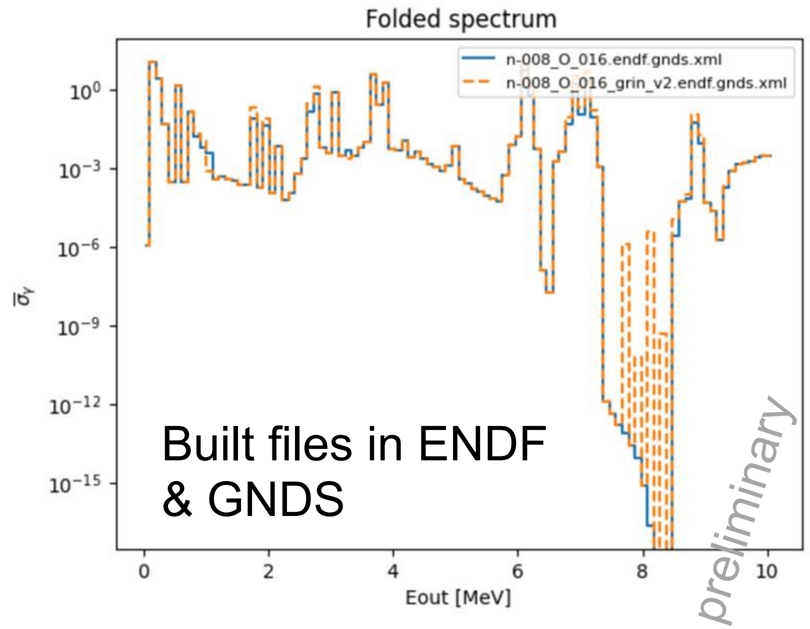




Primaries flagged

Primary gamma-ray energy dependence on neutron incident energy

I just changed **LP = 0 to LP = 2** for the primaries



This includes inelastic fixes

LP indicator of whether or not the particular photon is a primary:

- LP=0 origin of photons is not designated or not known, and the photon energy is EG_k;
- LP=1 for non-primary photons where the photon energy is simply EG_k;
- LP=2 for primary photons where in the center-of-mass frame the sum of the photon energy EG'_k and kinetic energy of the residual K_r is

From the ENDF manual (pg 201)

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

C – flagged primaries, submitted to ENDF phase1, also GNDS files we can use for testing coincidence modeling

Si – flagged primaries, submitted to ENDF phase1, also GNDS files we can use for testing coincidence modeling

^{14}F – flagged primaries (phase1)

^{16}O – flagged primaries (phase1), fixed missing inelastic gammas (waiting to be submitted), can't do much for other O

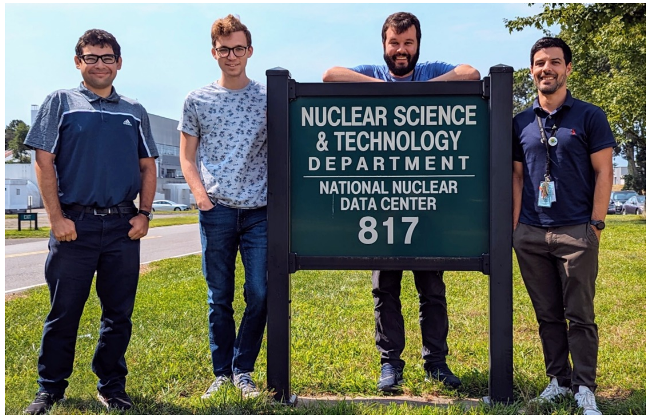
^{32}S – "close"; can't do much for $^{33+}$S (low abundance – bad data)

^{207}Pb – experimental ENDF file that uses MT900-999 (n, gamma[i]) format (Thank you Amanda!)

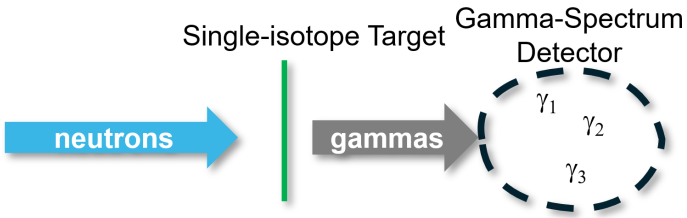
Rethinking formats and API for e-by-e: discrete levels

GEANT4's implementation of gamma emission is so so wrong

Michael Allen & Mauricio Cerda



Emanuel & Andrea (BNL-Staff)



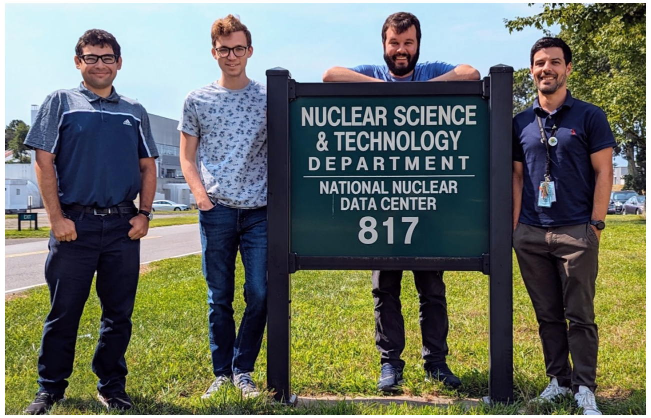
Gamma-ray multiplicity

Simple idea:

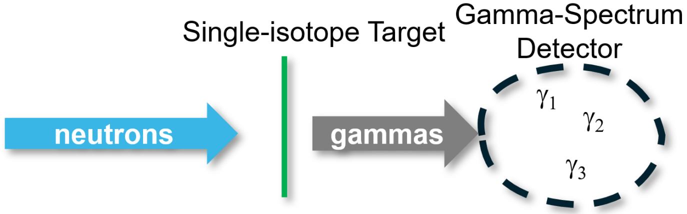
- Verify how Geant4 uses ENDF/B to simulate neutron capture.
- How that affects the capture gamma-ray simulation

GEANT4's implementation of gamma emission from (n_{th},g) is limited

Michael Allen & Mauricio Cerda



Emanuel & Andrea (BNL-Staff)



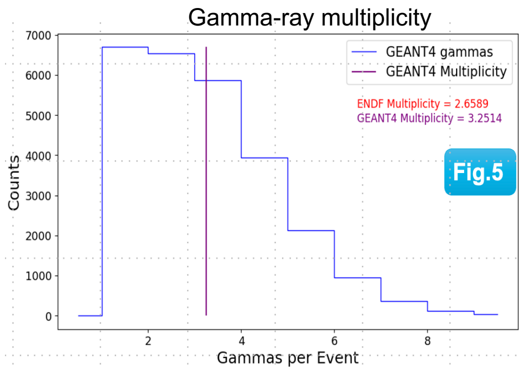
Simple idea:

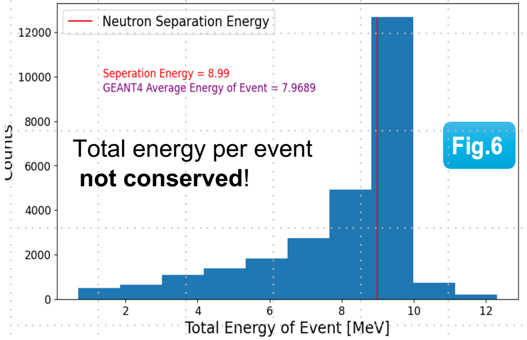
- Verify how Geant4 uses ENDF/B to simulate neutron capture.
- How that affects the capture gamma-ray simulation

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

When using ENDF/B inputs only:

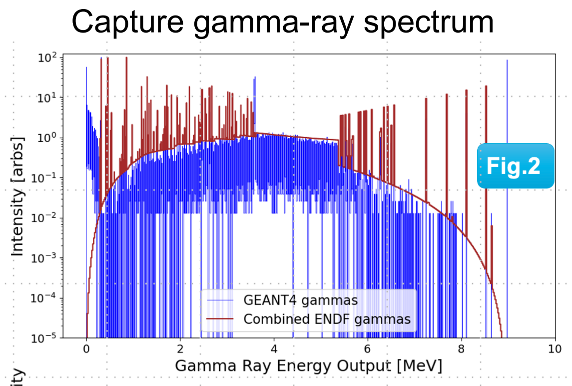
- **Geant4 does not distinguish primaries from secondaries even when ENDF/B does (G4NDL is built with ENDF + …)**
- **No gamma-ray correlations**
- **Energy is not conserved on event-by-event**
- **Gamma-ray multiplicity is affected by the problems above**

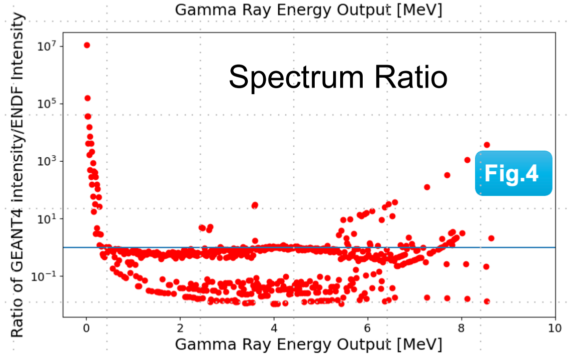




$(n,g)^{58}$Ni

@ thermal





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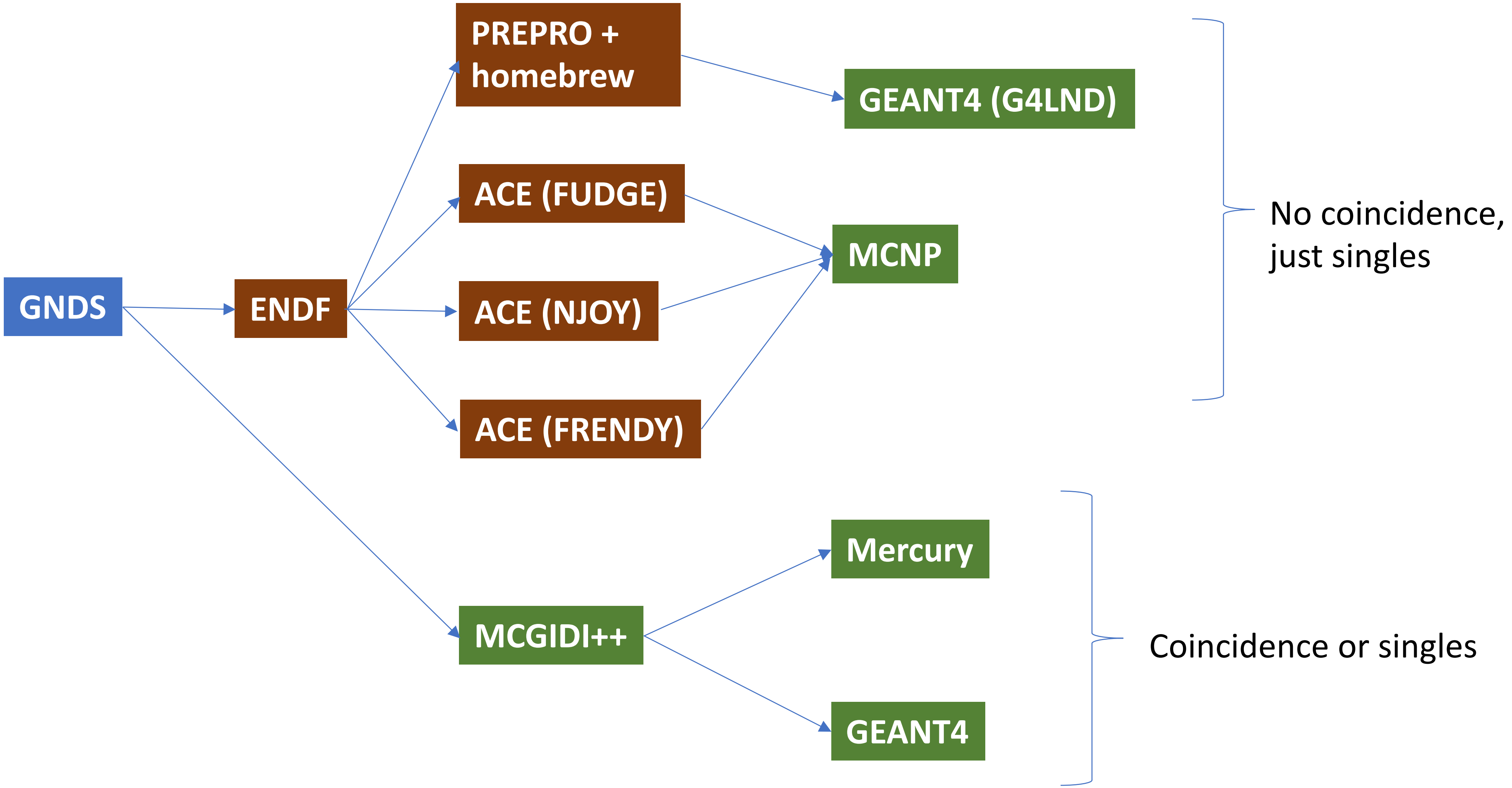
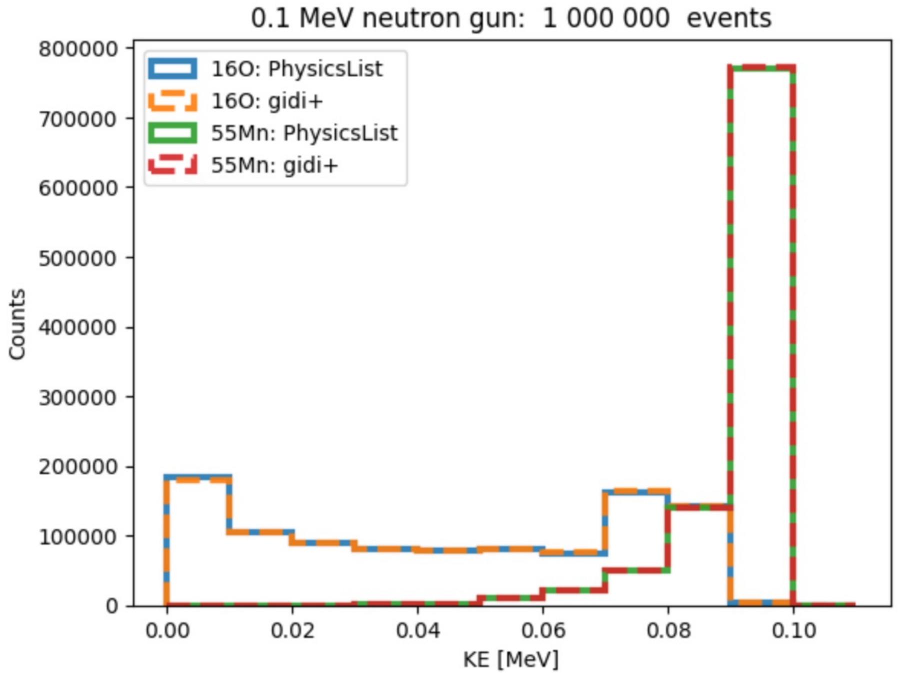
To understand our strategy to fix, it is useful to understand whole processing chain



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

- Part of GIDI+: https://github.com/LLNL/gidiplus
- 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)



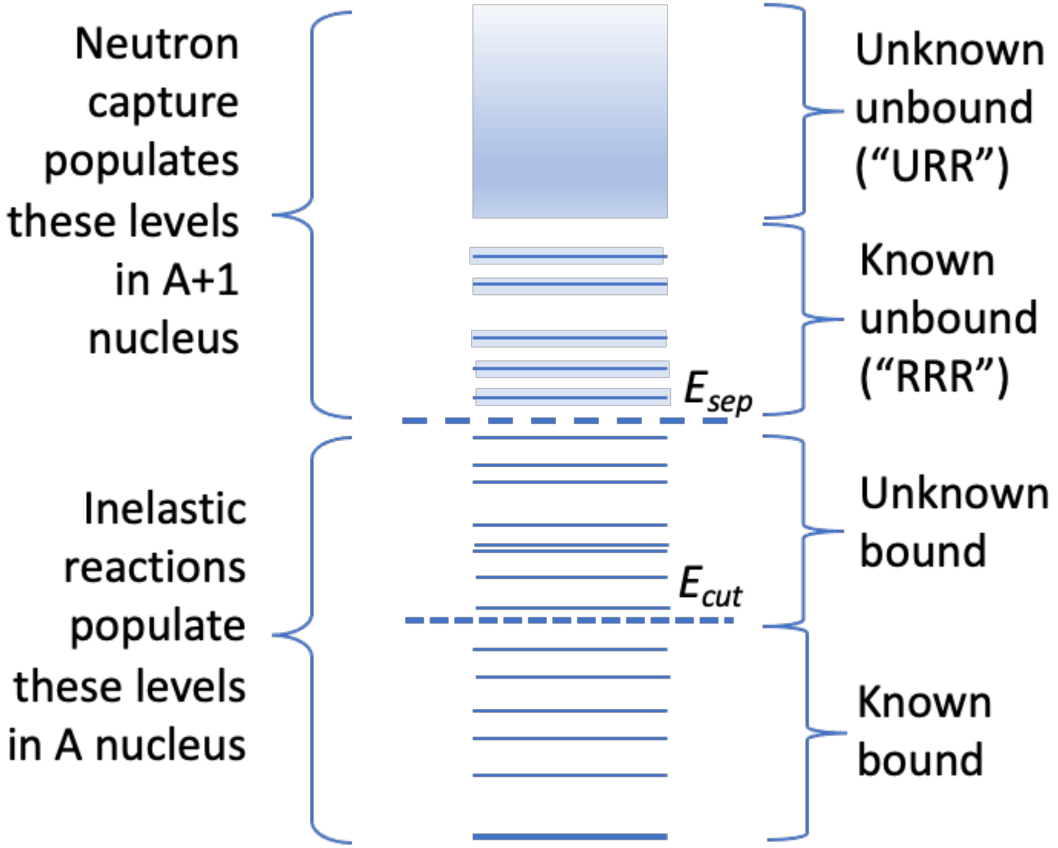
We have not tested the event-by-event capability of GIDI yet.

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



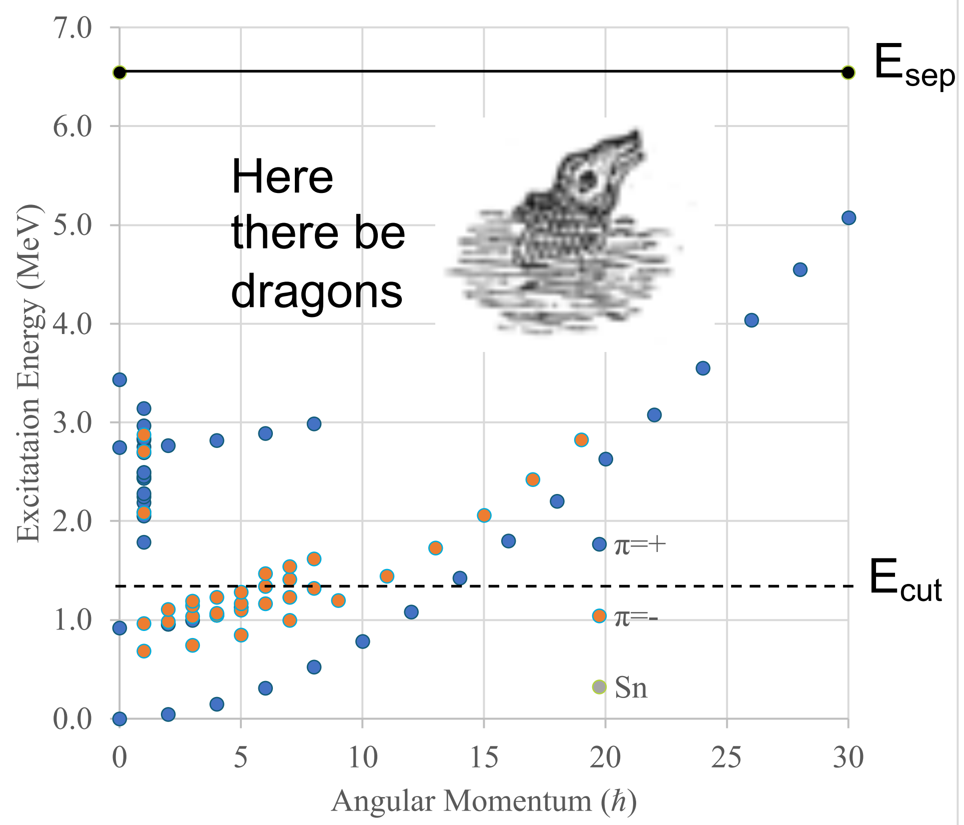
The essential problem when modeling

The level scheme above a certain energy E_{cut} is not well known (if at all)

Above the neutron separation energy E_{sep} we have resonance data

We do have information about what happens between E_{sep} and E_{cut}:

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



^{236}U level scheme (adapted from L. Bernstein)

Pros and Cons of some competing codes

DICEBOX
γ 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

RAINIER Public
Development repo for the nuclear decay code
HTML 3 2

- 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

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

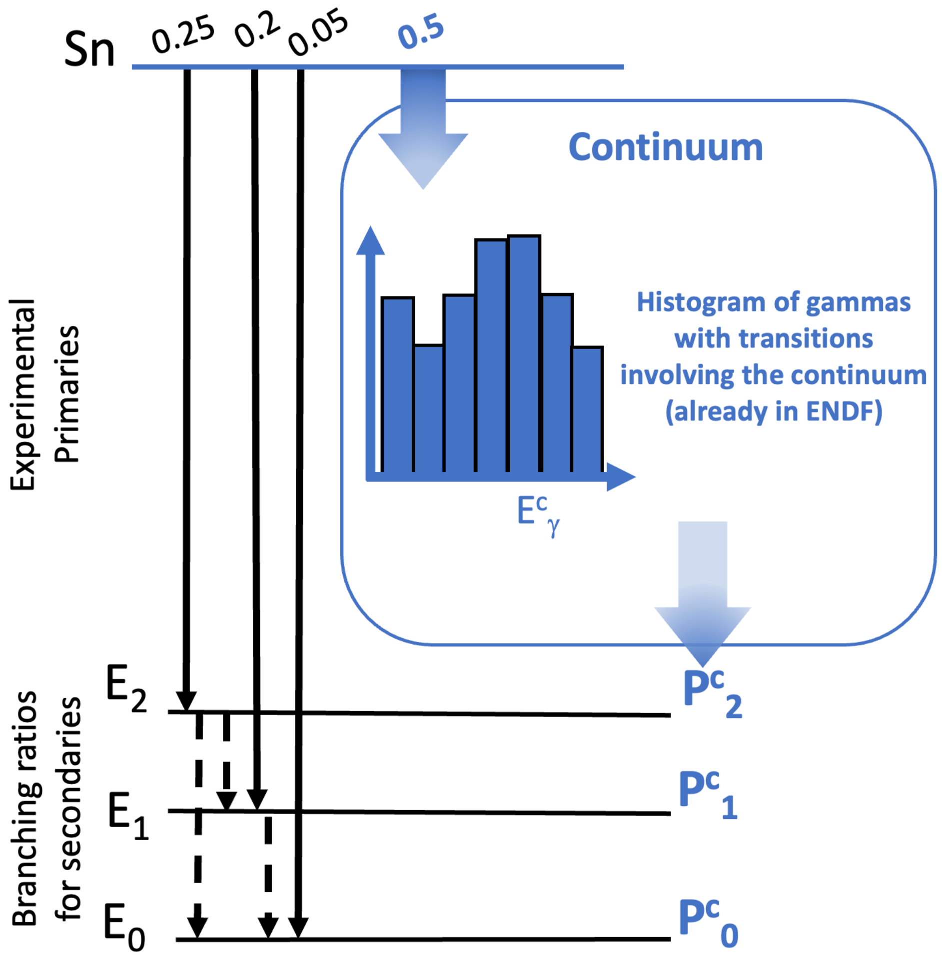
EMPIRE
Nuclear Reaction Model Code

- Reaction code;
- FORTRAN;
- “Simple” input file;
- Modeling of various nuclear reactions including γ-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

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

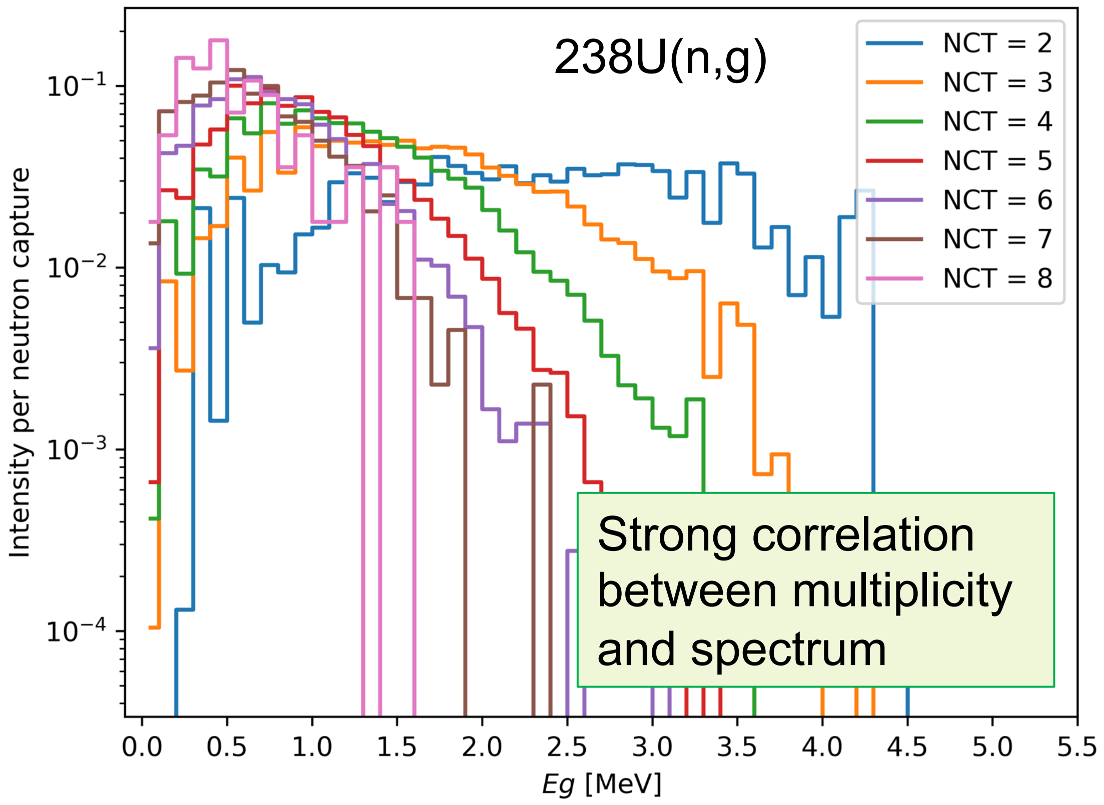
Approach #2: All levels, all branching ratios

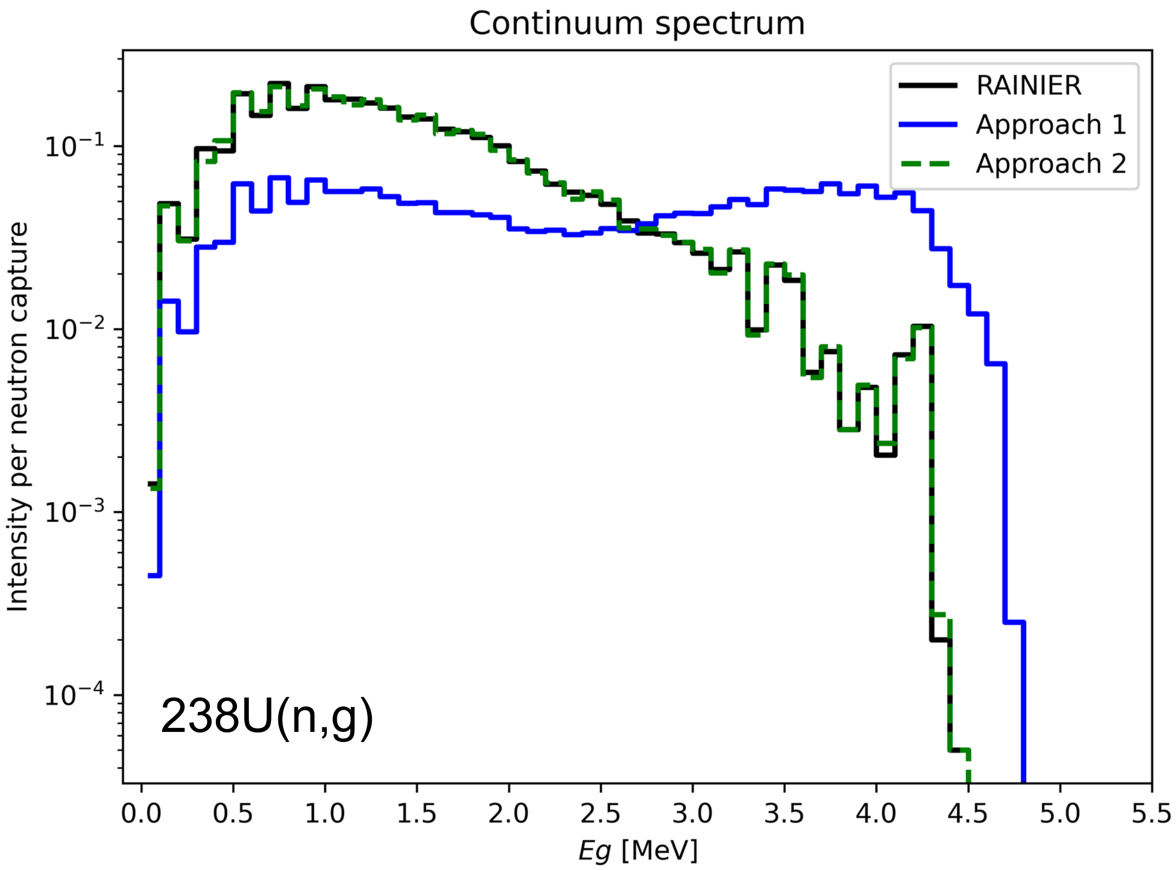
- Needs (i.e. evaluator provides):
  - Simulated level scheme (can be fixed width/spacing bins)
  - Population of all simulated levels
  - Simulated branching ratios out of simulated levels

EMPIRE, RAINIER & CoH provide this

- 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!)

Approach #1 fails for most nuclei





NCT=Number Continuum Transitions

Validation

Lining up folks to validate tools & evaluations

Us

Our fan base

NDWG FY24-FY26

FAIR FY24-FY26

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	^{252}Cf source, many materials
RPI	Yaron Danon*	MCNP	Yes, event list	RPI ToF, segmented NaI detector: ^{56}Fe, ^{55}Mn, ^{59}Co, ^{181}Ta, and ^{238}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	$MnSO_4$ bath, ^{252}Cf source, gamma spectrum

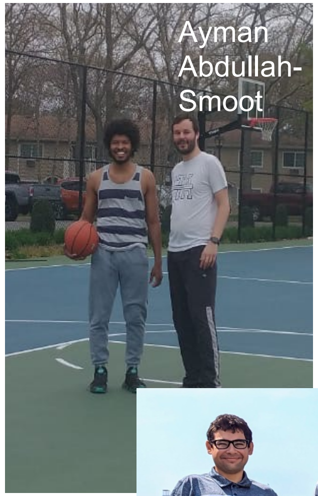
Where we are now

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 follow-on validation projects
-- thermal neutron capture cascades (Yaron Danon)
-- more for 14 MeV neutrons (Patrick Peplowski +)

Our Interns



Rest of the GRIN team:
D. Brown, C. Morse, S. Ota, A. Hurst, B. Beck, C. Mattoon, G. Gert, A.Lewis

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, https://pypi.org/project/pyEGAF/ (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. Mat- toon, E. A. McCutchan, C. Morse, G. Nobre, S. Ota, D. Brown, The current status of in- elastic 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

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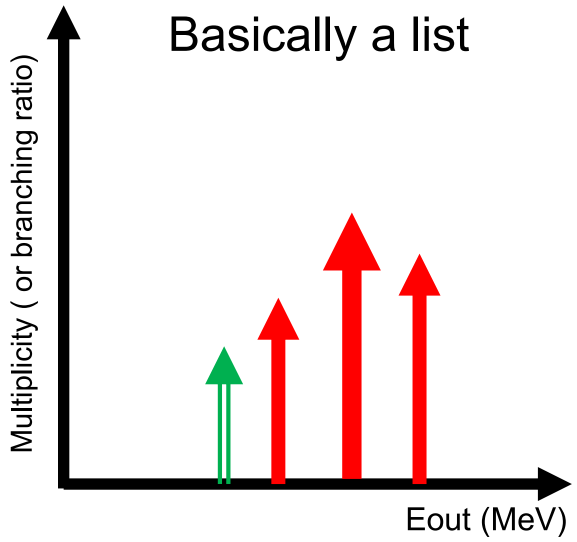
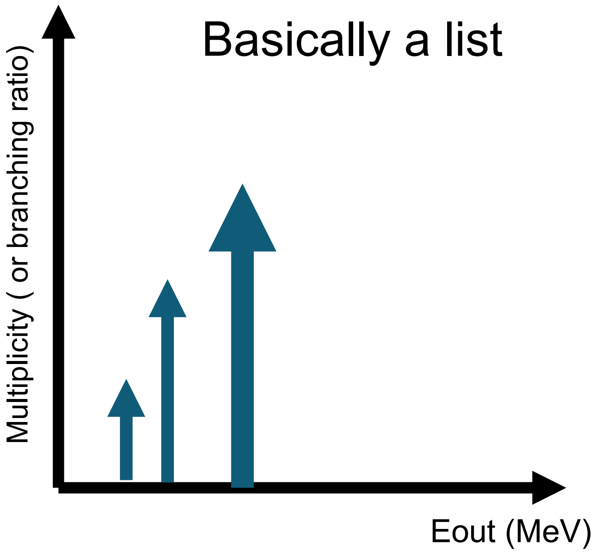
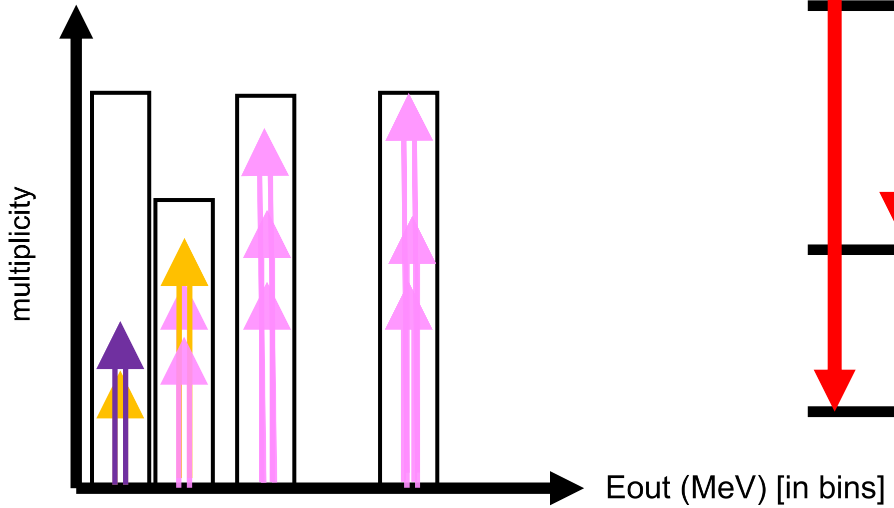
Backup Slides

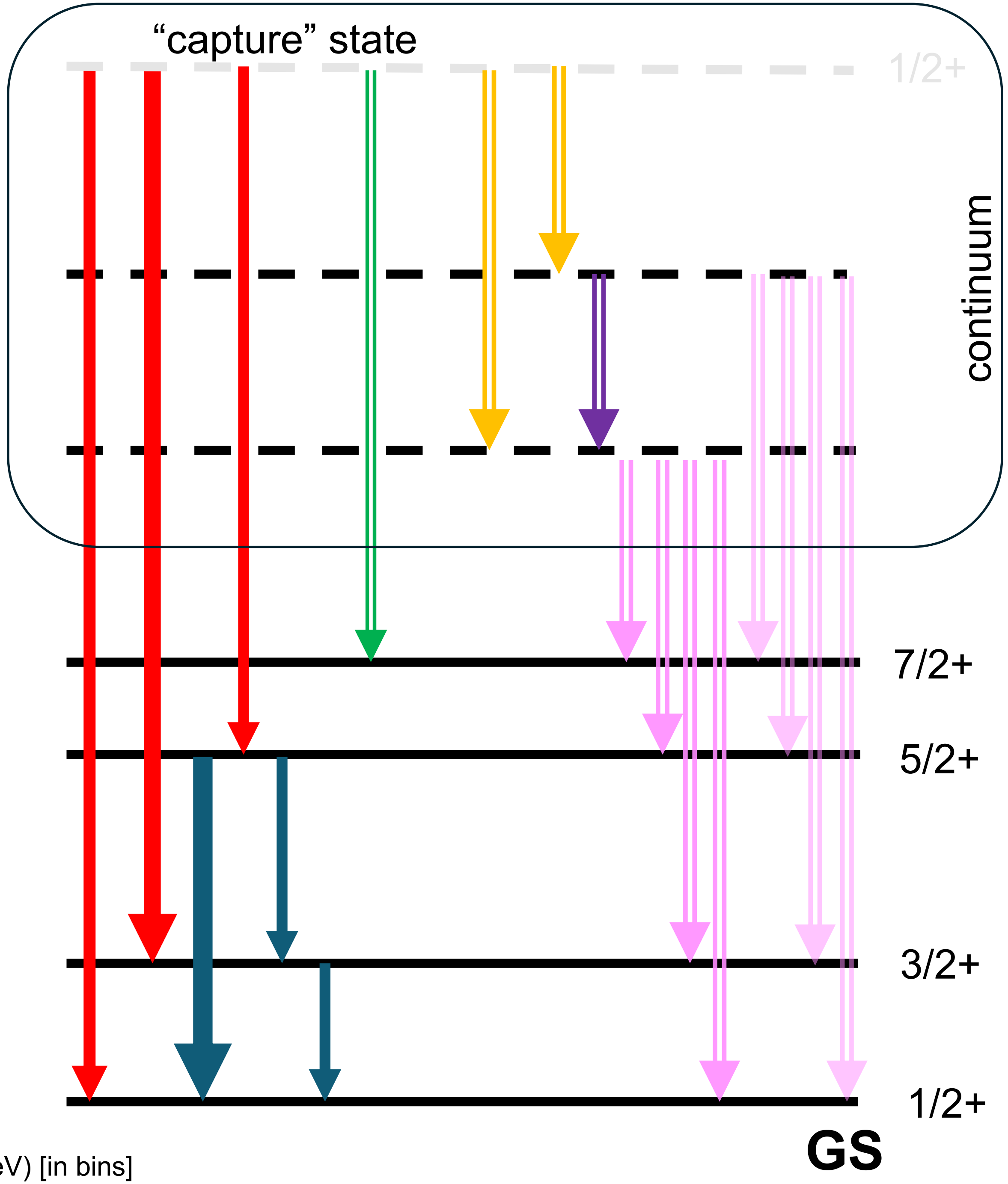
Gamma emission distributions in the GNDS/ENDF file





all gammas related to "continuum"





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CEA work: Cordero Ramirez & Jouanne

https://indico.frib.msu.edu/event/52/contributions/981/attachments/597/2268/ND2022_CORDERO.pdf

Inelastic

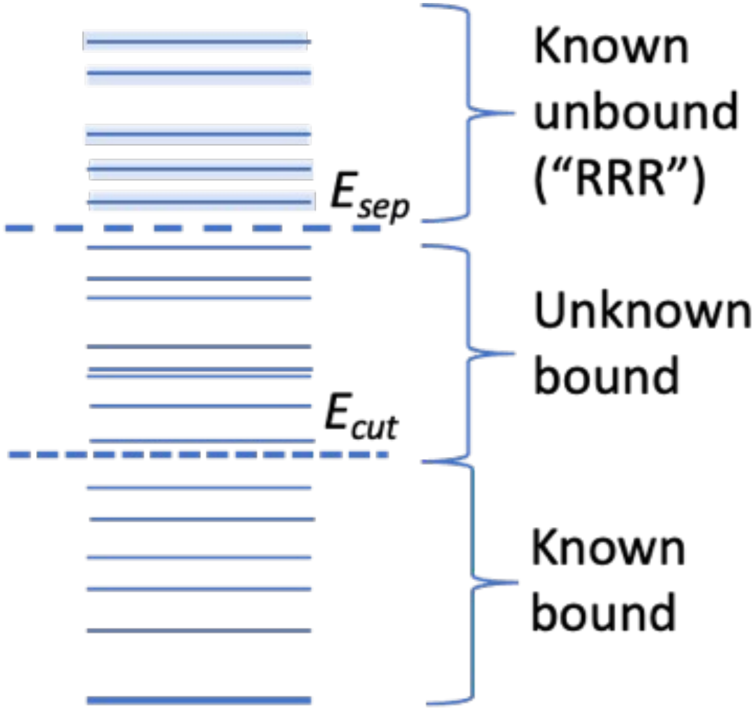
- Found a mix of MF12 and MF6 data (depending on the MT)
- Very strange
- Is apparently allowed in ENDF format
- Uncommon in JEFF-3.3
- TK (LANL) does this in CoH/Dece

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^{Π}
  - Short range spacing rule (GOE, fixed, …)

  levels

  - Multipolarity of gammas (including mixing)
  - Rule for width sampling
  - Gamma ray strength function

  BR's

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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

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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

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