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U.S. DEPARTMENT OF ENERGY

Gamma Rays Induced by Neutrons

Year 3 Report

David Brown (National Nuclear Data Center, Brookhaven National Laboratory)

GRIN Collaboration:

E. Chimanski, E. Ricard, G. Nobre, S. Ota, C. Morse (BNL),
A. Hurst, L. Bernstein (LBNL), C. Mattoon, B. Beck, G. Gert (LLNL), A. Lewis (UTK)

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WANDA 2024

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

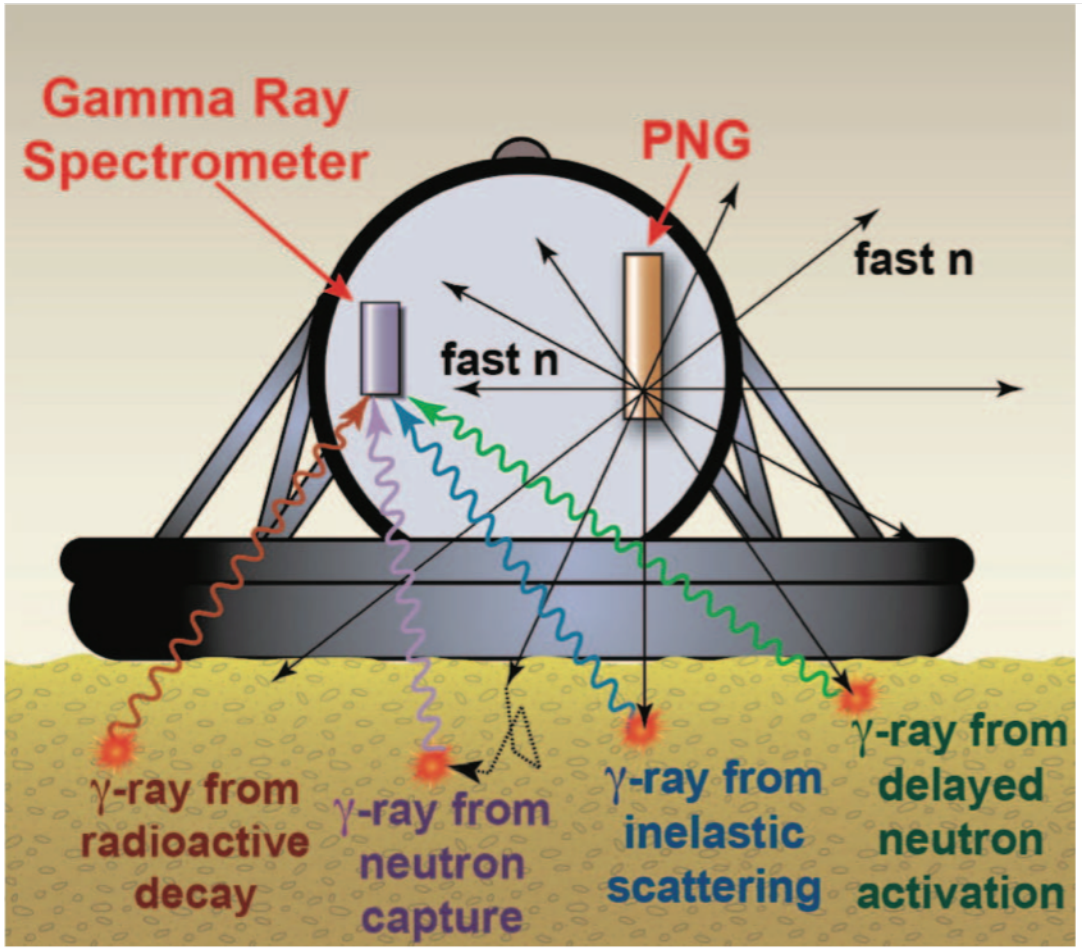


Figure 1: The Bulk Elemental Compositional Analyzer (BECA) instrument proposed for a future NASA mission to Venus. From Fig 1. of [Parsons 2016].

GRIN is 3-year NA-22 project with these Intended Goals

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

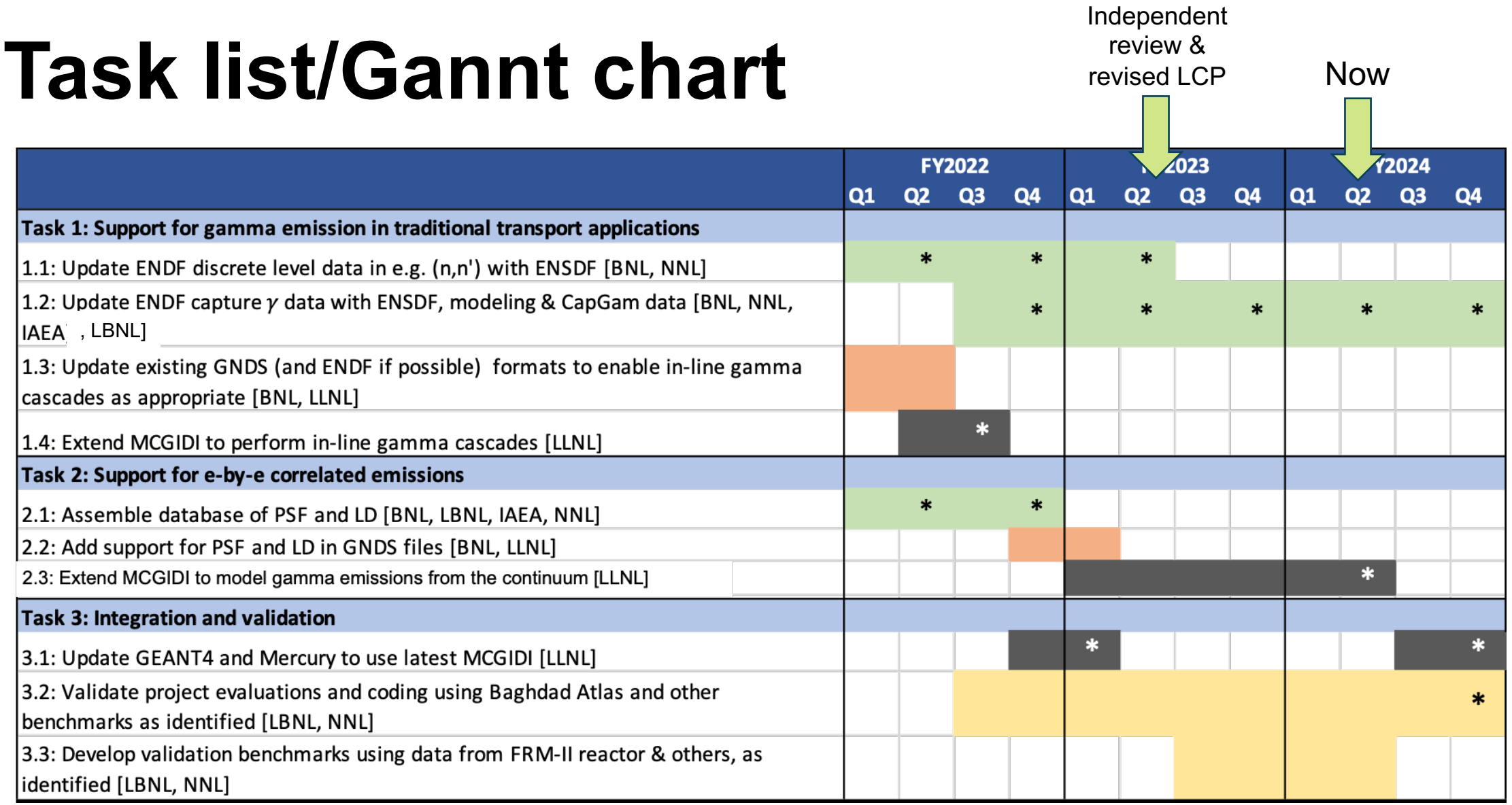
For event-by-event user (correlations!): need to rethink the API & what data we store in an evaluation

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

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

And we need to test the final product!

Task list/Gannt chart



Task list/Gannt chart

✓ done
✓ part done, more to go!

Independent review & revised LCP

Now

	FY2022 Q1	FY2022 Q2	FY2022 Q3	FY2022 Q4	FY2023 Q1	FY2023 Q2	FY2023 Q3	FY2023 Q4	FY2024 Q1	FY2024 Q2	FY2024 Q3	FY2024 Q4
Task 1: Support for gamma emission in traditional transport applications												
✓ 1.1: Update ENDF discrete level data in e.g. (n,n') with ENSDF [BNL, NNL]		*		*		*						
✓ 1.2: Update ENDF capture γ data with ENSDF, modeling & CapGam data [BNL, NNL, IAEA , LBNL]				*		*		*		*		*
✓ 1.3: Update existing GNDS (and ENDF if possible) formats to enable in-line gamma cascades as appropriate [BNL, LLNL]												
✓ 1.4: Extend MCGIDI to perform in-line gamma cascades [LLNL]			*									
Task 2: Support for e-by-e correlated emissions												
✓ 2.1: Assemble database of PSF and LD [BNL, LBNL, IAEA, NNL]		*		*								
2.2: Add support for PSF and LD in GNDS files [BNL, LLNL]												
2.3: Extend MCGIDI to model gamma emissions from the continuum [LLNL]										*		
Task 3: Integration and validation												
✓ 3.1: Update GEANT4 and Mercury to use latest MCGIDI [LLNL]					*							*
3.2: Validate project evaluations and coding using Baghdad Atlas and other benchmarks as identified [LBNL, NNL]												*
3.3: Develop validation benchmarks using data from FRM-II reactor & others, as identified [LBNL, NNL]												

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Task 1: fixing the ^%#@$ evaluations

Task 1: traditional user support *modeling and evaluation – evaluation status*

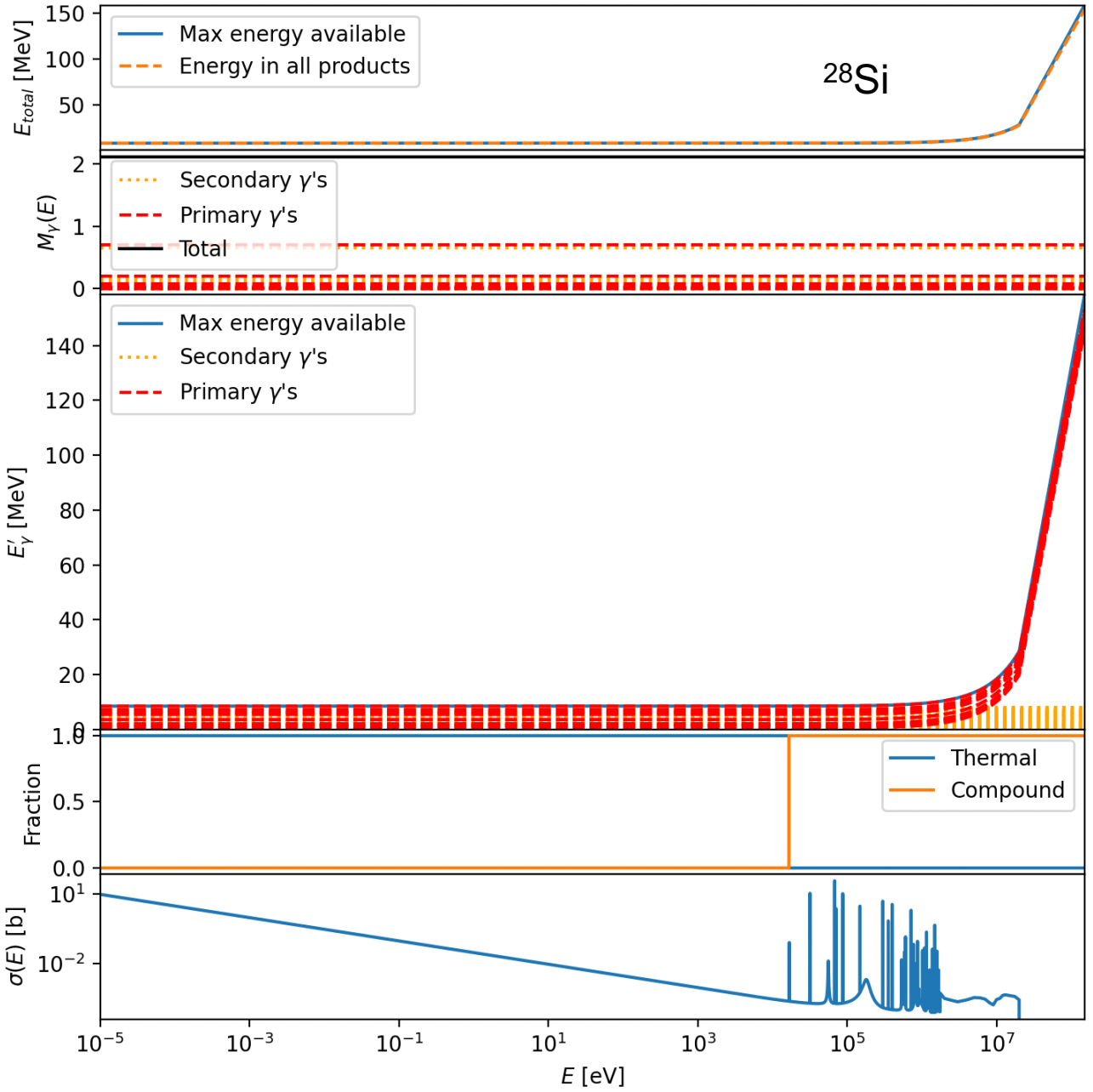
- ✓ H [OK]
- ✓ ^{12}C [OK], ^{13}C [done FY24]
- ✓ ^{16}O [done FY23], ^{17,18}O [to do]
- ✓ ^{19}F [done FY23]
- • ^{28}Si [done FY23], $^{29\text{-}32}$Si [*in progress*]
- ✓ $^{32\text{-}34}$S [done FY23],
- • ^{55}Mn [OK (IAEA)], ^{54}Mn [to do]
- • ^{208}Pb [*in progress by RPI*], ^{204}Pb [to do], ^{206}Pb [to do], ^{207}Pb [done by AL]
- • ^{238}U [OK (INDEN)], rest of U isotopes [to do]
- • Next: N, Na, Al, Cu, Fe, W, Pu, He, Li, Be, B, Cl, Cr, Ni, Ge, Br, Cd, I, Cs, La, Mg, P, Ar, K, Ca, Ti, As, Kr, Mo, Sn, Sb, Xe, Gd, Bi, Np, Np, Am

Isotope priority
First
Follow-up
Remaining

File	Inelastic	Capture	Status
n-006_C_013.endf	BRs and energies updated.	Included from EGAF	ENDF/B-VIII.1β3
n-008_O_016.endf	BRs and energies included	Updated: Primaries flagged	ENDF/B-VIII.1β3
n-009_F_019.endf		Updated: Primaries flagged	ENDF/B-VIII.1β3
n-014_Si_028.endf	BRs and energies updated	Updated: Primaries flagged	ENDF/B-VIII.1β3
n-016_S_032.endf	BRs and energies updated	Formatting	ENDF/B-VIII.1β3
n-016_S_033.endf	BR and energies updated	We need more data	ENDF/B-VIII.1β3
n-016_S_034.endf	BRs and energies updated	We need more data	ENDF/B-VIII.1β3

Outline of a typical fix

- Replace inelastic-like BR's with ENSDF if needed
- Replace thermal capture gammas with EGAF/ENSDF
- For RRR capture, either:
  - Replace RRR gammas with CN model or
  - Keep as all primary and extrapolate to higher energies
- Fixes made to GNDS files, translated back to ENDF
- Scheme coded in our *grin-formatter* code



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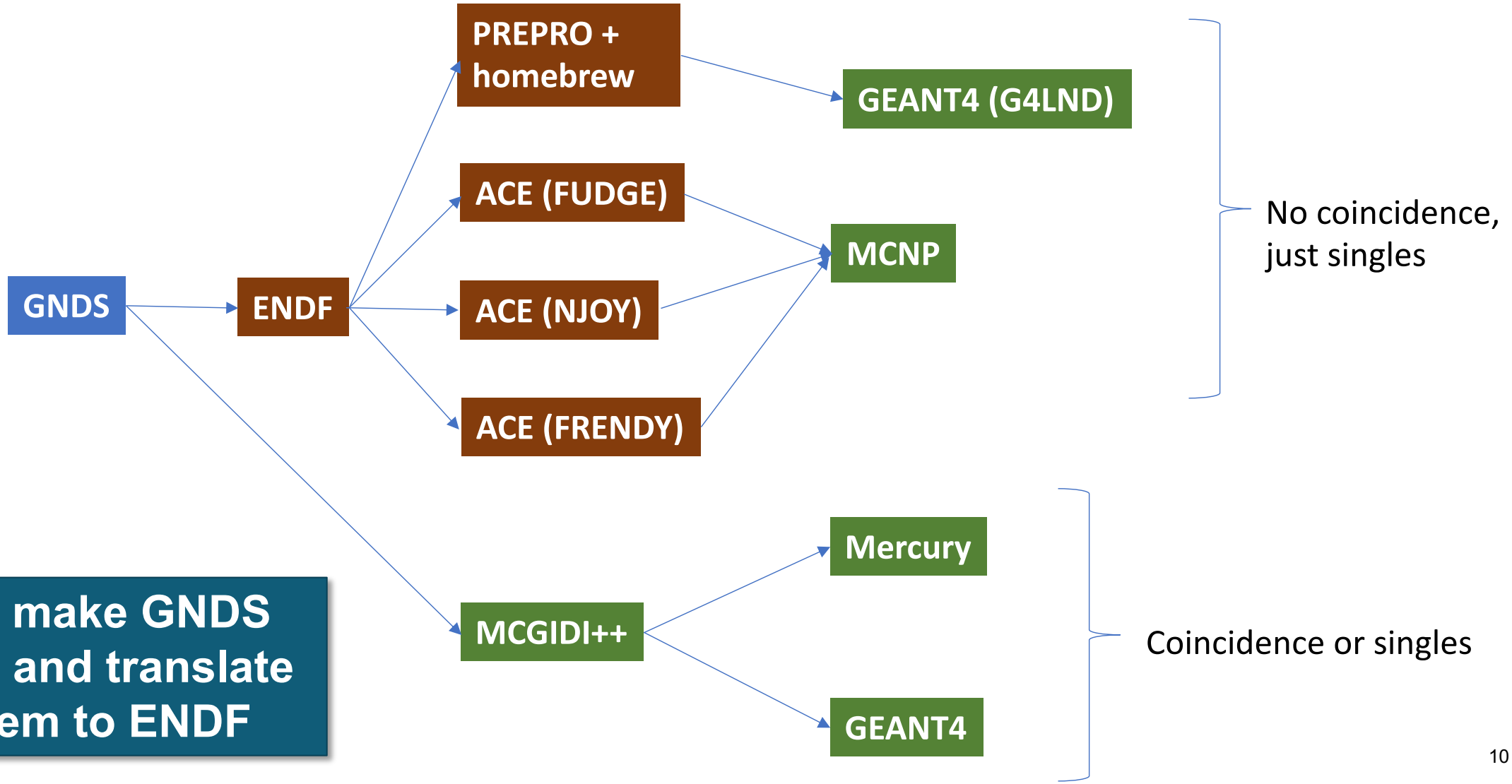
All the processing pathways we consider



We make GNDS files and translate them to ENDF

Task 2: enabling correlations

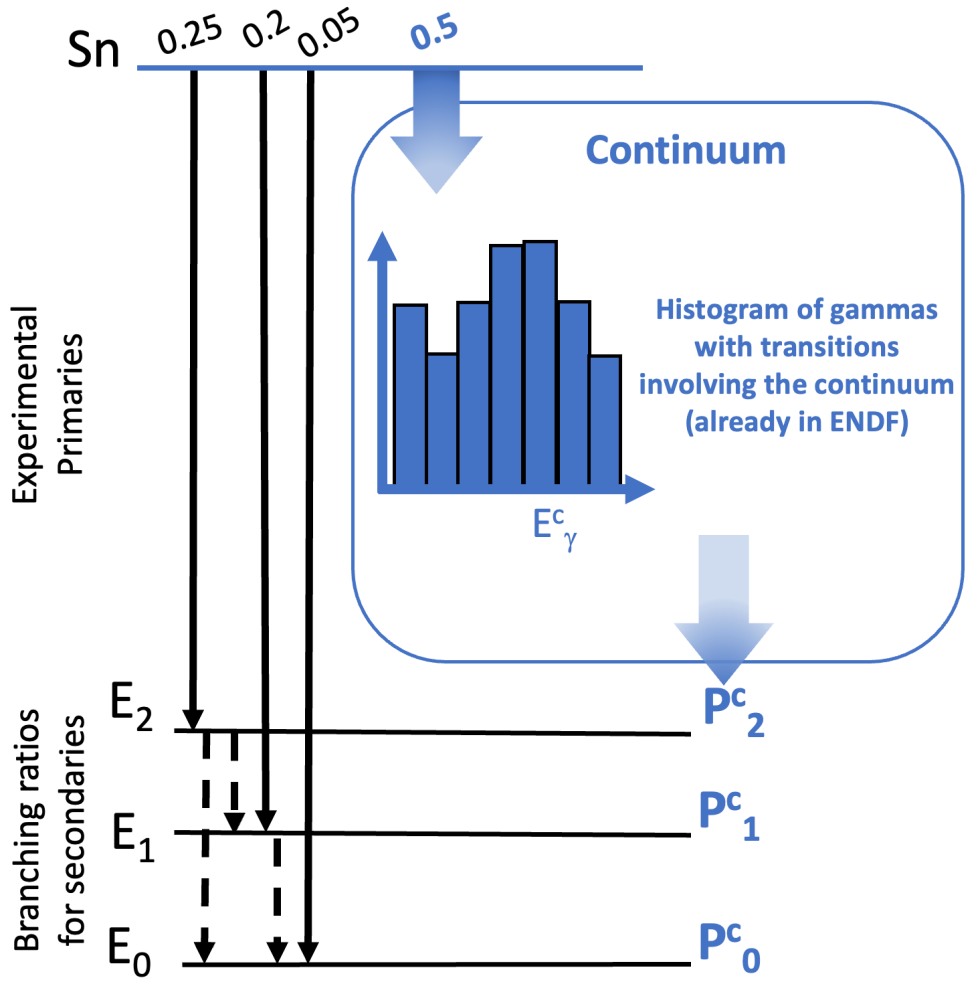
Task 2: event-by-event modeling support

Trying to develop efficient e-by-e scheme:

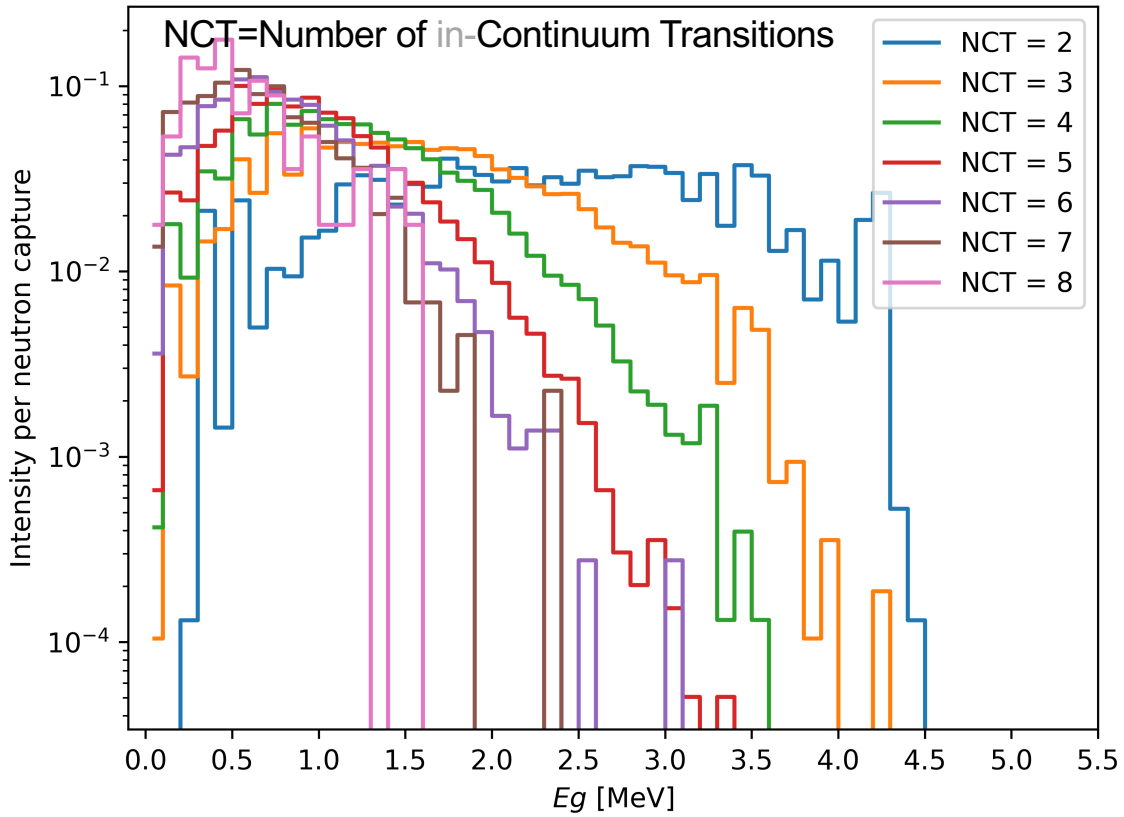
- "Small" files
- Fast sampling
- Correct physics

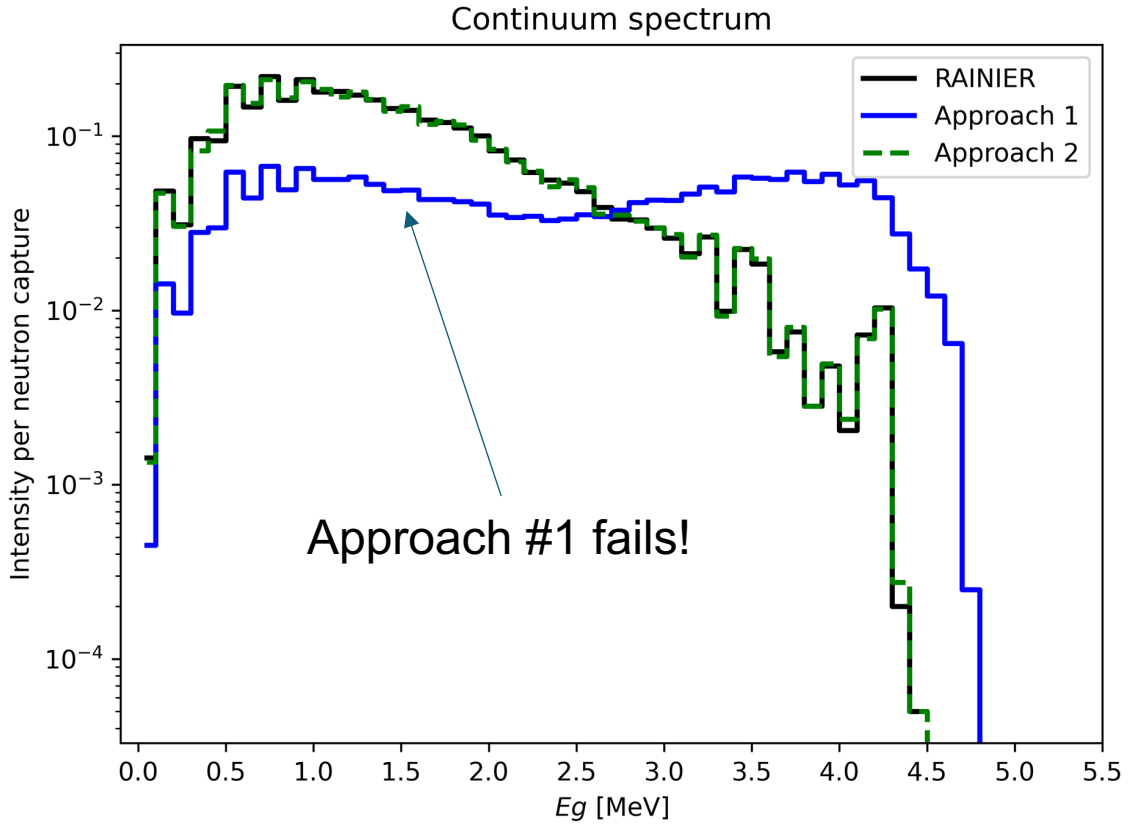
Two approaches:

1. Two emissions in Continuum
2. All levels, all branching ratios



We must adopt approach #2





Approach #2 needs:

- **Simulated level scheme**
- **Population of all simulated levels**
- **Branching ratios from simulated levels**

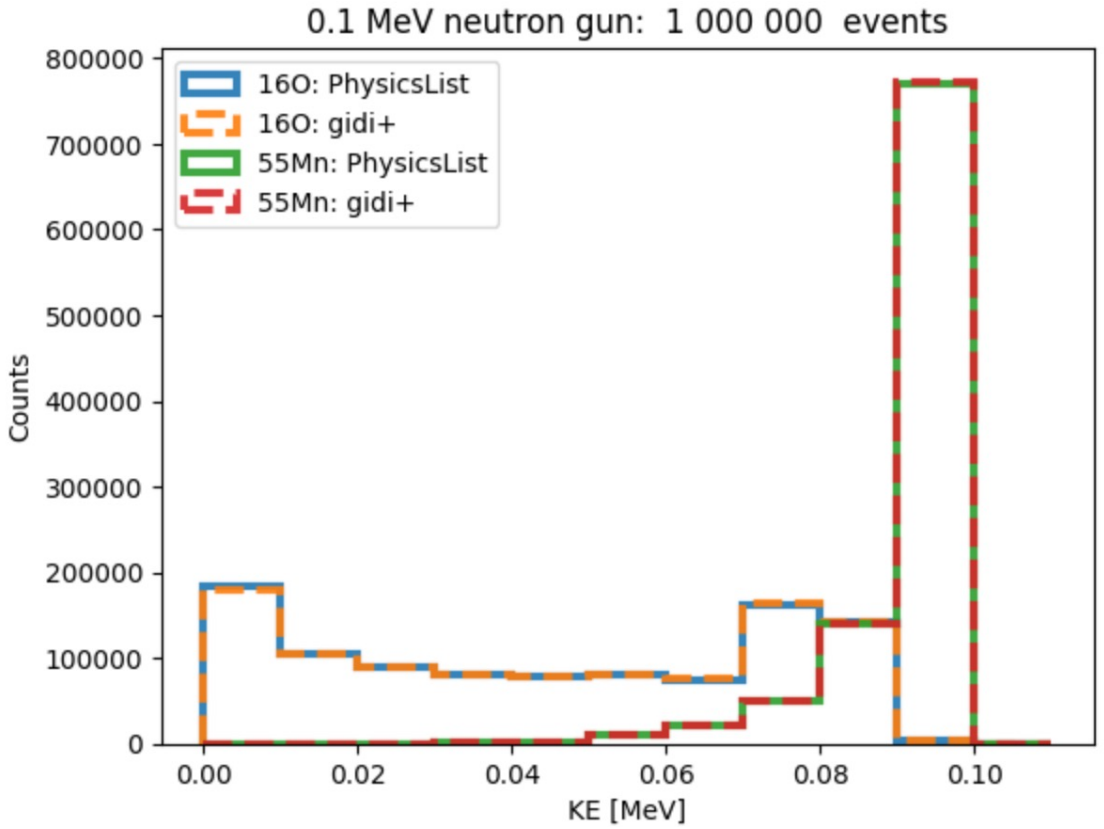
Task 3: making it all work

Task 3: Integration and validation

GIDI is now working as an event generator in GEANT4 using vanilla ENDF data, but in GNDS format

https://github.com/LLNL/gidiplus

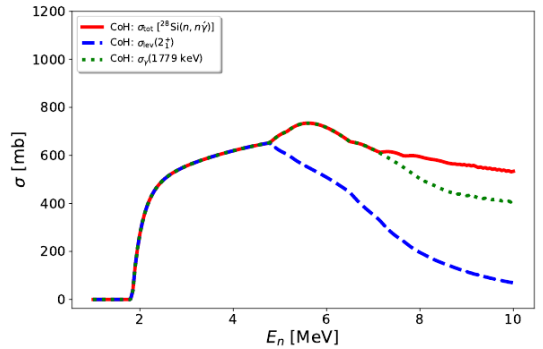
Testing inline cascade & correlation capabilities using evaluated data files

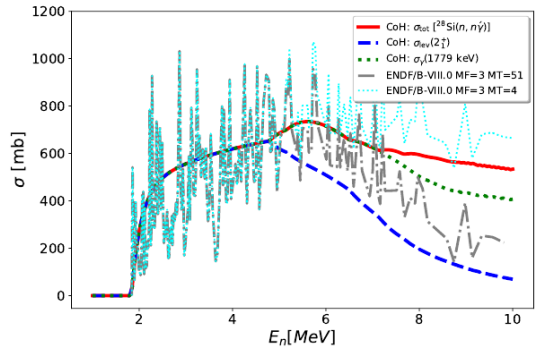


Task 3: Integration and validation

The Baghdad IRT-M Reactor and (n, n'γ) data
https://nucleardata.berkeley.edu/atlas/

CoH vs. ENDF for ^{28}Si$(n, n'\gamma)$: 1779 keV





- Deduce flux-weighted averages for all graphed quantities cf. ^{56}Fe.
- Results indicate: $\frac{\langle\sigma^{CoH}_{lev}\rangle}{\langle\sigma^{CoH}_{tot}\rangle} \approx \frac{\langle\sigma^{ENDF}_{lev}\rangle}{\langle\sigma^{ENDF}_{tot}\rangle}$.
- Find $\langle\sigma^{ENDF}_{\gamma}\rangle \approx \langle\sigma^{ENDF}_{tot}\rangle \frac{\langle\sigma^{CoH}_{\gamma}\rangle}{\langle\sigma^{CoH}_{tot}\rangle}$.

We are working hard to stand up a validation framework for outgoing gamma data

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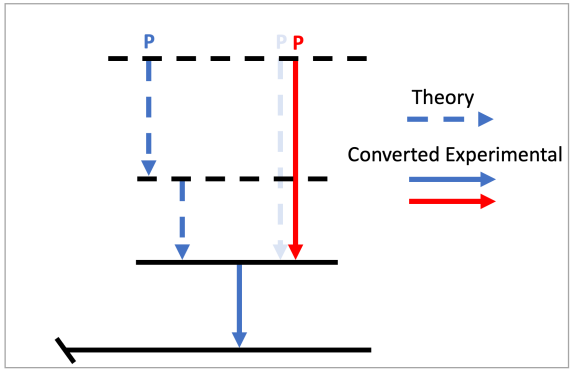
What next?

Involving students

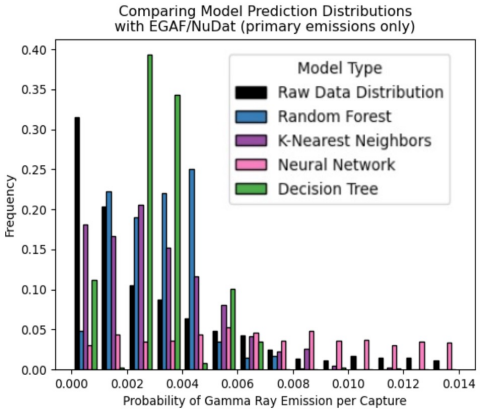
Science Undergraduate Laboratory Internships (SULI)

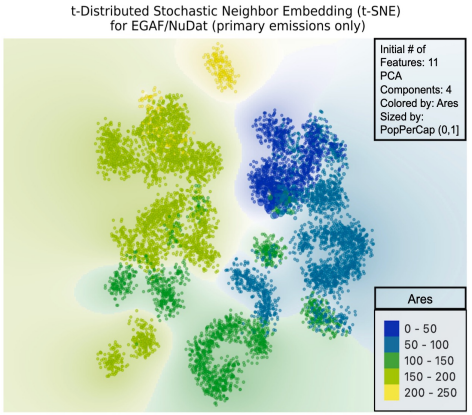
EGAF vs. RAINIER primary gammas



Ayman Abdullah-Smoot (TSU)

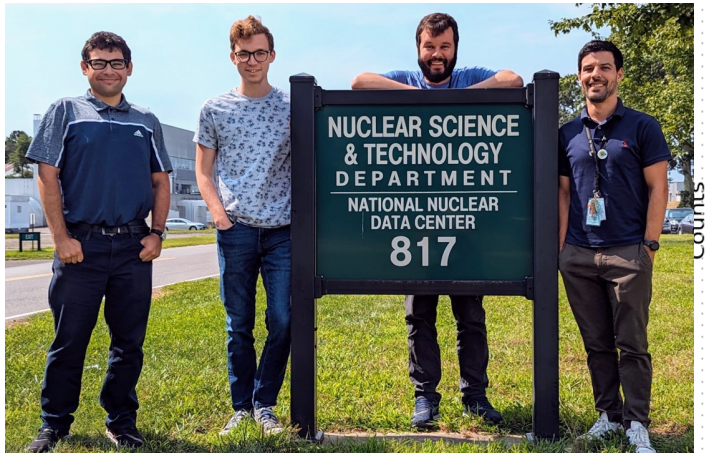
Can we model/predict Primaries with ML?

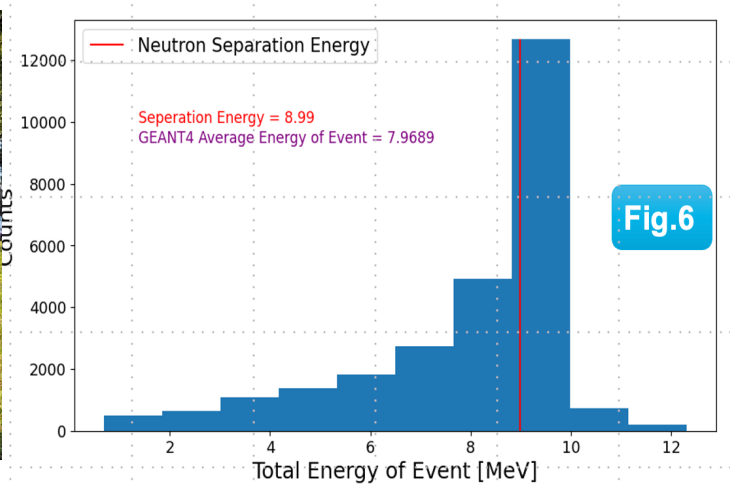




Ana Pereira (FSU)

Implementing GIDI & GRIN data in GEANT4





Michael Allen (TAMU), Mauricio Cerda (Texas Tech) & Andrea (BNL-Staff)

Two follow-on projects

- **The Berkeley Atlas: A database of absolute cross sections for inelastic, gamma-ray production with 14 MeV neutrons**
- Patrick Peplowski (Johns Hopkins University Applied Physics Laboratory)

- **Development Of Benchmark Measurements For Capture Gamma Cascades**
- Yaron Danon (Rensselaer Polytechnic University)

**We are working hard to stand up a validation framework for outgoing gamma data,
but this is a bigger job than GRIN can handle**

Reports and codes

- Aaron M. Hurst et al., pyEGAF: An open-source Python library for the Evaluated Gamma-ray Activation File, Nucl. Instrum. Methods Phys. Res. Sect. A 1057, 168715 (2023); doi:10.1016/j.nima.2023.168715; URL https://pypi.org/project/pyEGAF/
- 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 inelastic and capture gamma-ray production evaluations 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
- 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)
- C. Mattoon, B. Beck and G. Gert, “Managing and Processing Nuclear Data Libraries with FUDGE”, EPJ Web of Conferences 284, 14010 (2023), https://doi.org/10.1051/epjconf/202328414010
- A.M.Hurst, R.B. Firestone, E.V. Chimanski, pyEGAF: Modernization of the EGAF database, J. Radioanal. Nucl. Chem. (2024); doi:10.1007/s10967-023-09316-2
- 7 evaluations (to date) included in ENDF/B-VIII.1 beta libraries