CASCADE: a data-driven implementation of the neutron capture gammas in GEANT4

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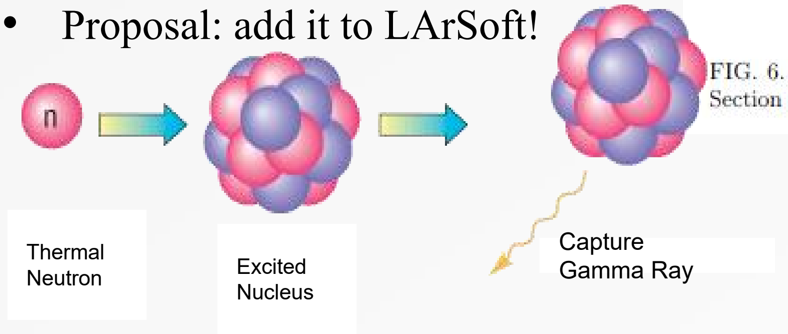
Pulsed neutron source call, DUNE Collaboration - 22 August 2024

Introduction

- Neutron capture gammas: fundamental for DUNE background and signal for MeV-scale searches, as well as the PNS calibrations
- Class in GEANT4 developed by Leo Weimer, with the supervision of Prof. Westerdale, motivated by MeV-scale searches in liquid argon detectors
- Proposal: add it to LArSoft!



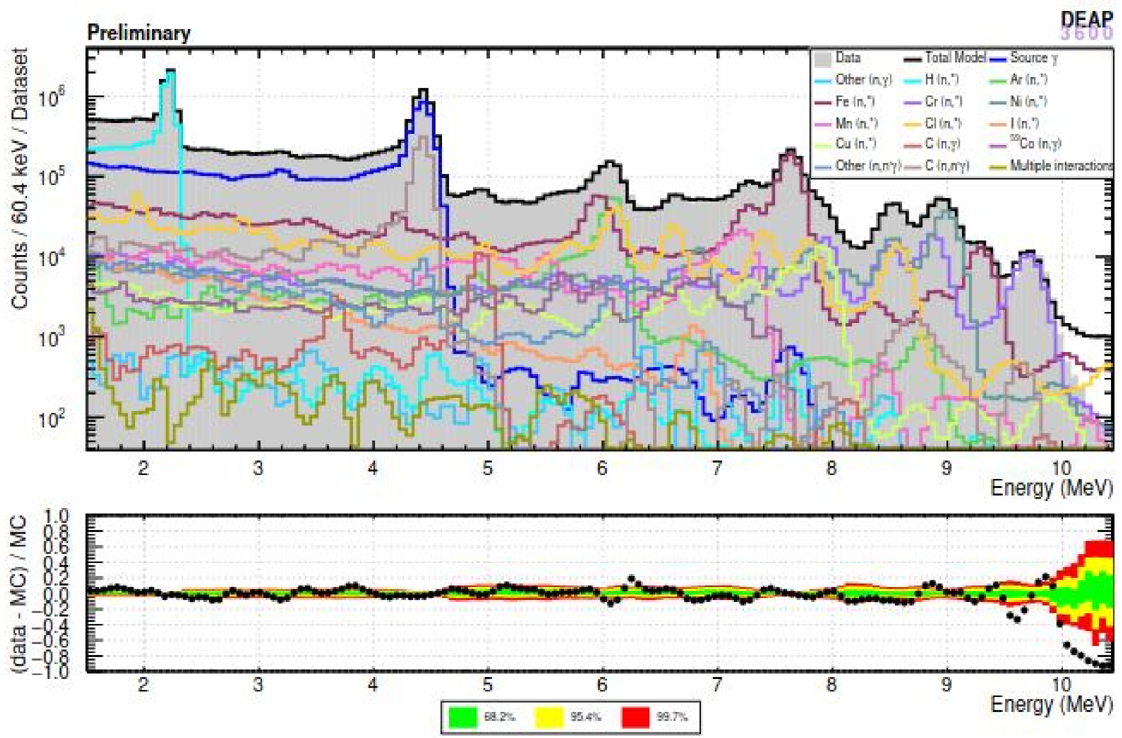
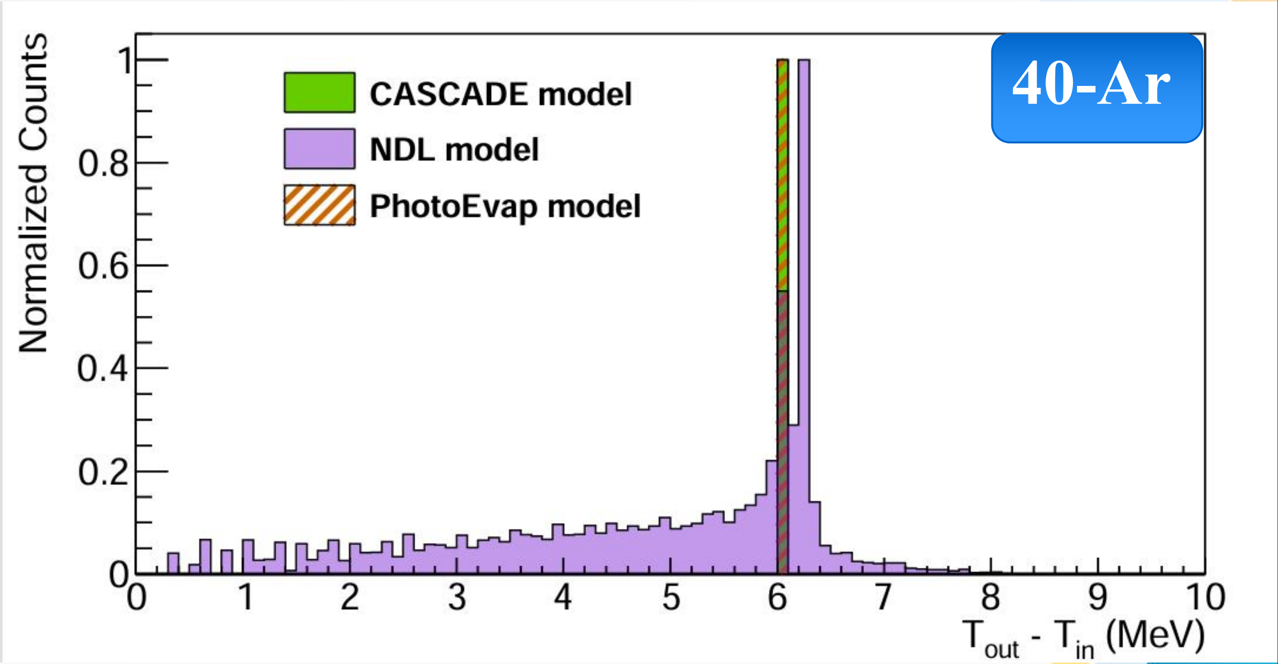


FIG. 6. The complete AmBe BAT fit that provided the response function priors for the physics fit discussed in Section VIII B. The lower plot includes statistical and systematic uncertainties.

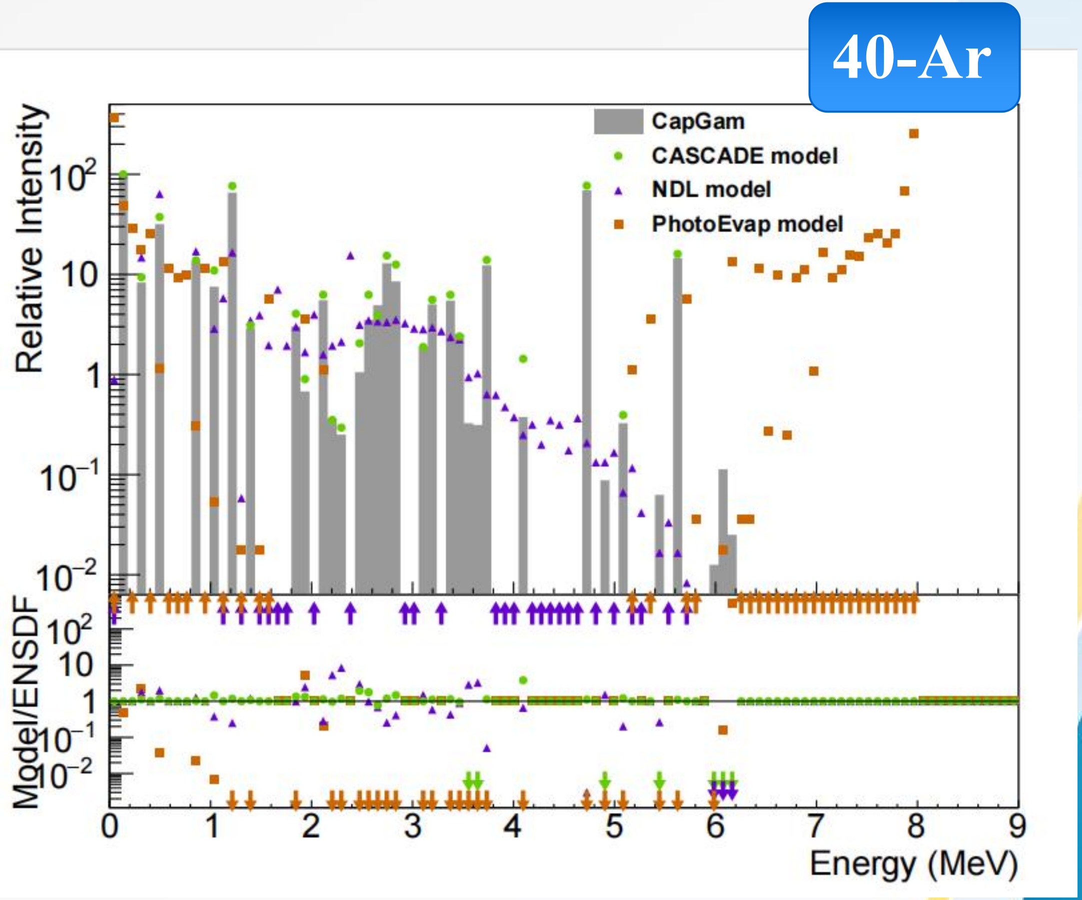
G4NDL

- G4NDL models <20 MeV neutron transport using data libraries for cross-sections, probability functions, and energy-angle distributions for emitted particles, when available
- Still does not conserve the energy of the gammas, giving a broad distribution for the Q-value



G4Photoevaporation

- G4Photoevaporation generated the gamma cascade according to statistical models
- Energy is conserved, but huge discrepancy with the relative gamma intensity (observed intensity normalized to the maximum intensity)
- CASCADE clearly improves the agreement, while still assuring the energy conservation

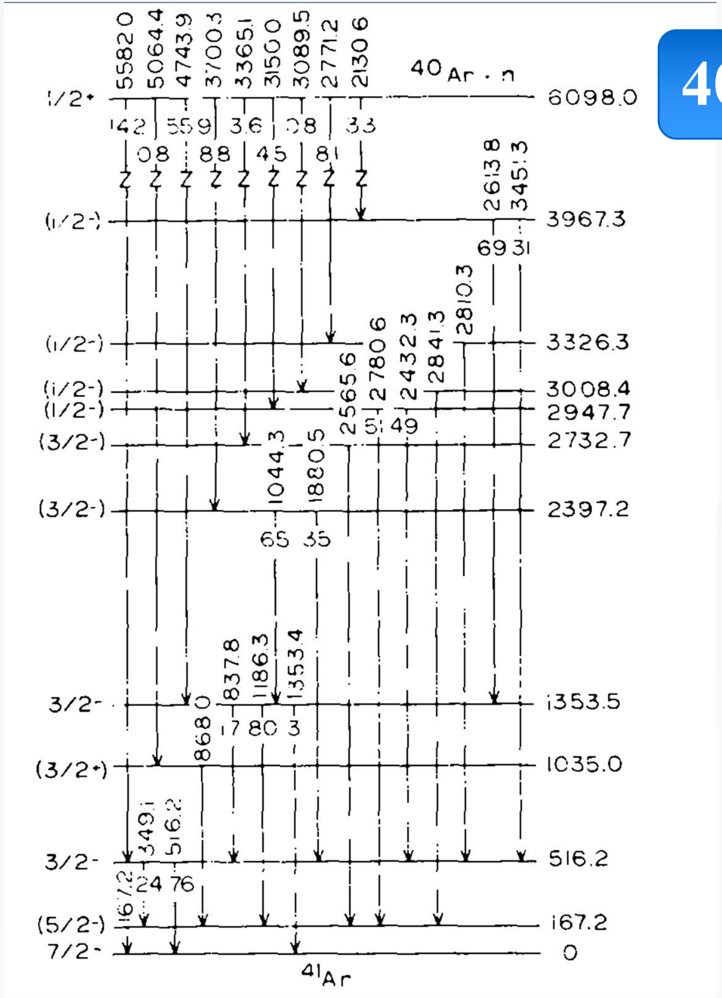


The gamma-cascade

- Looking in more detail, here is the gamma cascade as generated in G4Photoevaporation

- gamma: energy =   516 keV
- gamma: energy = 1.825 MeV
- gamma: energy = 167.3 keV
- gamma: energy = 867.4 keV
- gamma: energy = 167.3 keV

This clearly does not agree with the actual gamma cascade as measured, messing the relative gamma intensities



40-Ar

CASCADE

$$\mathrm{BR} = \mathtt{RI}.$$

$$\mathrm{BR} = \frac{\mathtt{TI}}{1 + \mathtt{CC}}.$$

- CASCADE: Geant4 **C**ode for **A**llowing **S**imulation of n-**C**apture and **D**e-excitation with **E**NSDFgamma
- It simulates de-excitation by moving down the level structure according to branching ratios
- For each transition, the Relative Intensity (RI) and the Total Intensity (TI) are multiplied by normalization factors, NR and NI

CASCADE

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- For each transition, the Relative Intensity (RI) and the Total Intensity (TI) are multiplied by normalization factors, NR and NI
- If also a conversion coefficient CC is defined, also a inner shell conversion electron is emitted. giving atomic relaxation and Auger cascades handled by G4RDAtomicDeexcitation

- Electrons removed from the atom according to fixed percentages.
  - Emitted from K shell with 89% probability
  - Emitted from L shell with 8.9% probability
  - Emitted from M shell with 1.8% probability

$$\mathrm{BR}_\gamma = \mathtt{RI} \text{ or } \frac{\mathtt{TI}}{1 + \mathtt{CC}}$$

$$\mathrm{BR}_e = \mathrm{BR}_\gamma \times \mathtt{CC}.$$

CASCADE

Example of the simulated n, gammas on 40-Ar in CASCADE :

- gamma: energy = 2.131 MeV
- gamma: energy = 2.614 MeV
- gamma: energy = 1.187 MeV
- gamma: energy = 167.3 keV

Data shows consistent correlation with level structure!

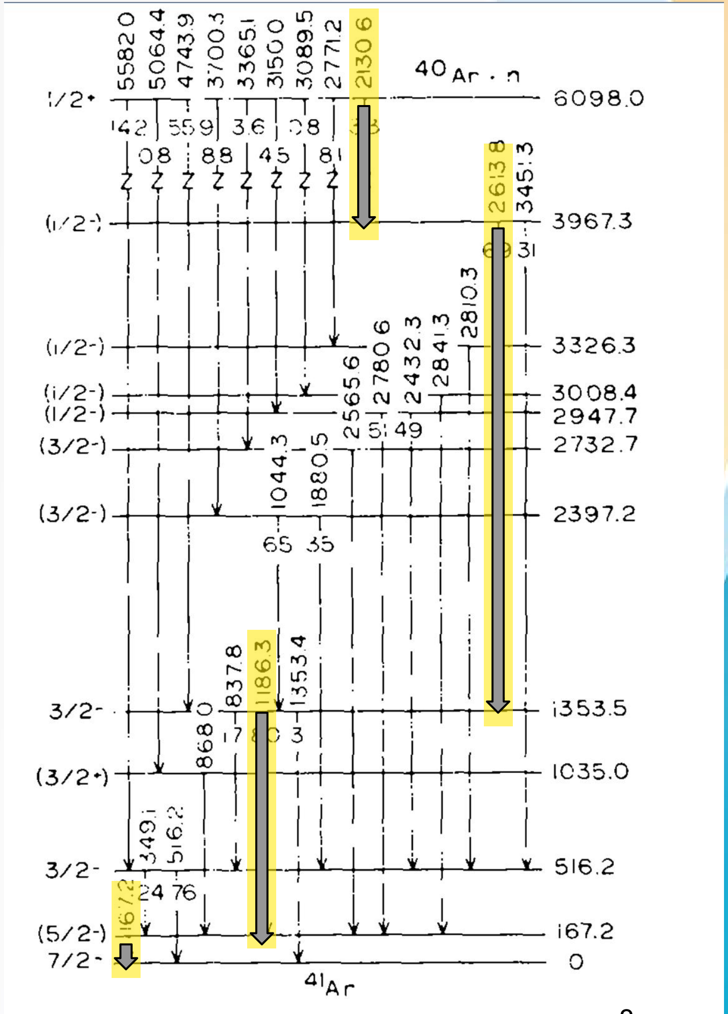
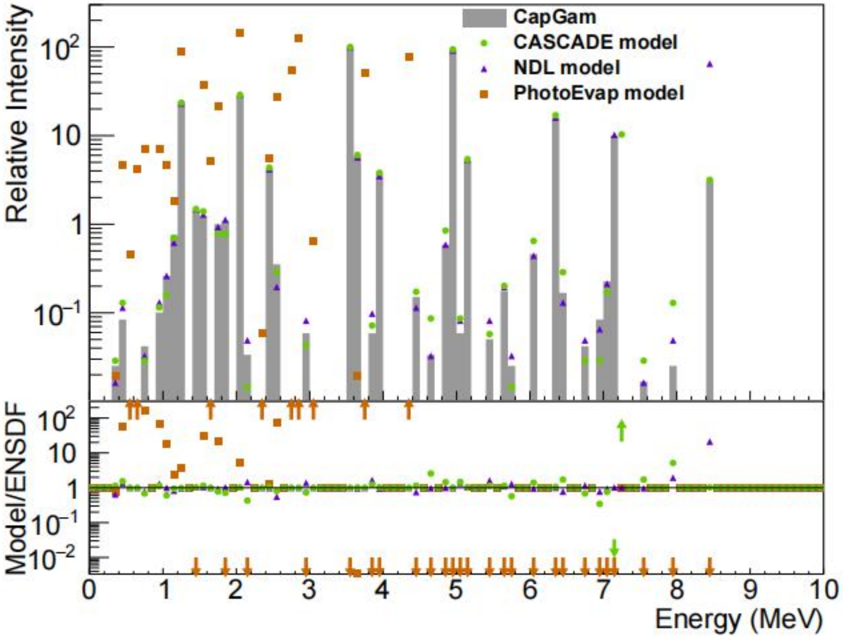


Fig. 5. Decay scheme for the $^{40}Ar(n,\gamma)^{41}Ar$ reaction.

Unplaced Gammas?

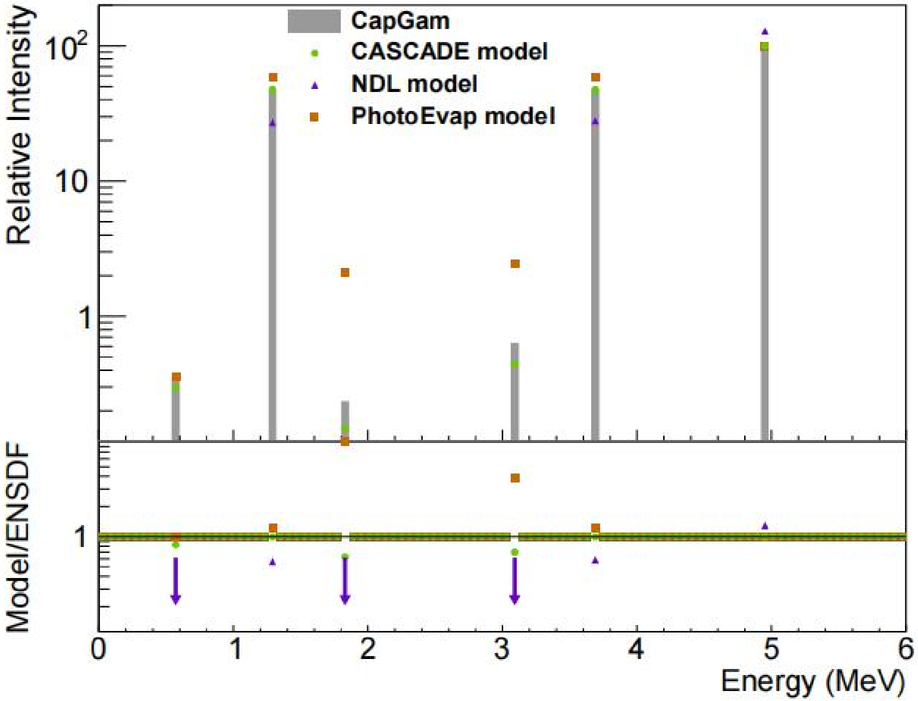
- The biggest challenge for CASCADE is the lack of ENSDF neutron capture data for some isotopes.
- Some gammas in ENSDF are not placed in a particular level. These are optionally simulated in CASCADE by going from the top level to a dead end level using this gamma, then deexciting from there using Photon Evaporation.
- Photon Evaporation conserves energy, and prevents high energy non-physical gammas from forming.
- Relative intensity agreement is maximized by having this option disabled, but it can be useful for producing specific peaks which otherwise wouldn't have appeared, especially in high Z isotopes.

28-Si



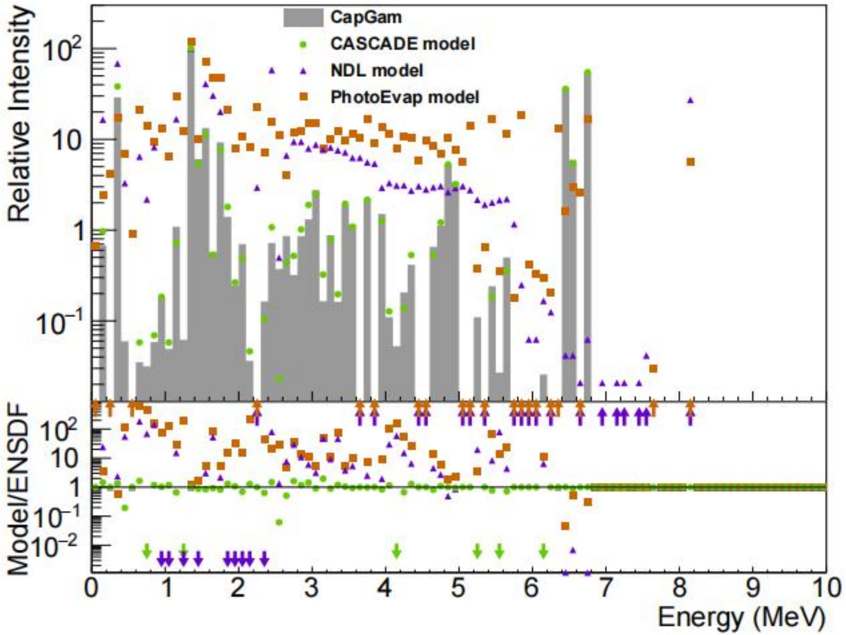
CapGam
CASCADE model
NDL model
PhotoEvap model
Relative Intensity
Model/ENSDF
Energy (MeV)

12-C



CapGam
CASCADE model
NDL model
PhotoEvap model
Relative Intensity
Model/ENSDF
Energy (MeV)

48-Ti


CapGam
CASCADE model
NDL model
PhotoEvap model
Relative Intensity
Model/ENSDF
Energy (MeV)

56-Fe

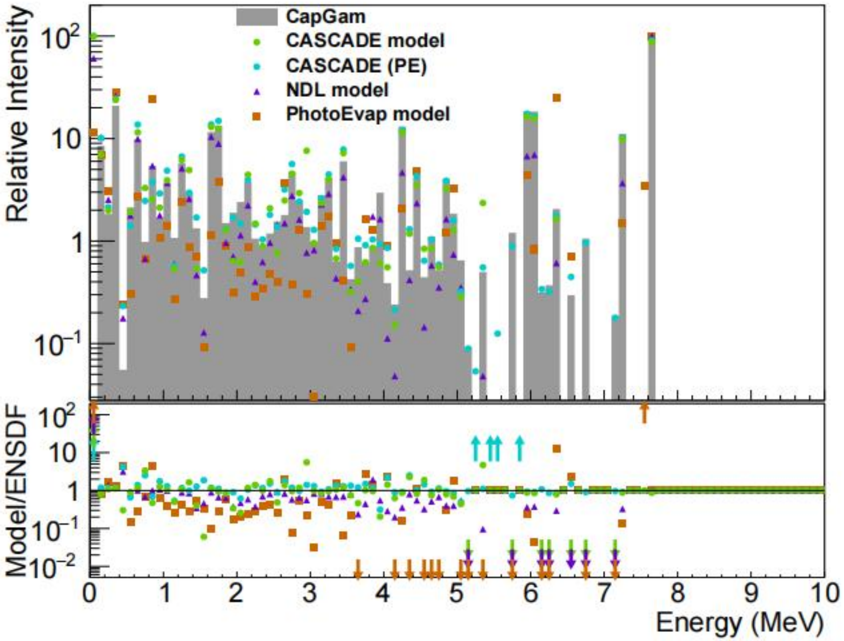

CapGam
CASCADE model
CASCADE (PE)
NDL model
PhotoEvap model
Relative Intensity
Model/ENSDF
Energy (MeV)

Table 1 Comparisons for G4NDL, G4PhotonEvaporation, G4CASCADE, and G4CASCADE with unplaced γ-ray lines completed by G4PhotonEvaporation, color-coded according to RMS (blue for lowest, indigo second, purple third, and red for highest). Three metrics summarize residuals (model − data): (top) maximum, (middle) average, and (bottom) RMS.

Isotope		G4NDL	G4PhotonEvaporation	G4CASCADE	G4CASCADE (PE)
^{12}C	Max	27	10	0.20	0.20
	Mean	0.55	-0.24	0.0072	0.0072
	RMS	3.8	1.5	0.035	0.035
^{28}Si	Max	64	100.	10.	10.
	Mean	-0.68	-1.5	-0.028	-0.028
	RMS	6.4	20.	1.4	1.4
^{40}Ar	Max	69	58	10	10
	Mean	0.48	-1.6	-0.49	-0.49
	RMS	9.6	8.5	1.7	1.6
^{48}Ti	Max	70.	46	9.8	10.
	Mean	-4.1	-4.6	-0.069	-0.11
	RMS	14	11	1.0	1.1
^{56}Fe†	Max	12	23	7.3	6.0
	Mean	0.68	0.74	-0.27	-0.38
	RMS	2.2	4.5	1.3	1.1
^{129}Xe	Max	39	100.	47	40.
	Mean	-2.6	-3.6	-0.91	-3.0
	RMS	5.8	16	6.9	7.6
^{155}Gd	Max	56	91	91	91
	Mean	1.3	2.7	3.1	2.0
	RMS	11	19	17	18

† Neglecting the 14 keV γ-ray emitted by the first excited state, the intensity of which is not unambiguously measured

Future steps

- So far for Geant v.10, need to extend to Geant4 v.11
- Comparison with other neutron capture improvements (FIFRELIN, etc.)
- More complete nuclear level data would improve CASCADE performance
- Grad student from UCR will work on the integration with LArSoft

ArXiv:2408.02774

https://github.com/UCRDarkMatter/CASCADE