(α,n) yield calculations with NeuCBOT

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(α,n) yield in low background experiments

Workshop in CIEMAT, Madrid (2019)

NeuCBOT
(nook-bot)

- Neutron Calculator Based On TALYS
  - https://github.com/shawest/neucbot/
  - Westerdale, S., and P. D. Meyers. “Radiogenic Neutron Yield Calculations for Low-Background Experiments.” NIM A 875 (Dec, 2017): 57–64.
- Design principles:
  - Easy to use (Python, not Fortran!)
  - Flexible

User inputs

- Material composition
  - List of…
    - Chemical symbols
    - Mass numbers (0 for natural abundance)
    - Percent mass

```
# Example Semi-Heavy Water
H 1 5.3
H 2 10.5
O 0 84.2
```

- α energy list **OR**
  - List of…
    - Energy [MeV]
    - Percent relative intensity

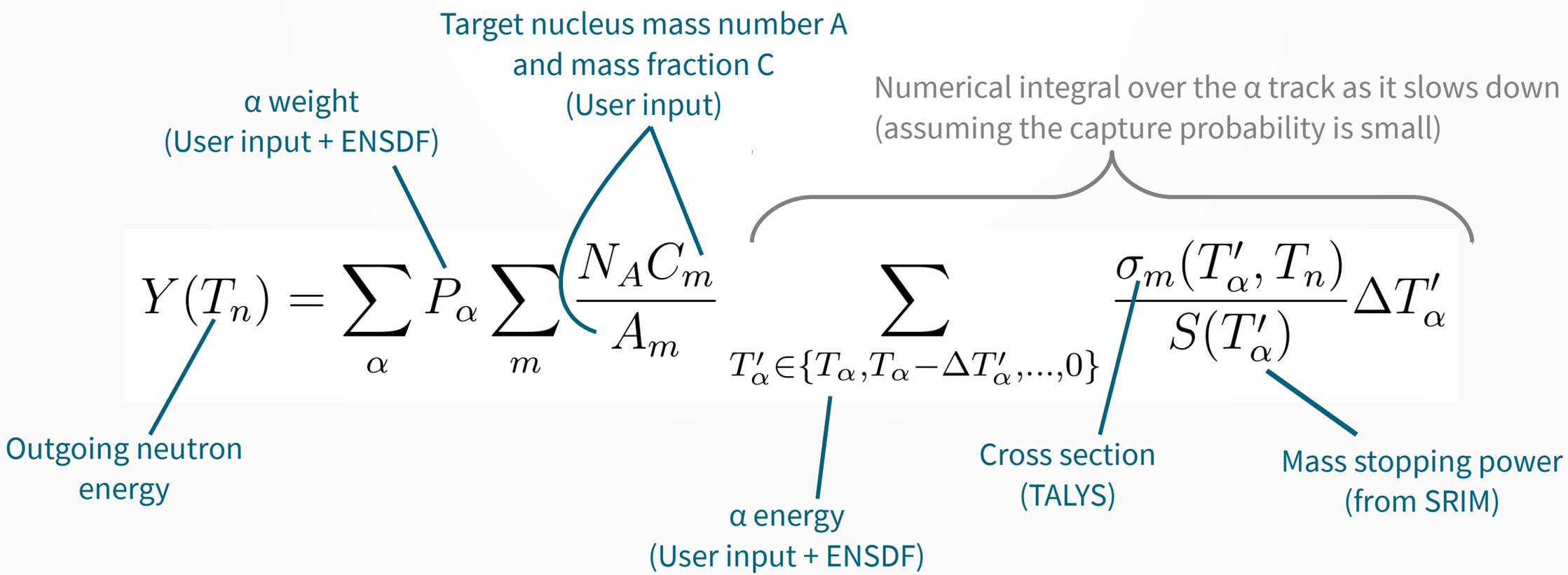
```
# Example Alpha Source
5 100
6 50
```

- Isotope list
  - List of…
    - Isotope symbol
      - (e.g. Th232)
    - Percent relative intensity

```
# Th232 Decay Chain Alpha-emitters
Th232 100
Th228 100
Ra224 100
Rn220 100
Po216 100
Bi212 35.94
Po212 64.06
```

Decay info scraped from NNDC's ENSDF database and compiled into a local database

The underlying calculation



Speeding up calculations with an effective α spectrum, rather than simulating each α individually

```
# Example α list
6  30
5  100
4  20
3  90
```

Two possible executions →

$$0.30\int_0^6 f(x)dx + 1.0\int_0^5 f(x)dx + 0.20\int_0^4 f(x)dx + 0.90\int_0^3 f(x)dx$$

OR

$$0.30\int_5^6 f(x)dx + 1.3\int_4^5 f(x)dx + 1.5\int_3^4 f(x)dx + 2.4\int_0^3 f(x)dx$$

NeuCBOT does this, because it is faster

Databases: downloaded by default

- NeuCBOT comes with some data automatically, and generates a local database with additional data as needed
- Elemental isotopic abundance:
  - ./Data/abundances.dat
  - From P. De Bievre and P.D.P. Taylor, “Table of the isotopic compositions of the elements,” Int. J. Mass Spectrom. Ion Phys. 123, 149 (1993).
  - Used for determining default abundances when “0” is specified for the mass number in the material file – relevant for slowing and capturing α’s
- Elemental stopping powers:
  - ./Data/StoppingPowers/*.dat (* = chemical symbol, lower case)
  - One file for every element
  - Contains SRIM stopping power tables for α’s in pure element from 10 keV to 10 MeV)

Databases: Populated as needed

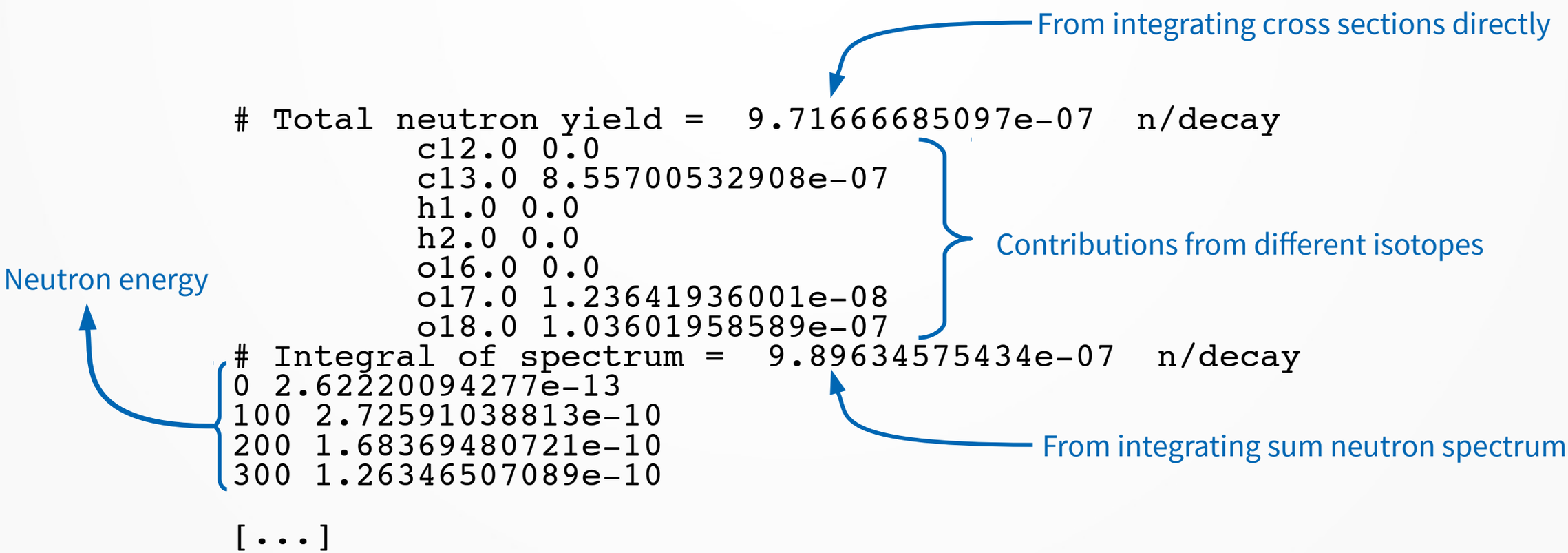
- Isotope decay data:
  - ./Data/Decays/ensdf[Isotope].dat
  - Populated when NeuCBOT is run with an isotope list by retrieving ENSDF files from NNDC's website
  - Contains α-decay data about the isotope (energy and branching ratio) – can also be used to retrieve data about correlated γ emission, but not implemented yet
- Cross section calculations:
  - ./Data/Isotopes/[Ele]/[Isotope]/NSpectra/ – neutron energy spectrum, generated by TALYS
  - ./Data/Isotopes/[Ele]/[Isotope]/TalysInputs/ – auto-generated input files for running TALYS
  - ./Data/Isotopes/[Ele]/[Isotope]/TalysOut/ – detailed output file from TALYS describing α reactions, outgoing γ's and excited daughters
  - Can be auto-generated by a local installation of TALYS (-t option) or pulled from a pre-generated database with TALYS-1.6 (-d option)
    - Pre-generated database contains data for all naturally occurring isotopes for α energies up to 10 MeV

Usage

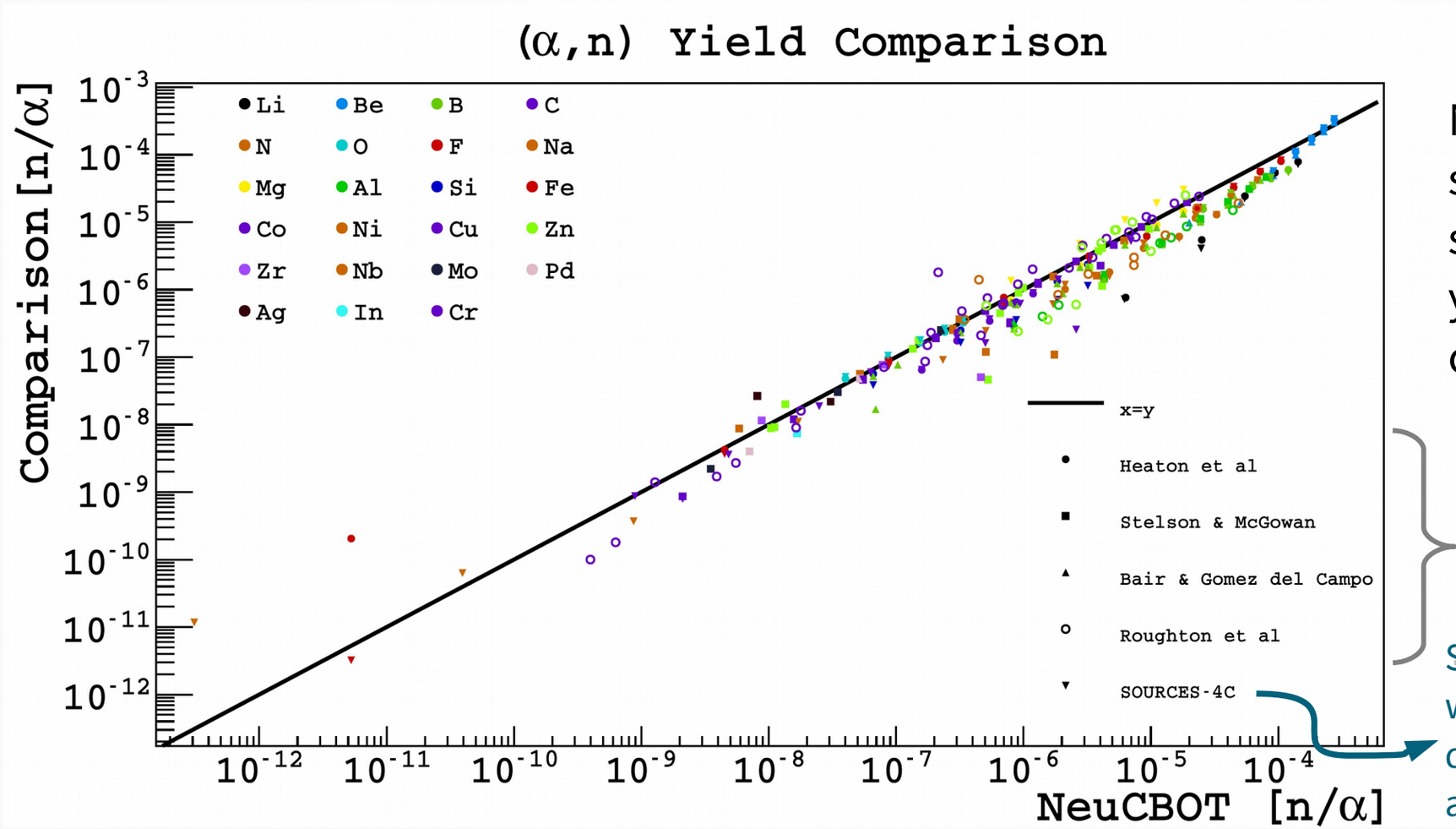
```
./neucbot.py -h
Usage: You must specify an alpha list or decay chain file and a target material file.
You may also specify a step size to for integrating the alphas as they slow down in
MeV; the default value is 0.01 MeV
    -l [alpha list file name]
    -c [decay chain file name]
    -m [material composition file name]
    -s [alpha step size in MeV]
    -t (to run TALYS for reactions not in libraries)
    -d (download isotopic data for isotopes missing from database)
    -o [output file name]
```

- ./neucbot -c Chains/Rn222Chain.dat -m Materials/Acrylic.dat -o outputRn22inAcrylic.dat

Example output



Yield comparisons to other calculations

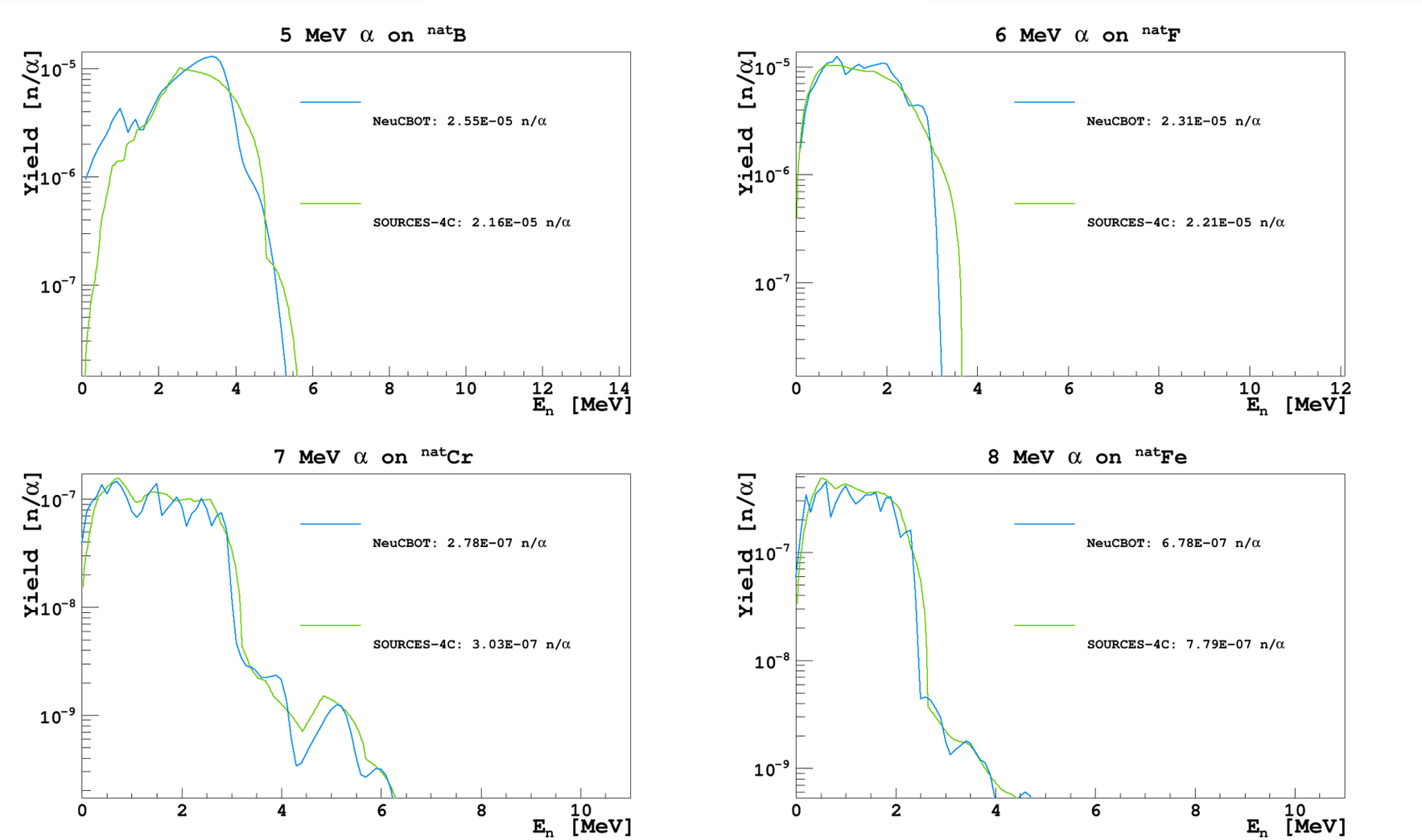


NeuCBOT systematically gives somewhat higher yields than other calculations by ~30%

Direct (α,n) measurements

S4-C calculations, with JENDL when available (typically same data as above measurements), and EMPIRE cross sections when not

Neutron spectra generally agree with SOURCES-4C, but with typically sharper features

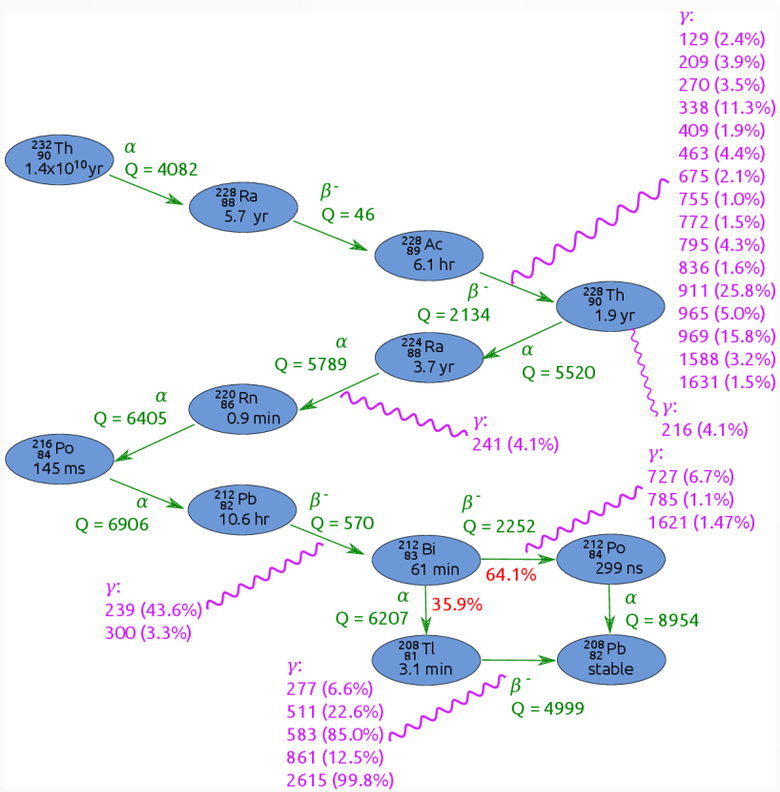


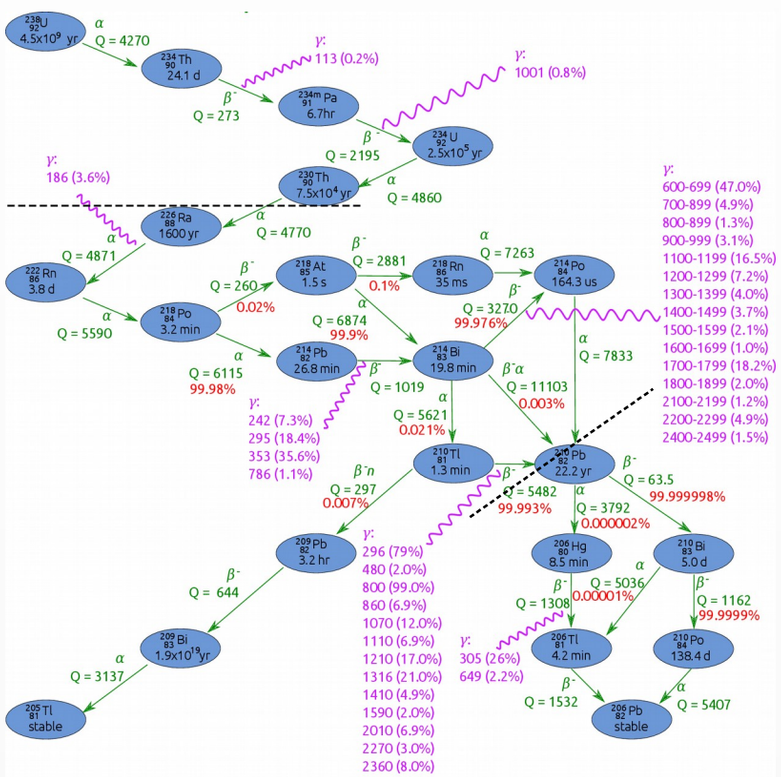
Uncertainties in (α,n) calculations: In NeuCBOT and more generally

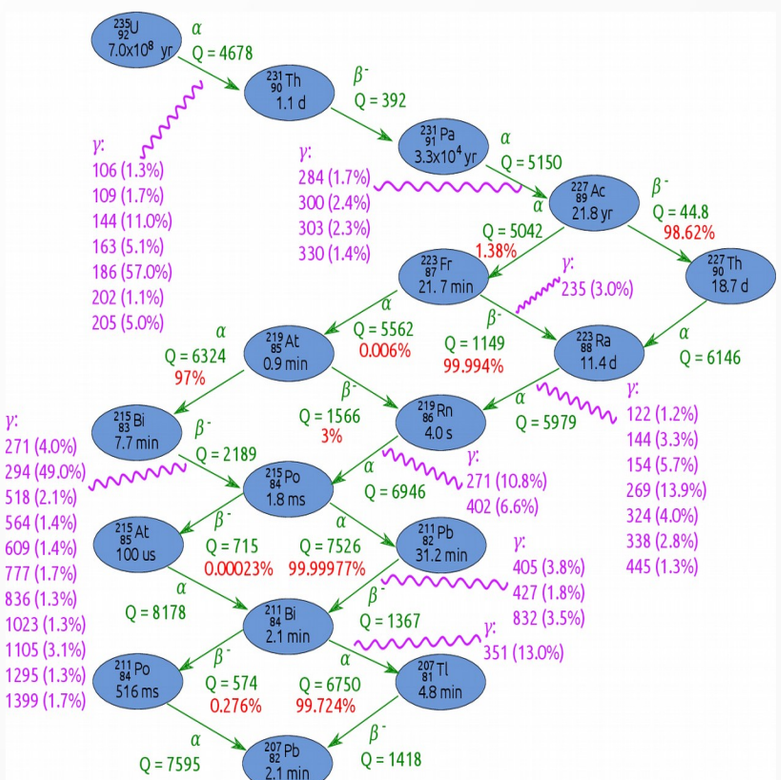
- Materials
  - **Material compositions:** for some proprietary materials, the exact composition is left vague by the supplier; for others, industry tolerances may allow for significant variation
    - E.g. for 304L stainless steel, companies seem to report compositions that vary by ~5% for most elements, and C, Mg, P, S, Si, N are reported as upper limits
    - A few percent uncertainty in composition is small, but whether or not an isotope appears at all can make a bigger difference
  - **Natural abundances:** there is some variance and uncertainty in reported isotopic abundances between references; most are consistent within uncertainties

Uncertainties in (α,n) calculations: In NeuCBOT and more generally

- Where to assume secular equilibrium in decay chains?
  - Typical assays are restricted to γ-emitters and the heads of chains
  - There is significant ambiguity about where the chains should actually be broken, especially ^{238}U







Uncertainties in (α,n) calculations: In NeuCBOT and more generally

- Stopping power calculations
  - NeuCBOT uses SRIM
    - Ziegler, James F., M. D. Ziegler, and J. P. Biersack. “SRIM – The Stopping and Range of Ions in Matter (2010).” NIM B, 268, no. 11–12 (June 2010): 1818–23.
    - Uses models with corrections to match data
      - For α’s, 70% of data are within 5% of calculation, 87% of data within 10%
  - Bragg’s rule for multi-elemental compounds (summing the mass stopping powers weighted by mass fractions)
    - Usually agrees with data to within 20%
    - Thrown off by chemical bonds – significant for simple molecular targets and light elements
    - SRIM can account for this w/ “Köln Core and Bond” approach, though NeuCBOT doesn’t use this
  - Another option: ICRU 49

Uncertainties in (α,n) calculations: In NeuCBOT and more generally

- Cross sections
  - NeuCBOT uses TALYS, which is largely based on theoretical nuclear models.
    - Generally pretty good, but there are some isotopes where its predictions disagree significantly with measurements
  - Another option for model-based calculations: EMPIRE
  - Compilations of cross section measurements in JENDL and ENDF/B-VIII
    - Cross section measurements are not always available for isotopes at needed energies (some of which may be significant)
    - Uncertainties on measurements are typically large (often in the 10-20% range)
    - Measurements of the same isotopes by different groups differ by up to 40%
    - There are a lot of tricky systematics in these measurements

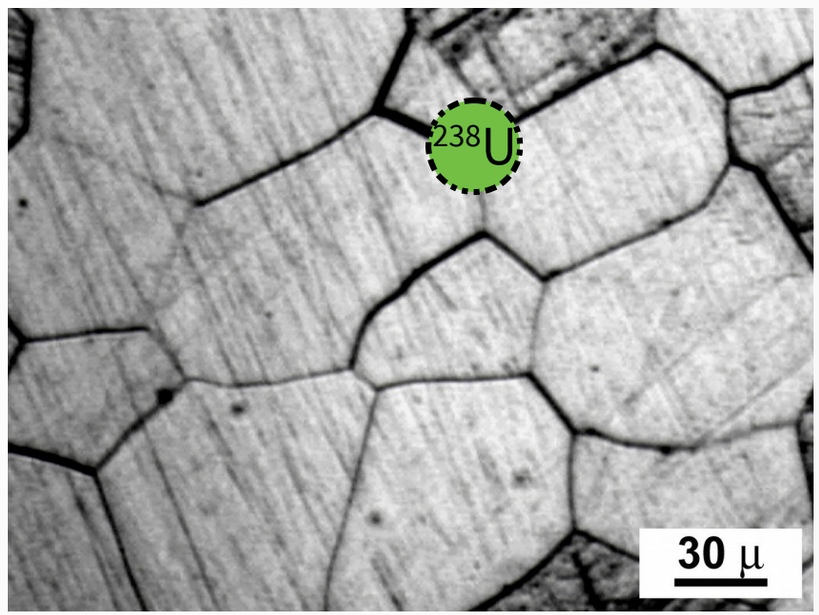
Uncertainties in (α,n) calculations: In NeuCBOT and more generally

- Neutron spectra
  - In theory, this is easy to calculate…
    - … if you know the structure of all relevant nuclei
  - NeuCBOT lets TALYS and its models handle all of this
  - In general, uncertainties and lack of knowledge regarding nuclear structure can significantly impact the neutron spectrum calculations
  - A. Robinson points out that SOURCES-4C assumes isotropy in the center of mass frame – the calculation should account for the differential cross section and the change of reference frame correctly
    - Tsujimura, N., T. Yoshida, and T. Momose. “Calculations of Anisotropy Factors for Radionuclide Neutron Sources Due to Scattering from Source Encapsulation and Support Structures.” Radiation Protection Dosimetry 126, no. 1–4 (Aug., 2007): 168–73.

How good is the homogeneous mixture assumption?

If the material has grains that are large compared to the α track length, the location of the α-emitters may actually matter, and the α won't see all isotopes equally.

This will also throw off stopping power calculations

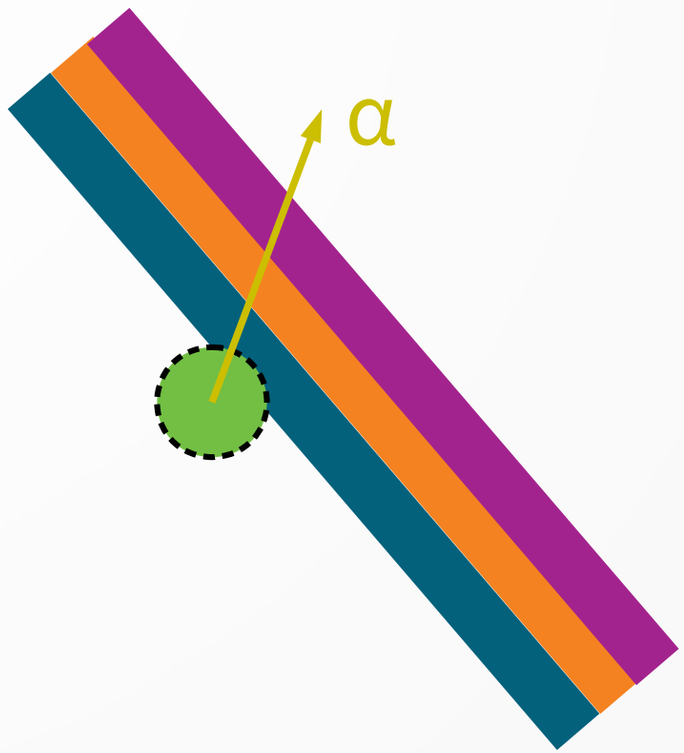


What about thin films?

NeuCBOT doesn't currently have the ability to simulate thin films (where α doesn't stop in material)

But this can be added in a future upgrade

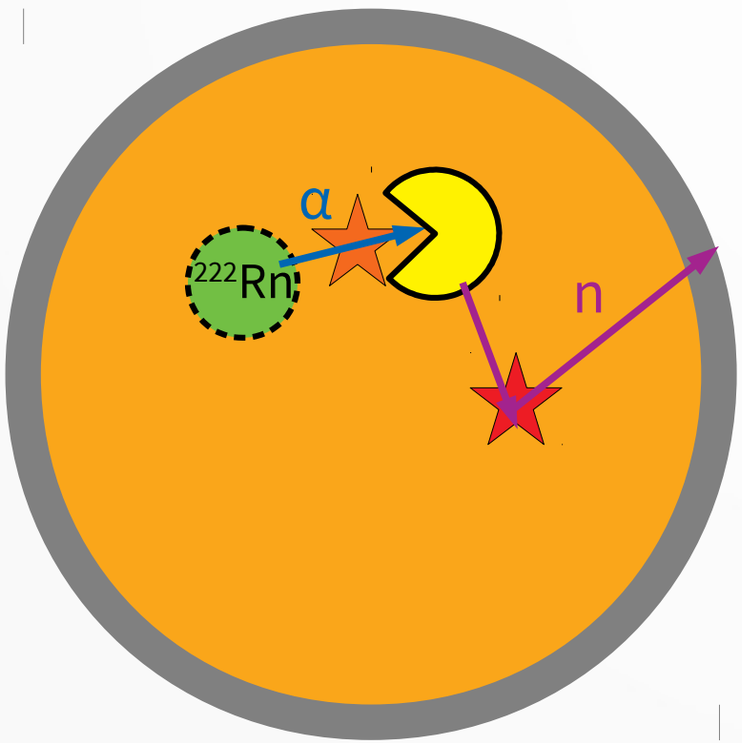
Geant4 and SOURCES-4C both have capacity to do this.



NeuCBOT wish list

- Implement option to use a graphical user interface or a web interface
- Update pre-generated TALYS database to use the latest version
- Calculate energy loss by the α before it captures
- Output γ's (or other secondaries) emitted in coincidence with the neutron
- Add the ability to perform calculations with different cross section libraries
- Add option to switch between SRIM and ICRU 49 stopping power calculations, add "Core and Bond" calculations for composite materials where possible
- Option for thin-film and multi-layer calculations
- Other ideas?

Wish list: Calculate energy lost by α before it captures



Can α-emitters dissolved in the detector's active material or plated on the surface (e.g. Rn and its progeny) produce neutron backgrounds?

Does scintillation from the α before it captures remove these events from the equation?

Wish list: Calculate energy lost by α before it captures

Speeding up calculations with an effective α spectrum, rather than simulating each α individually

```
# Example α list
6 30
5 100
4 20
3 90
```

Two possible executions →

$$0.30\int_0^6 f(x)dx + 1.0\int_0^5 f(x)dx + 0.20\int_0^4 f(x)dx + 0.90\int_0^3 f(x)dx$$

OR

$$0.30\int_5^6 f(x)dx + 1.3\int_4^5 f(x)dx + 1.5\int_3^4 f(x)dx + 2.4\int_0^3 f(x)dx$$

NeuCBOT does this, because it is faster

S. Westerdale (INFN) (α,n) yield in low bkgd experiments 5

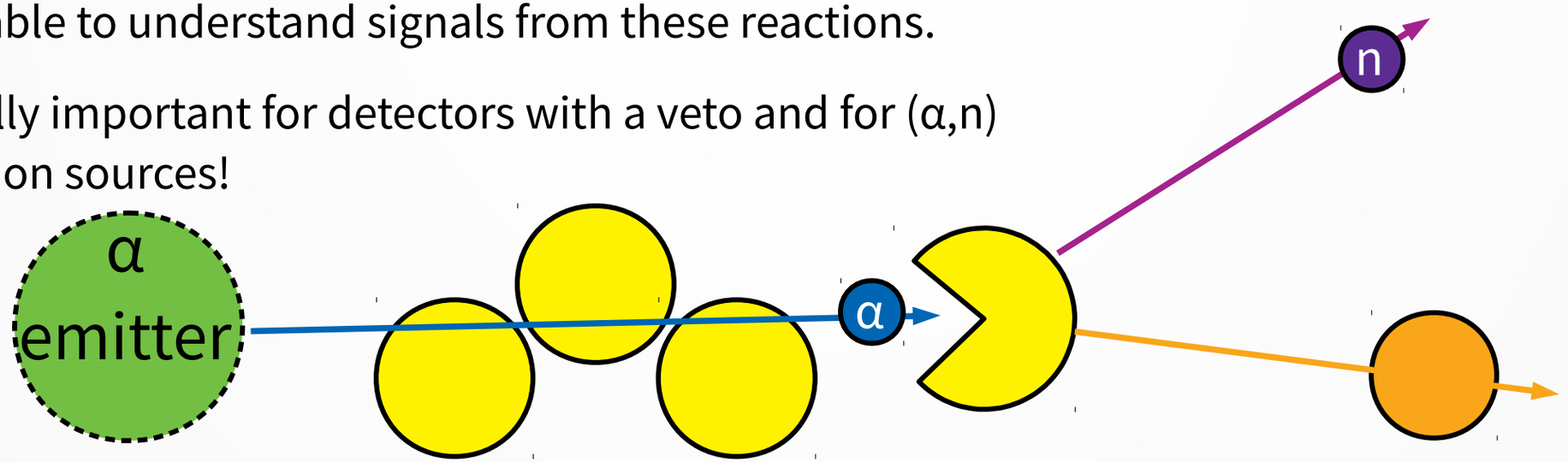
The current "fast" calculation does not track the α's initial energy, and so information about energy loss prior to capture is lost

Would need an option to use the "slow" calculation

Wish list: Output γ's (or other secondaries) emitted in coincidence with the neutron

The more of these processes we can account for, the better we will be able to understand signals from these reactions.

Especially important for detectors with a veto and for (α,n) calibration sources!



Emitted with α

Emitted by daughter of α-emitter

Emitted by inelastic collisions as α slows down

Emitted by compound nucleus

Emitted by daughter nucleus

Wish list: Add the ability to perform calculations with different cross section libraries

Other sources:

- JENDL
- ENDF/B-VIII
- EMPIRE
- User-added

Need to make sure we properly account for the differential cross section and COM→lab frame

```
# Example material file (my vision)
C 12 34.56 TALYS
C 13 12.12 JENDL
N  0 20.19 EMPIRE
O 16 33.13 ./Data/Isotopes/O/O16/CustomXSect/
```

Question: Do want a default library, or should the library be a required input?

- **Pro:** More user-friendly – users do not need to be experts and know the differences
- **Cons:** Are we prepared to vouch for one library over others by makig it default?

Other thoughts: Integration with Geant4?

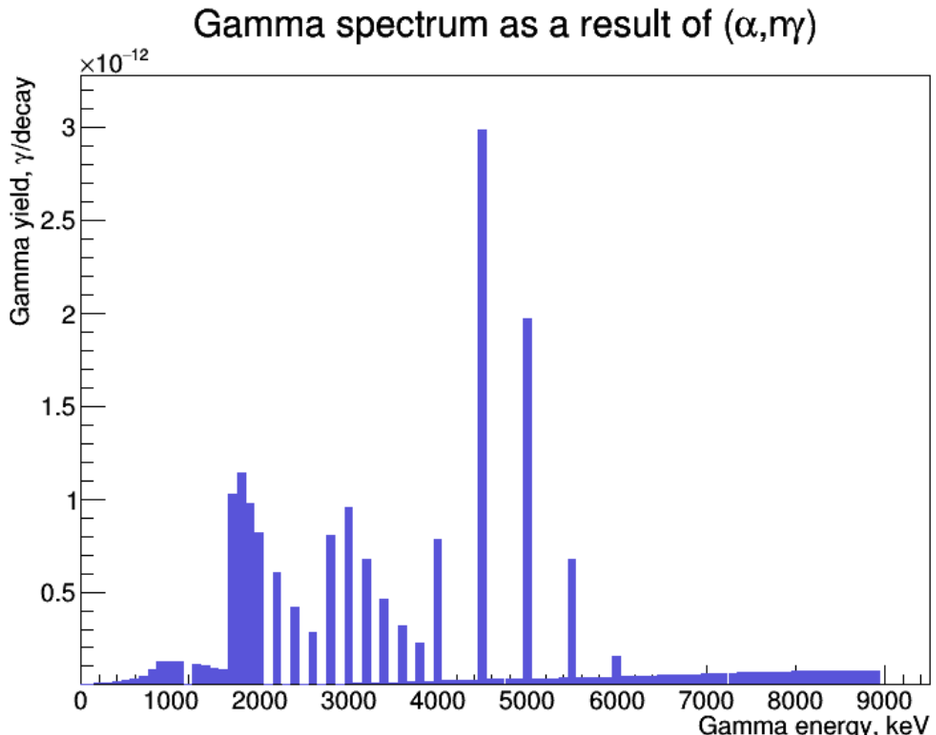
- We've seen that Geant4 can successfully simulate (α,n) reactions
  - E. Mendoza et al. "Neutron production induced by α-decay with Geant4" arXiv:1906.03903 [hep-ph] (Jun., 2019).
  - See the upcoming talk by E. Mendoza Cembranos
- Can we integrate this into the back-end or into a generator so that users can toggle between default Geant4 libraries and NeuCBOT calculations
  - This will allow for a better probe of the systematics by comparing multiple calculations from within a set Geant4 framework

Work being done

- Alan Robinson has done some work with his student Tia adding some additional cross section libraries
  - Still in progress
- Maxim Grobov and his student Vardui have added (α,nγ) calculations
  - Future plans:
    - More cross section libraries
    - Functionality to visualize and compare spectra
    - Graphical interface
- Interested in getting involved? Let me know!

Progress implementing (α,nγ) calculations

From Maxim Gromov and Vardui Barbaryan



Pure acrylic (neutron yield, n/decay)				
^{232}Th	^{235}U	^{238}U lower,	^{238}U upper	Total
1.33×10^{-6}	1.42×10^{-6}	9.72×10^{-7}	2.19×10^{-7}	3.94×10^{-6}
Pure acrylic (γ yield, γ/decay)				
1.84×10^{-10}	1.85×10^{-10}	1.29×10^{-10}	2.90×10^{-11}	5.27×10^{-10}

Conclusions

- There are a lot of interesting directions to grow NeuCBOT – feel free to contribute
- Understanding the systematic uncertainties in these (α,n) yield calculations is hairy business
  - I'm hoping NeuCBOT's flexibility makes it possible to explore these uncertainties more thoroughly
  - What are the dominant uncertainties that matter most to low background experiments? Will it be possible to reduce them? What supplementary measurements do we need?
  - A systematic understanding of all of these uncertainties would be extremely valuable
- Multiple, independent tools for calculating (α,n) yields will allow us to more thoroughly understand the range of possible yields, given the substantial uncertainties
  - Great to have multiple tools for tackling this problem!
  - With different features, they also satisfy different niches
  - Let's make sure we are all on the same page about the details – this meeting is a great way to do this

END