Radiological Simulation

DUNE FD Sim/Reco Phone Meeting
May 18, 2023

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Outline

- New radiological model
- Test run with LArSoft
- Conclusions

New radiological model

- For details on new radiological model, see slides from recent LEP WG meetings
- Activities for backgrounds from previous radiological model adjusted based on assays
- New component: external gamma-rays
    - Simulated radioactivity in cavern wall with full 10-kt FD geometry, propagated to LAr
    - Obtained new neutron and gamma-ray spectra and fluxes

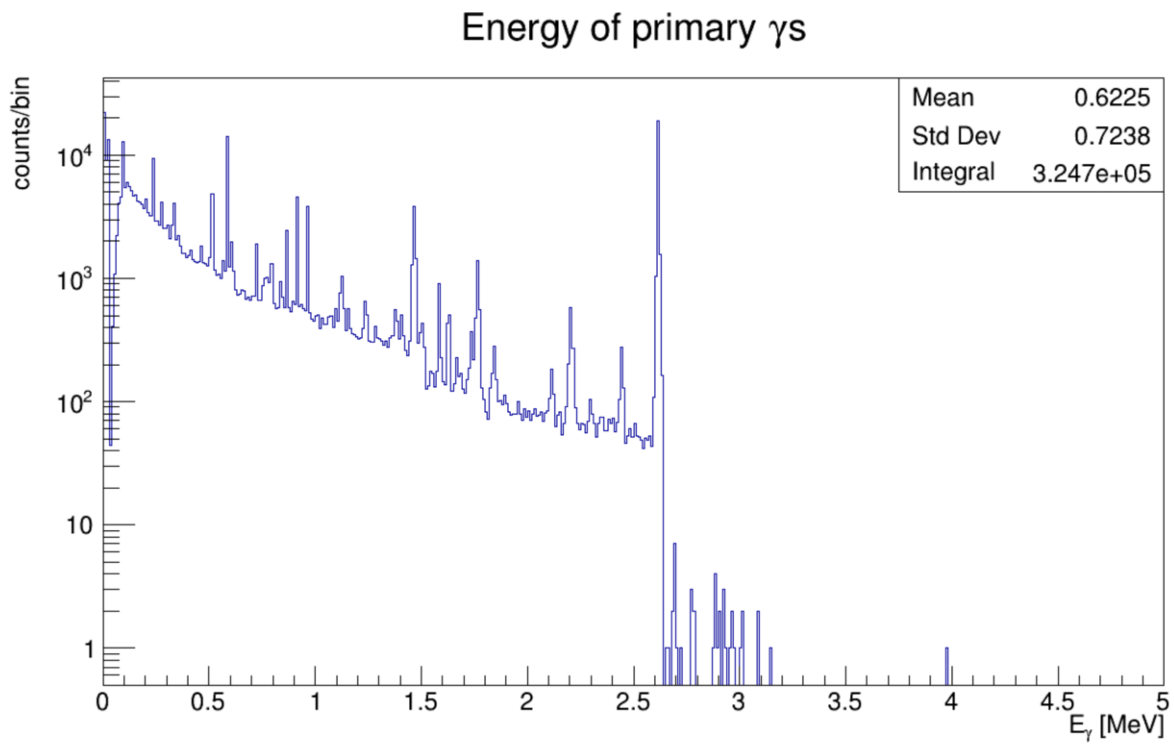
Test run with new LArSoft

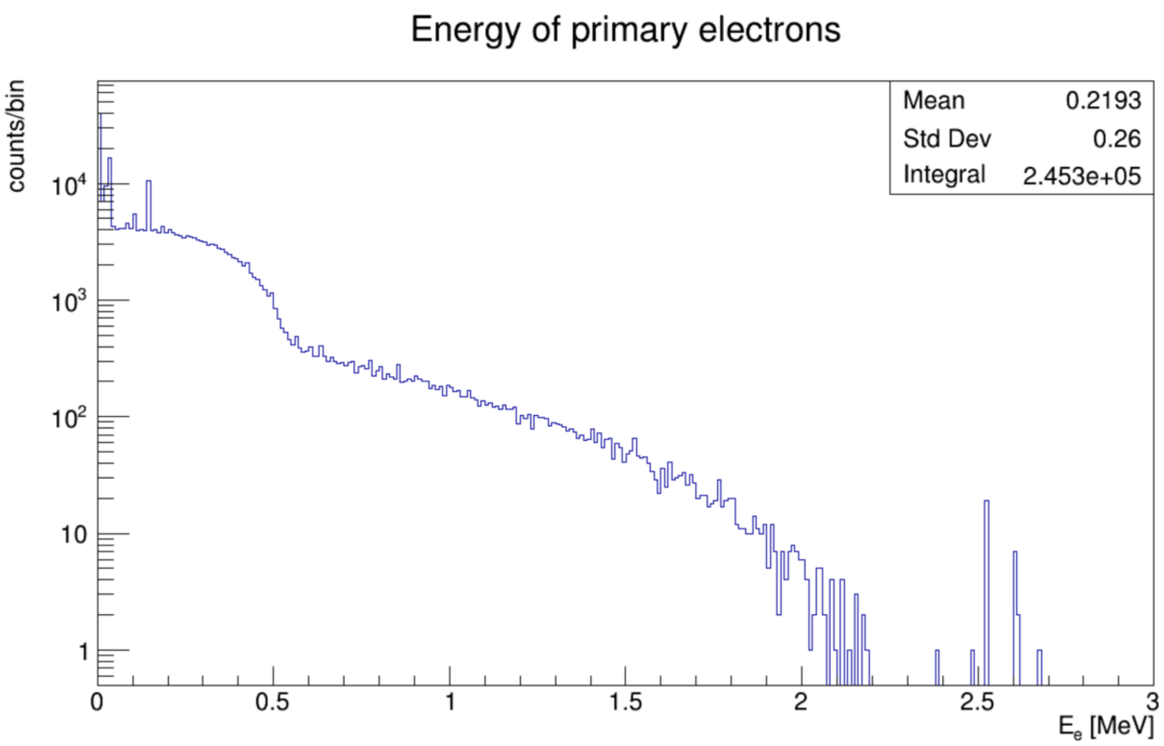
- Used DUNESW v09_72_00d00
  - Version from couple weeks ago
- Used 1x2x6 HD geometry and legacy LArG4
  - Are we planning to use refactored LArG4 for production?
- Simulated 1 event
  - Took ~1 hour total for gen, g4, detsim, reco stages
  - Resulting file ~600 MB
  - Is this acceptable for production?

Test run with old LArSoft

- Used DUNETPC v08_60_00 from ~2020
  - Use for background studies
  - Set up for quick analysis
- Simulation is faster
  - ~10 minutes per event
  - ~100 MB per event
  - What may cause this?

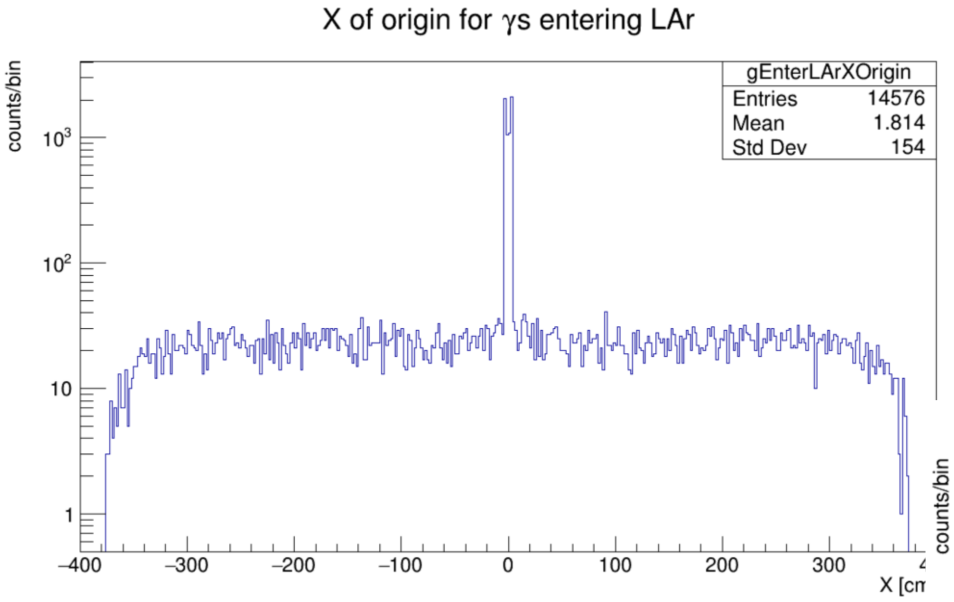
10 events with old LArSoft

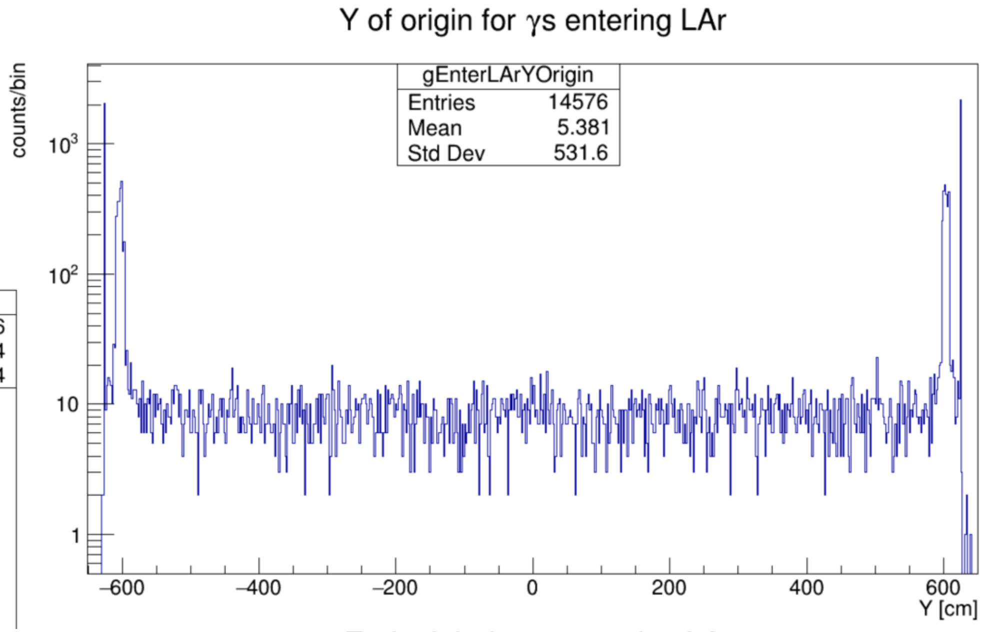


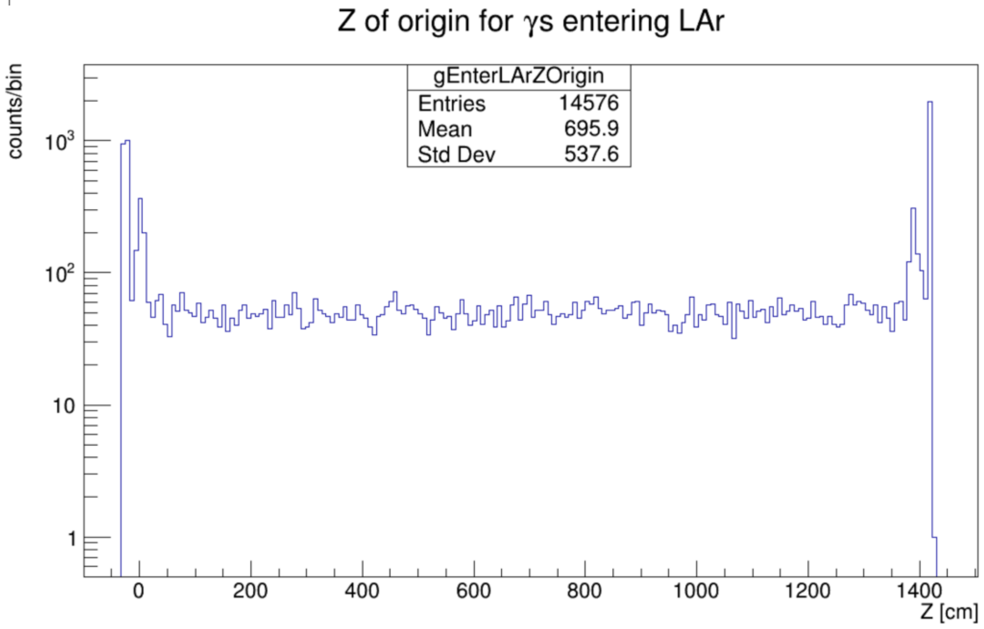


Energy spectra currently consistent with inputs
No neutrons generated

10 events with old LArSoft







Spatial distributions symmetrical and consistent with inputs

Continuing validation

- Need at least 20 seconds of simulation, better 100 seconds
  - Neutron capture rate in LAr is ~1 Hz
  - ~10,000 hours for new LArSoft (~3,000 hours for old LArSoft)
  - ~10 TB for new LArSoft (~1 TB for old LArSoft)
    - Space may not be issue if only final analysis output is recorded

Conclusions

- Produced FHiCL files for new radiological model for HD 1x2x6
    - Validating results of running them
- Finishing background FHiCL files for HD 1x2x2 and VD 1x8x14/1x8x6

Backup slides

Note on number of primary particles: fixed

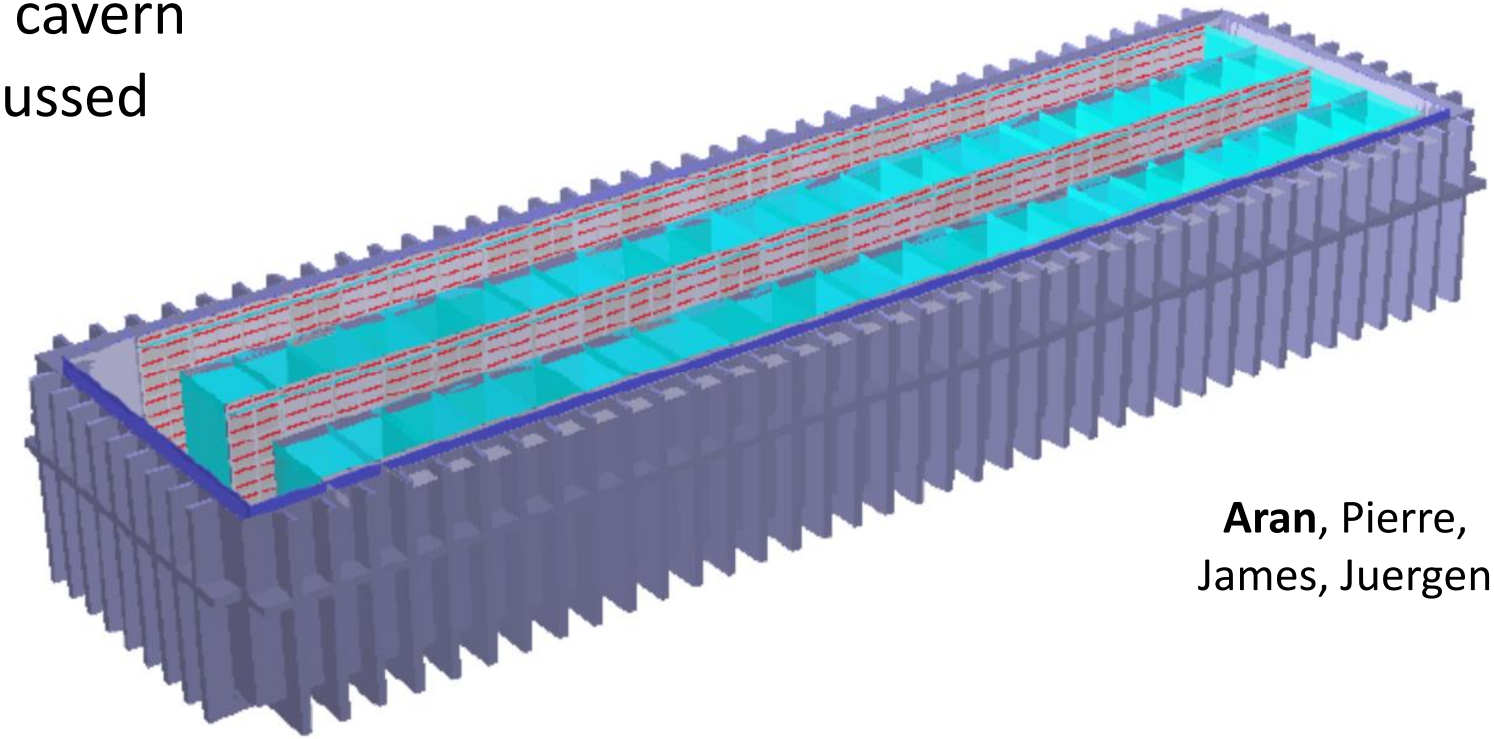
- Previously: why same number of primaries generated in each sample?
- Found that RadioGen generates same number of primaries for every job with same input parameters
  - Bug from using CLHEP method that does not use LArSoft random-number engine
    - Only affects number of primaries
- Easy fix
  - Change method used in RadioGen
    - One line of code
  - May make sense to fix this before upcoming production

LArSoft simulation

- Using DUNETPC v08_60_00 (older version from ~2020)
- Modified 10-kt geometry from Aran with inputs from our chemical assays and discussions on LBNF specifications
- Generating events with LArSoft Decay0 and RadioGen modules in cavern wall using our radiological-assay results (+Sources4 using also our chemical assays for target nuclei in previous neutron production)

10-kt DUNE Geometry

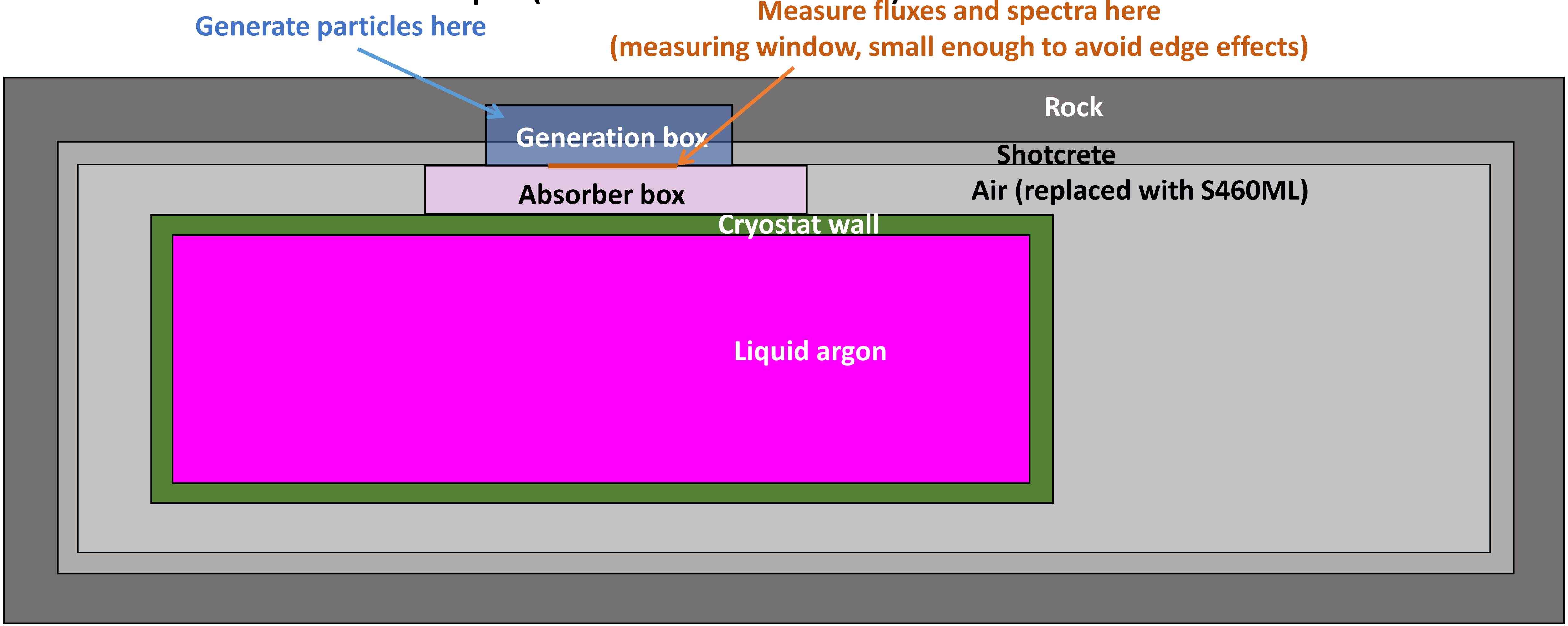
- Full HD DUNE 10-kt geometry from Aran (July 2022)
  - Includes detector, cryostat, cavern
  - Includes most changes discussed in backgrounds group
- Changed shotcrete thickness 4 inch → 6 inch
  - Important shielding effect of backgrounds from rock
  - No overlaps according to GeGeDe CheckOverlaps



Aran, Pierre, James, Juergen

- Available on DUNE GPVMs
  - /dune/app/users/gvsinev/dune10kt-backgrounds/srcs/dunetpc/dune/Geometry/gdml/larfd_rn200cm_noOpDet_shotcrete6in{,_nowires}.gdml

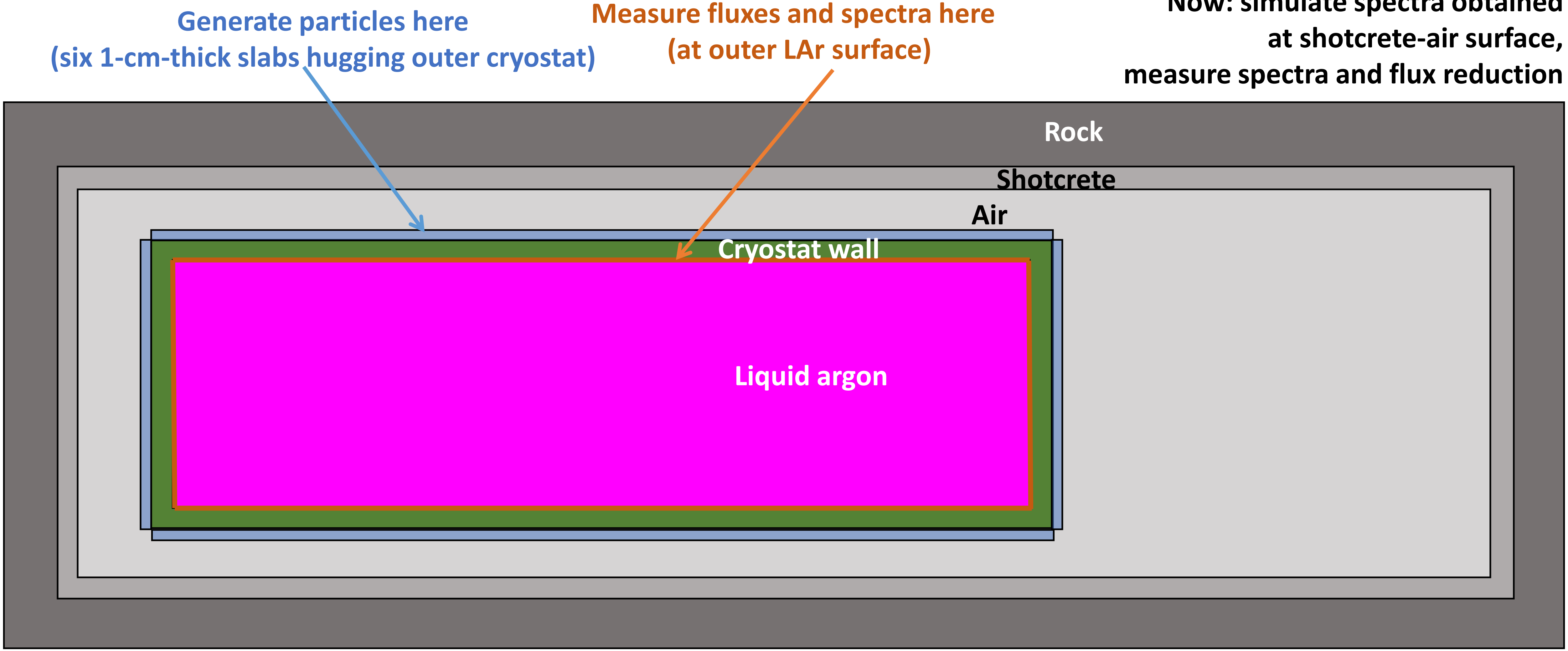
Cavern background simulation view from top (not to scale)



Previously: simulated ^{40}K outside cryostat, saw reduction of ~25 (used in VD production)

Cavern view from top (not to scale)

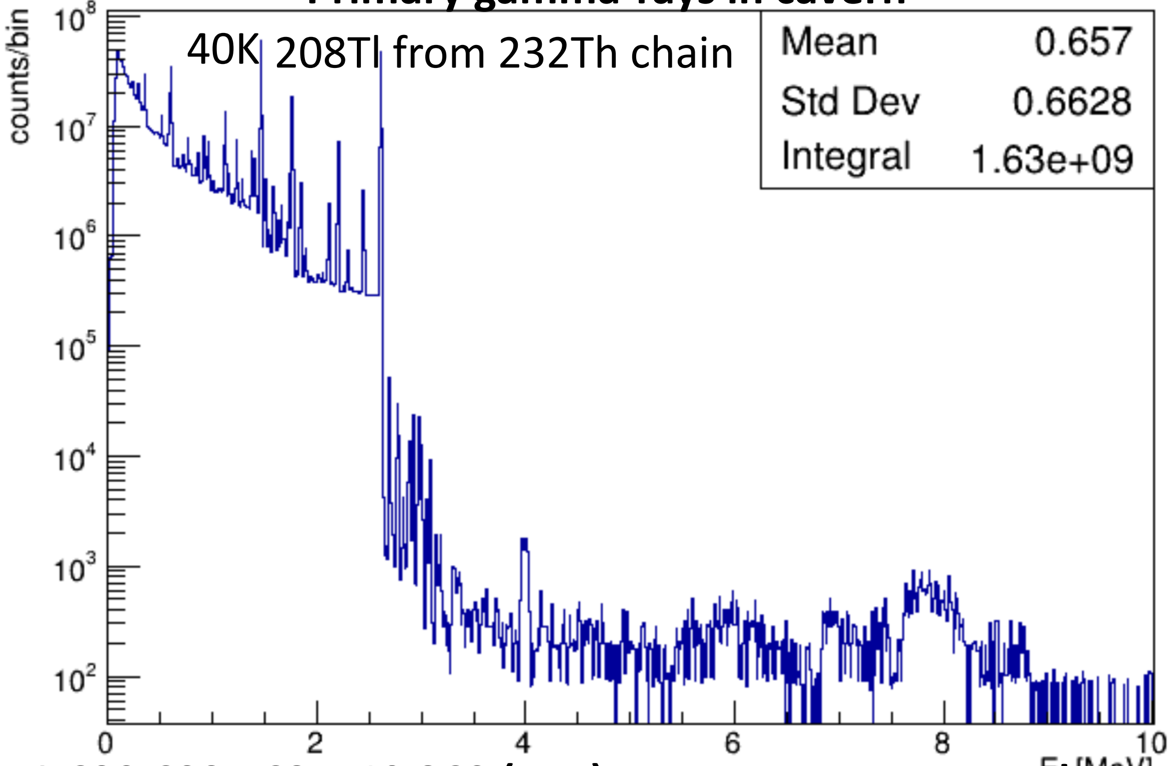
Now: simulate spectra obtained at shotcrete-air surface, measure spectra and flux reduction



Flux for VD production was 0.8 γ/cm²·s / 25 = 0.032 γ/cm²·s

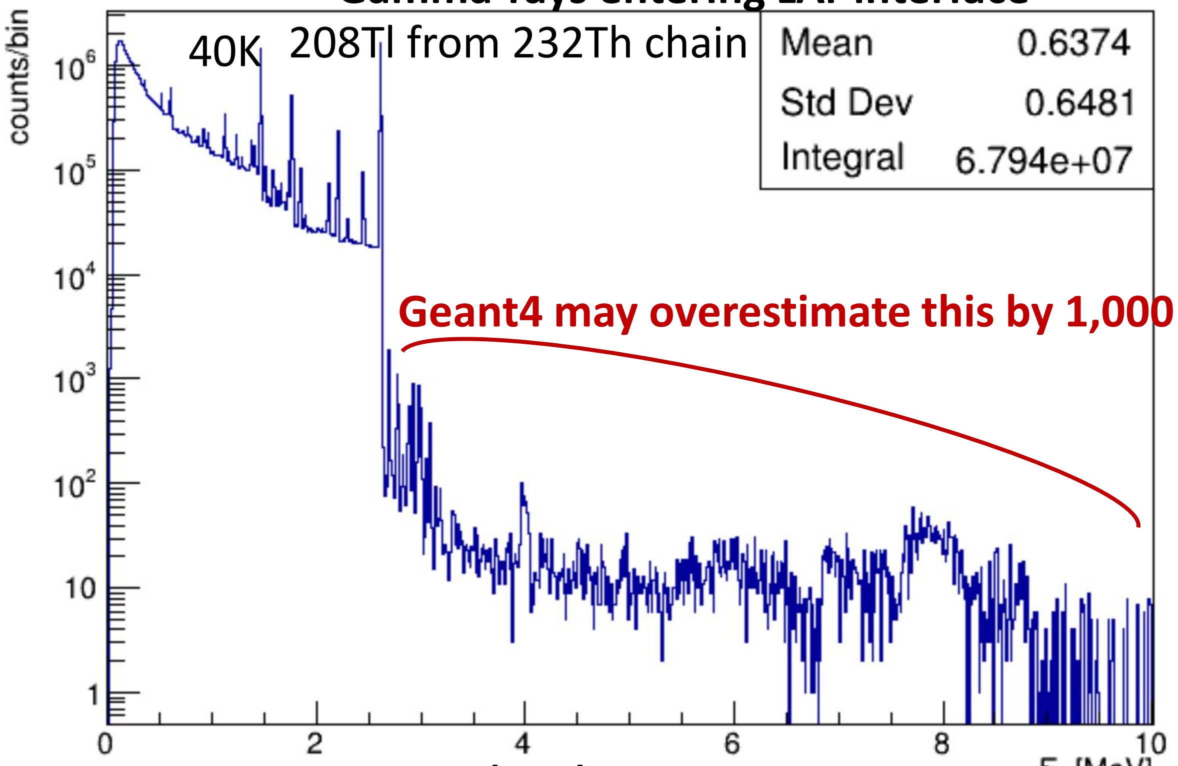
Propagating **cavern gamma-rays** through cryostat

Primary gamma-rays in cavern



1,629,622,763 ± 40,369 (stat) gamma-rays generated

Gamma-rays entering LAr interface



67,943,705 ± 8,243 (stat) gamma-rays measured

22,324 ± 149 (stat) gamma-rays >2.63 MeV

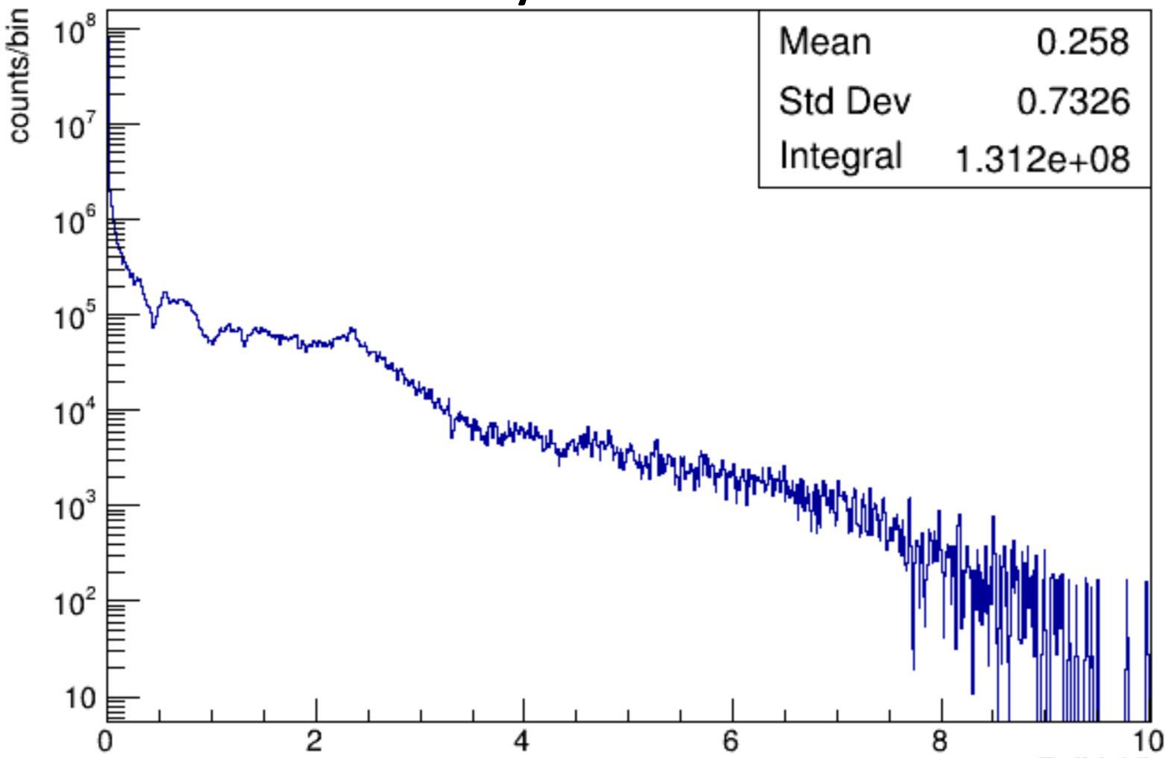
Reduction factor: 23.985 ± 0.003 (stat) (for gamma-rays >2.63 MeV: 73,000 ± 500 (stat))

2π γ-flux at LAr interface: (3.0697 ± 0.0005 (stat) γ/cm²·s) * $4\pi/2\pi$ / reduction factor = 0.25597 ± 0.00005 (stat) γ/cm²·s

2π γ-flux (>2.63 MeV) at LAr interface: = 84.1 ± 0.6 (stat) 10^{-6} γ/cm²·s

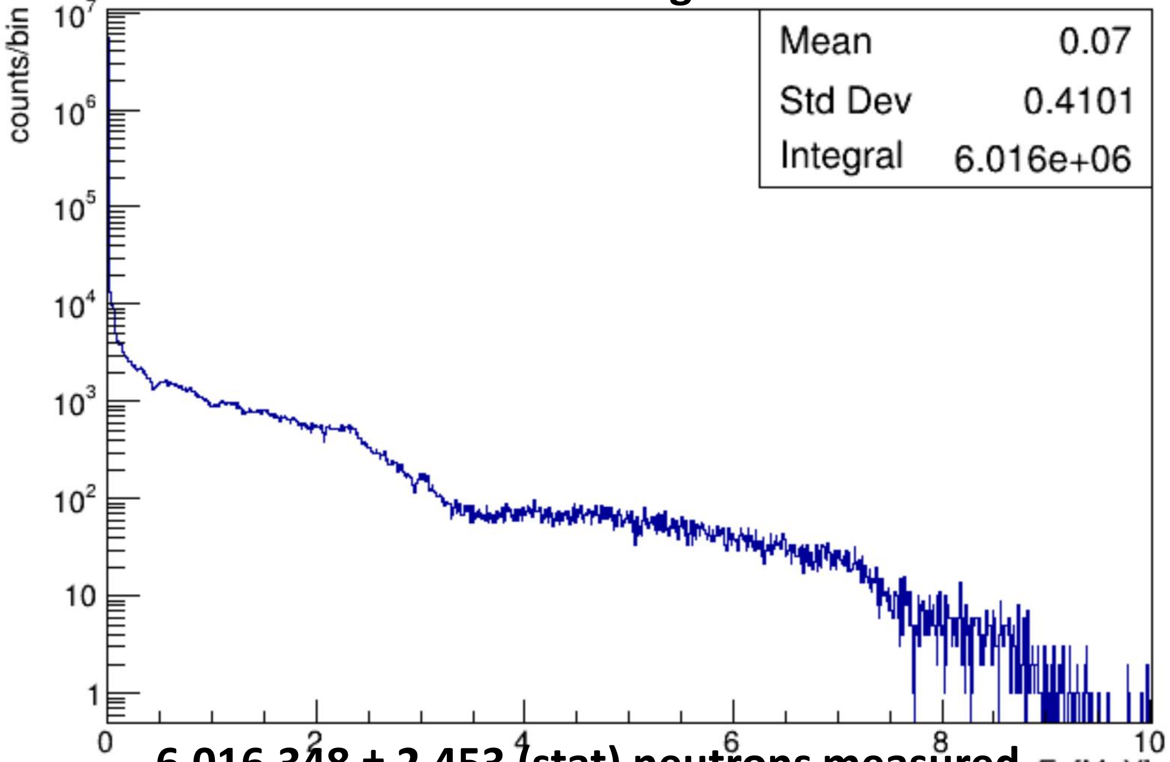
Propagating **cavern neutrons** through cryostat

Primary neutrons in cavern



131,249,863 ± 11,456 (stat) neutrons generated

Neutrons entering LAr interface



6,016,348 ± 2,453 (stat) neutrons measured

293,873 ± 542 (stat) neutrons > 0.1 MeV

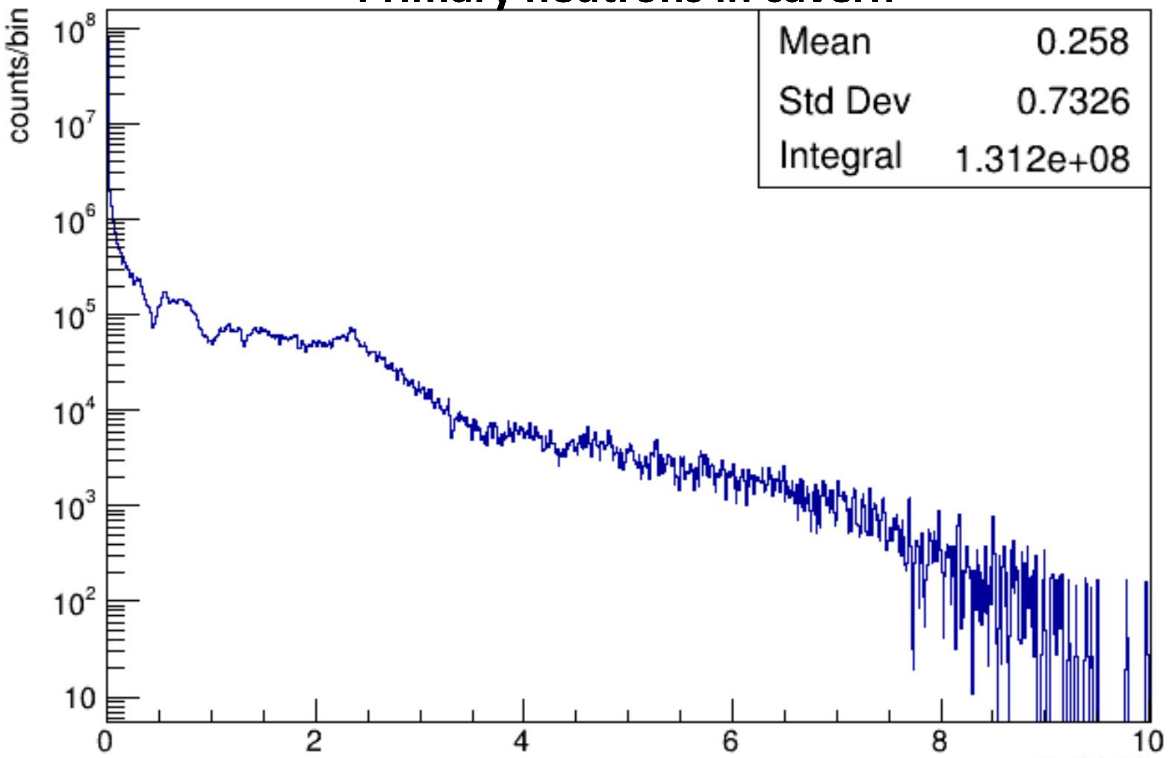
Reduction factor: 21.816 ± 0.009 (stat) (for neutrons >0.1 MeV: 446.6 ± 0.8 (stat))

2π n-flux at LAr interface: (1.0757 ± 0.0014 (stat) 10^{-6} n/cm^2·s) * $4\pi/2\pi$ / reduction factor = 0.09862 ± 0.00013 (stat) 10^{-6} n/cm^2·s

2π n-flux (>0.1 MeV) at LAr interface: = 0.004817 ± 0.000011 (stat) 10^{-6} n/cm^2·s

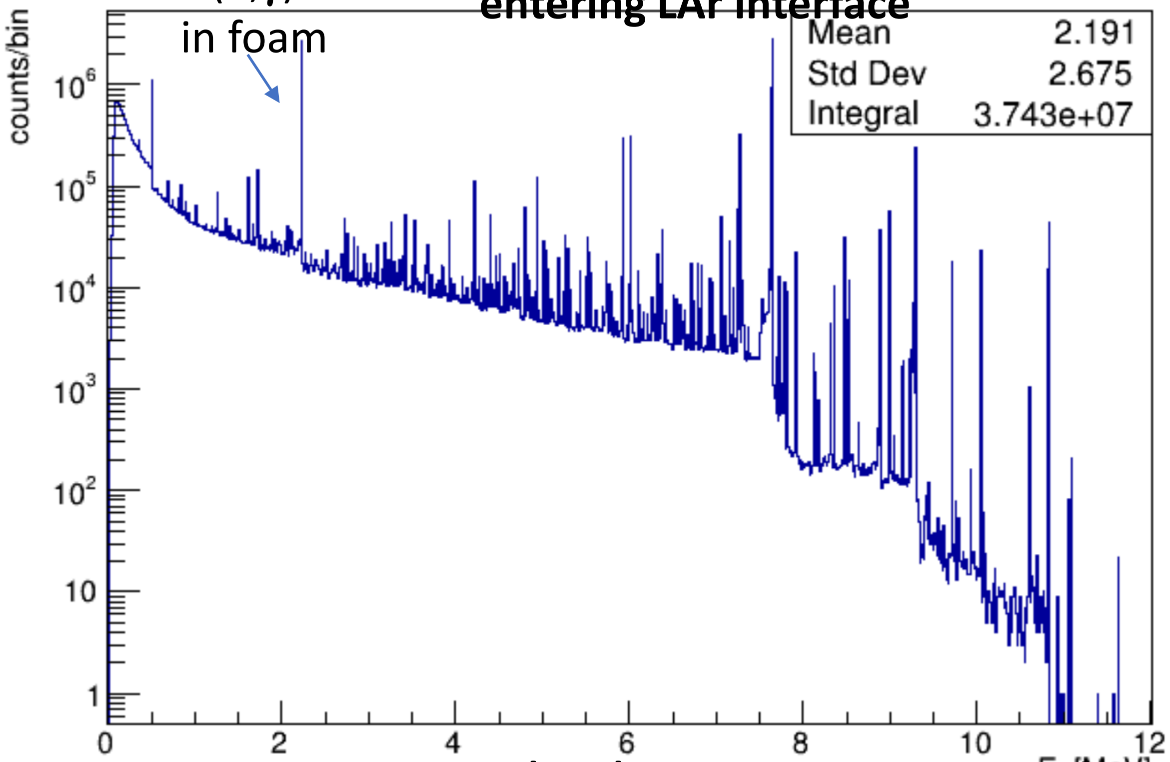
Cryostat propagation of cavern neutrons (& **capture γ-rays from cryostat**)

Primary neutrons in cavern



131,249,863 ± 11,456 (stat) neutrons generated

n-capture gamma-rays from cryostat entering LAr interface



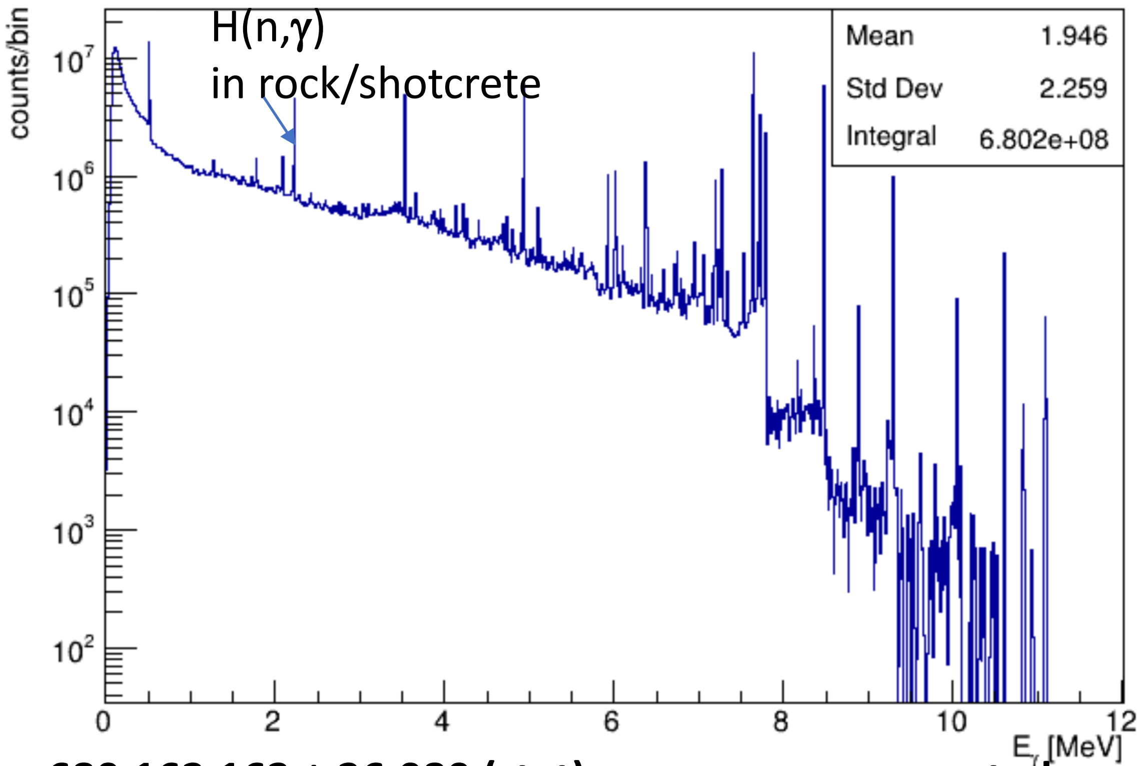
37,425,530 ± 6,118 (stat) gamma-rays measured

Conversion factor: 0.28515 ± 0.00005 (stat) γ/n

2π γ-flux at LAr interface: (1.0757 ± 0.0014 (stat) 10^{-6} n/cm²·s) * $4\pi/2\pi$ * conversion factor = 0.61347 ± 0.0008 (stat) 10^{-6} γ/cm²·s

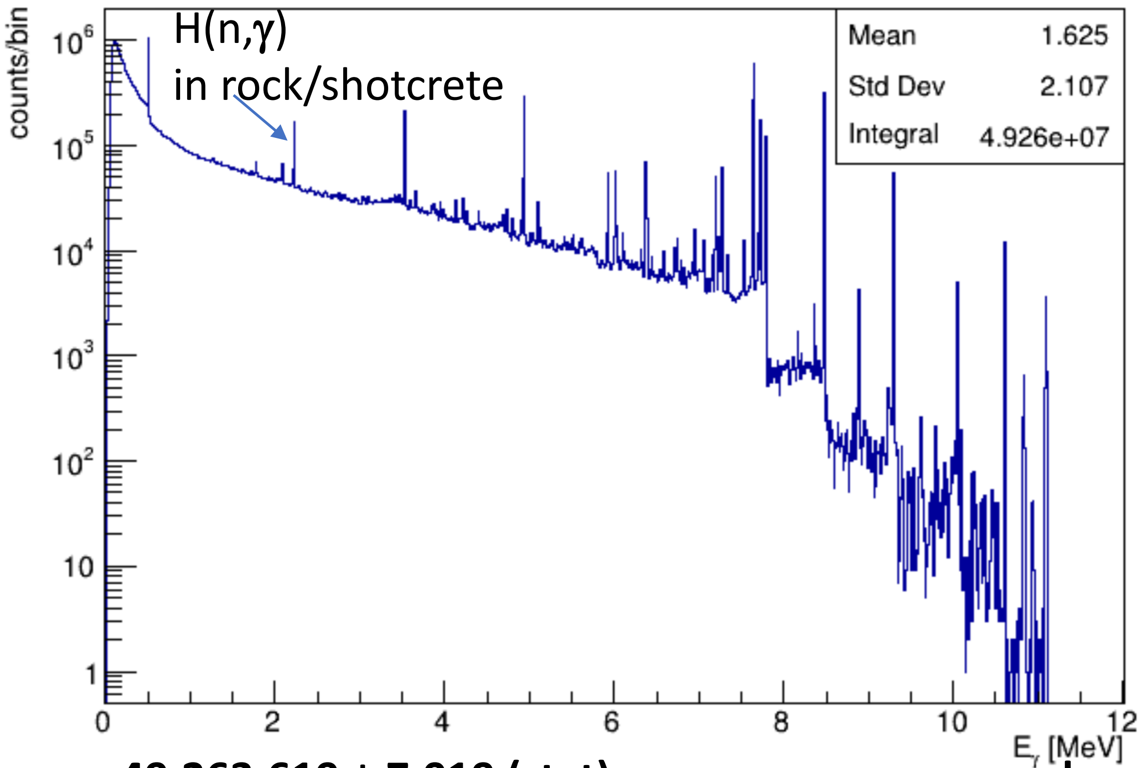
Cryostat propagation of cavern **n-capture γ-rays from rock/shotcrete**

Primary gamma-rays in cavern



680,162,163 ± 26,080 (stat) gamma-rays generated

Gamma-rays entering LAr interface



49,263,619 ± 7,019 (stat) gamma-rays measured

Reduction factor: 13.807 ± 0.002 (stat)

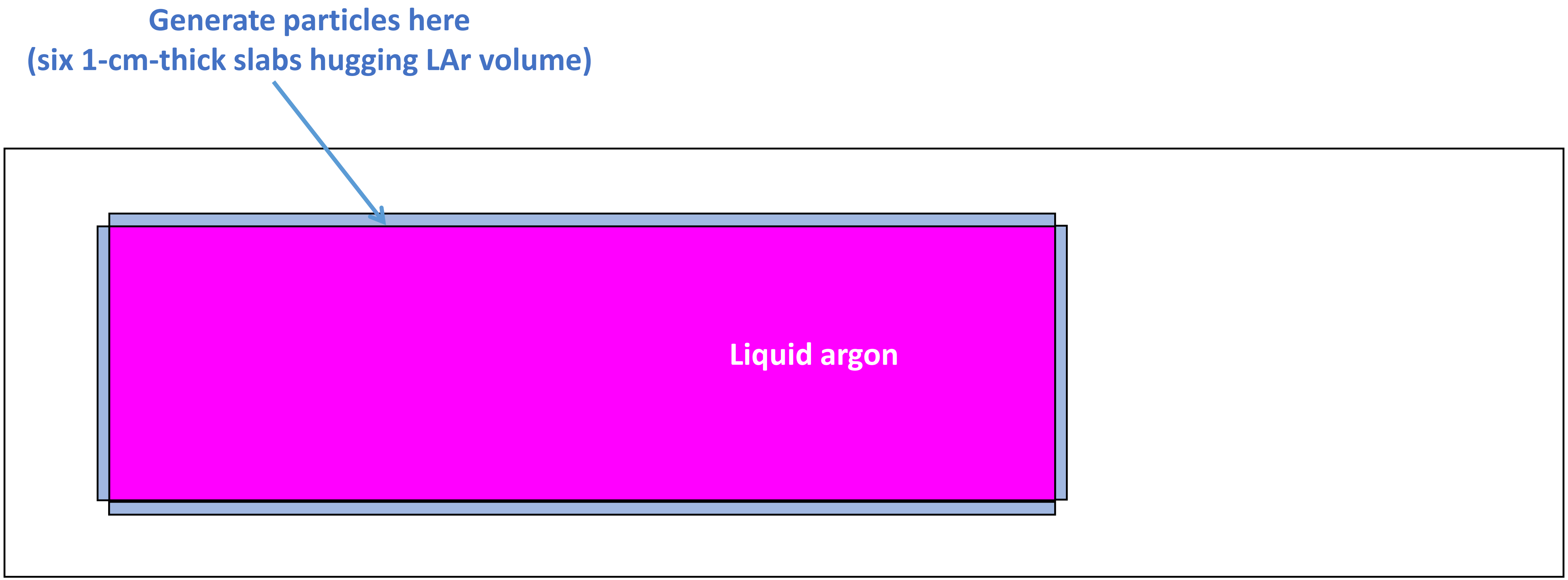
2π γ-flux at LAr interface: (1.3720 ± 0.0016 (stat) 10^{-6} γ/cm²·s) * $4\pi/2\pi$ / reduction factor = 0.1987 ± 0.0002 (stat) 10^{-6} γ/cm²·s

~1/3 of n-capture γ-rays from cryo!

Next steps: producing external background spectra and rates for background model in LAr

- γ, n, n-γ fluxes and spectra propagated to LAr surface will be used as external background
  - Add contributions from cavern and cryostat γ, n, n-γ
  - For cavern-gamma background, previously used reduction of 25 to quickly emulate effect of cryostat, but will correctly propagate background fully through cryostat in future
- External background in partial geometries (HD 1x2x6, VD 1x8x14, etc.)
  - Generate particles with previously calculated fluxes and spectra directly outside of LAr volume
    - Six 1-cm-thick slabs touching full? LAr volume from outside (truncated LAr volume for HD?)
    - Isotropic particles, and 2x inferred flux from outer LAr surface because of that

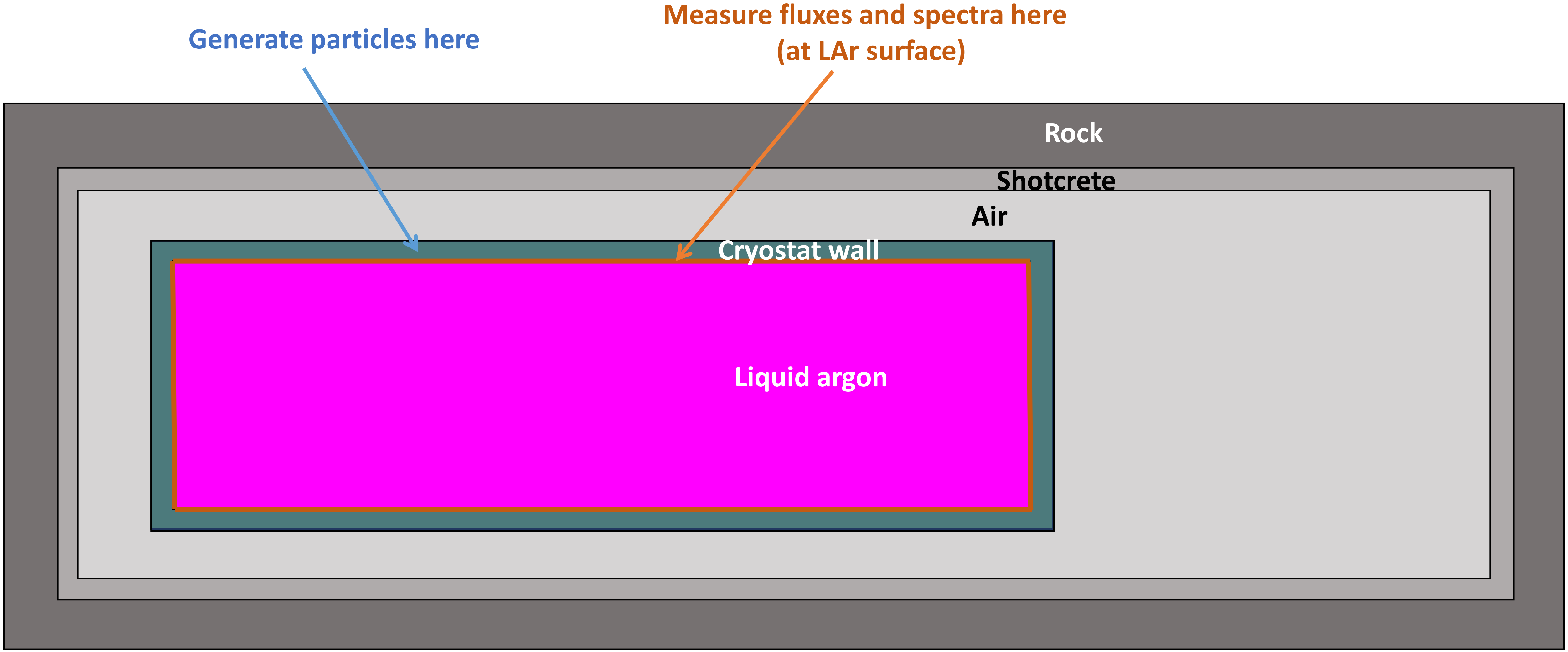
Truncated geometry (HD 1x2x6, VD 1x8x14, etc.) view from top (not to scale)



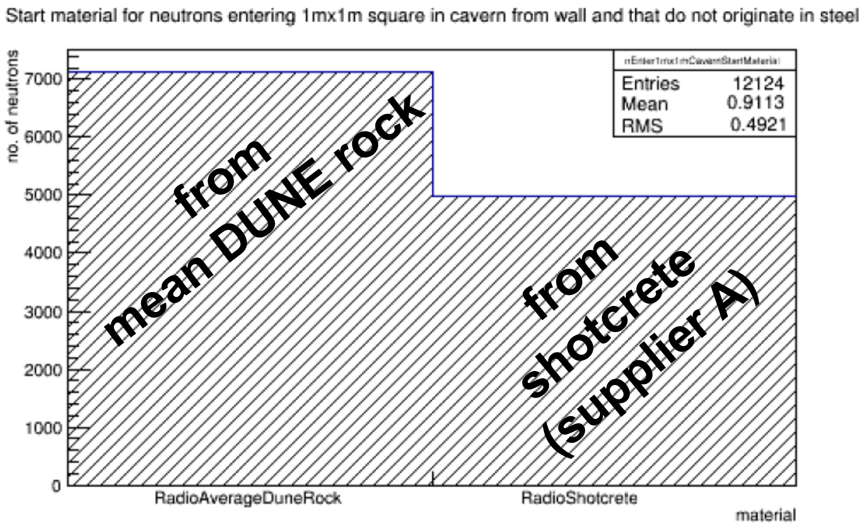
Next steps: simulating backgrounds in cryostat walls

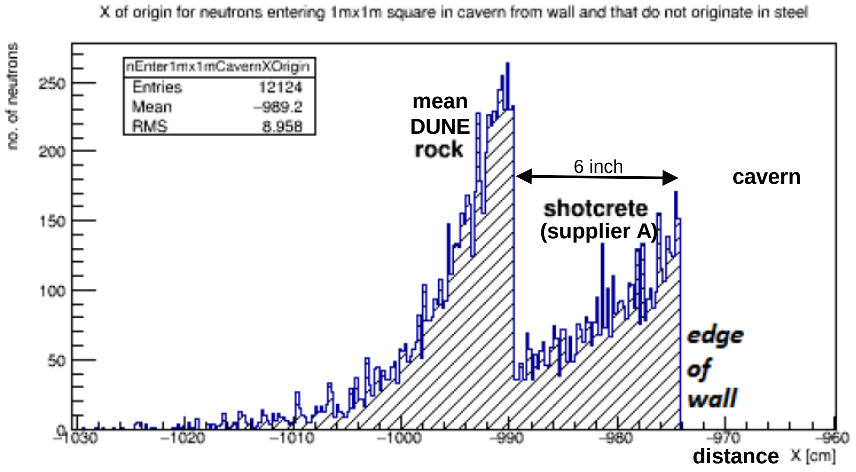
- Planning to simulate U/Th in cryostat steel, foam, other layers
- Will use our new radiological assay results for foam and cryostat steel as input
- Propagation will include new gamma-rays from cavern neutron captures in cryostat

Cavern view from top (not to scale)



Neutron Production from Cavern Walls





LArSoft simulated total cavern neutron flux:
(1.08 ± 0.2[syst.]) x 10^-6 neutron cm−2 s−1

with E_{kin} > 0.1 MeV (fast neutron flux in cavern):
(2.24 ± 0.5[syst.]) x 10^-7 neutron cm−2 s−1

Mean DUNE Rock:
66.7 ± 0.3 Bq/kg of 238U
31.8 ± 0.2 Bq/kg of 232Th

Worst rock (2x activity) could cause 60% increase to ≤ 1.7 x 10^-6 neutron cm−2 s−1

Shotcrete Supplier A (15 cm thick):
24.6 ± 0.4 Bq/kg of 238U
6.0 ± 0.2 Bq/kg of 232Th

Worst shotcrete (4x activity) could double neutron rate to ≤ 2.2 x 10^-6 neutron cm−2 s−1

Use worst case as indicated by our latest excavation site assays of shotcrete

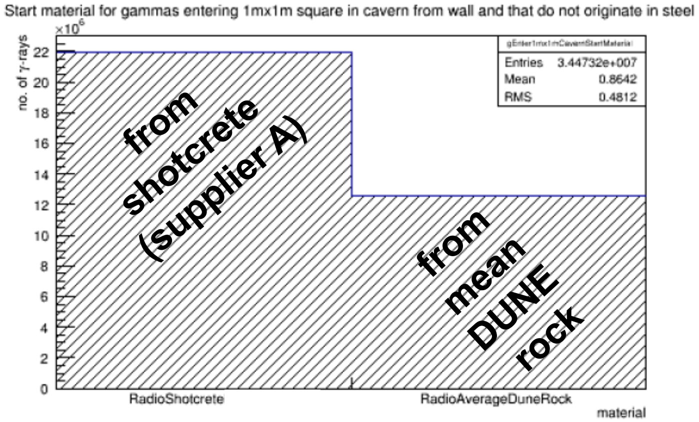
work in progress

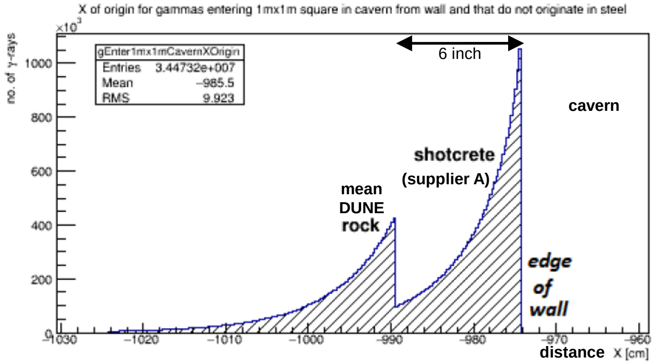
(simulation w/ LArSoft and Decay0 and new 232Th decay chain implementation)

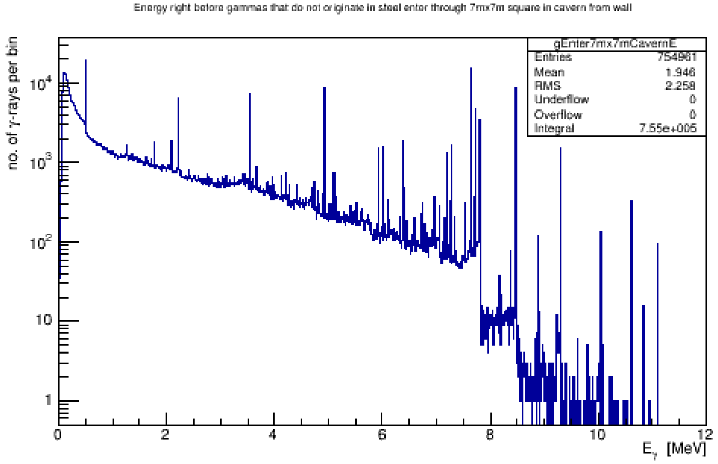
γ-Ray Production from Cavern Walls

(simulation w/ LArSoft and Decay0 and new 232Th decay chain implementation)

work in progress







Simulated DUNE cavern γ flux:

3.07 ± 0.2[syst.] γ cm−2 s−1

Mean DUNE Rock:
665.5 ± 1.4 Bq/kg of 40K
66.7 ± 0.3 Bq/kg of 238U
31.8 ± 0.2 Bq/kg of 232Th

Worst rock (2x activity) could cause 35% increase to ≤ 4.1 γ cm−2 s−1

Shotcrete Supplier A (15 cm thick ~2Λ):
105.8 ± 4.5 Bq/kg of 40K
24.6 ± 0.4 Bq/kg of 238U
6.0 ± 0.2 Bq/kg of 232Th

Worst shotcrete (4x activity) could triple γ rate to ≤ 9.2 γ cm−2 s−1

γ flux from neutron captures:
(1.37 ± 0.3[syst.]) x 10^-6 γ cm−2 s−1

Use worst case as indicated by our latest excavation site assays of shotcrete

Next steps: Background Explorer

- Will simulate individual layers and background components
  - Rock and shotcrete separately
  - Early and late U, Th chains separately
  - and others
- Then can combine components in Background Explorer
  - See e.g. talk by Sagar Sharma Poudel at September collaboration meeting: https://indico.fnal.gov/event/53964/contributions/250798/attachments/160136/210830/PresentBackground_Explorer_DUNE_Sept_Collaboration_meeting_Sagar.pdf
  - Will be able to build background models based on assays
  - Taking this over from Sammy Valder

Next steps: proposed sim improvements

- Vitaly Kudryavtsev suggested following improvements, need to think more about how to implement them
  - Saving particle directions at measuring surfaces and simulating them instead of isotropic particles at next stage
    - Saving this information should be easy (need to consider increased filesize), but not sure if can use current radiological generators to set particle direction
  - Define parallel worlds in Geant4 where particles stop instead of adding absorbers into existing volumes
    - Adding absorbers is easy through GDML, need to think about defining parallel worlds in LArG4
  - Make separate simulations for U, Th, K, early, late chains
    - Then will not have to resimulate for different assays/materials/composition
    - Currently separate γ, n, and n-γ

Thank you, Vitaly!

Cavern backgrounds

- Gammas and neutrons produced in DUNE cavern can be significant background, particularly for Vertical Drift module
  - No ~40 cm of passive LAr shielding in VD compared to HD
- Previous cavern-gamma simulation used in VD production
  - June 2022 created fast beta version of cavern spectra that Thiago used for VD sim
  - Found bug in RadioGen generation, also did not propagate energy dependence through cryostat due to shortness of time
- Produced new cavern-neutron simulation
- Previously used internal RadioGen 238U, 232Th and 40K generators, as there was no 232Th decay chain in Decay0 (232Th crucial for gamma background)
- Juergen implemented 232Th decay chain in Decay0 (with most relevant isotopes in decay chain)
  - allowed us to move to Decay0 for cavern background sims in Oct 2022
- Produced new cavern background sims (external gamma-rays and neutrons)
  - See e.g. Juergen's overview at DUNE January 2023 CM at CERN: https://indico.fnal.gov/event/53965/contributions/258266/attachments/163355/216219/DUNE_CM_AssaysStatusAndCavernWallBackgrounds_26Jan2023_CERN_JR.pdf
  - And e.g. Gleb's technical summary at DUNE January 2023 CM at CERN: https://indico.fnal.gov/event/53965/contributions/258267/attachments/163377/216249/cavern-cryo-backgrounds_20230126_v2.pdf

Note on Decay0

- Decay0 is simulation package used for background and signal simulations in neutrinoless double-beta experiments
- "Decay0" here means Decay0 LArSoft module (with larsimrad) written by Pierre Lasorak, see DUNE-doc-23595 https://docs.dunescience.org/cgi-bin/private/ShowDocument?docid=23595
  - Decay0 interface + features common with RadioGen (also added some new features)
- It lives in larsimrad (now one of LArSoft packages)
  - Depends on BxDecay0 (C++ port rather than original FORTRAN Decay0): https://github.com/BxCppDev/bxdecay0
- DUNETPC v08_60_00 BxDecay0 did not have all isotopes we needed
  - Installed locally later version, rebuilt larsimrad with it
- Defining decay chains explicitly
  - ^{40}K, ^{238}U taken from Pierre/Thiago, ^{232}Th implemented by Juergen

Note on statistical uncertainty

- Found that RadioGen generates same number of primaries for every job with same input parameters
  - Bug from using CLHEP method that does not use LArSoft random-number engine
- Assume this results in actual statistical uncertainty closer to sqrt(number of jobs used) times stat uncertainty I specified

Note on running with custom Decay0

- Decay0 available with dunetpc v08_60_00 lacks some decays
- Install latest version of BxDecay0 locally
- Set up local version of dunetpc
- Check out larsimrad with mrb
  - Change to tagged version appropriate for dunetpc version
- Set up ups BxDecay0 variables to point to local BxDecay0 version
  - BXDECAY0_{{,FQ_}DIR,INC,LIB,VERSION}
  - Also include local BxDecay0 lib in LD_LIBRARY_PATH
- Build local LArSoft
- Before running LArSoft, reset variables to local BxDecay0 (see above)

Note on running on FermiGrid

- Split simulation into 1,000 jobs
    - Not sure if good idea to run many more than this
- However, due to errors, had to run ~10% more jobs
    - ~1,100 jobs
    - Seems to be fixed as of late September 2022
- Total events per job selected to run about 1 day
    - As well as whatever resulted in good-looking number of total events
        - 10,000,000 events, 1,000,000,000 events
    - Gamma simulations are limited by space
        - Not sure if good idea to request much more than 60 GB of space per job
- Only saved final histograms
    - Intermediate data takes too much space + takes long to reprocess