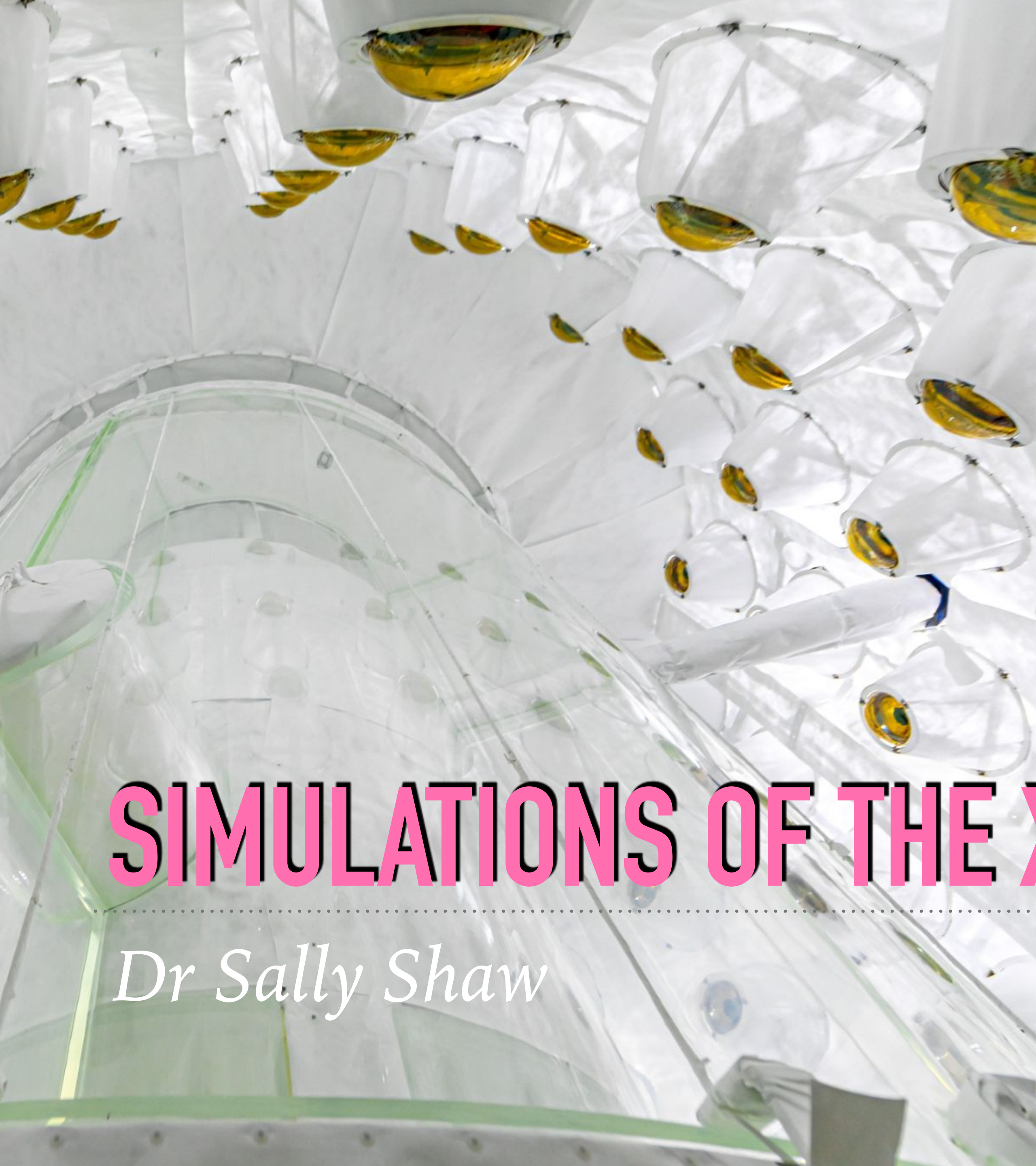
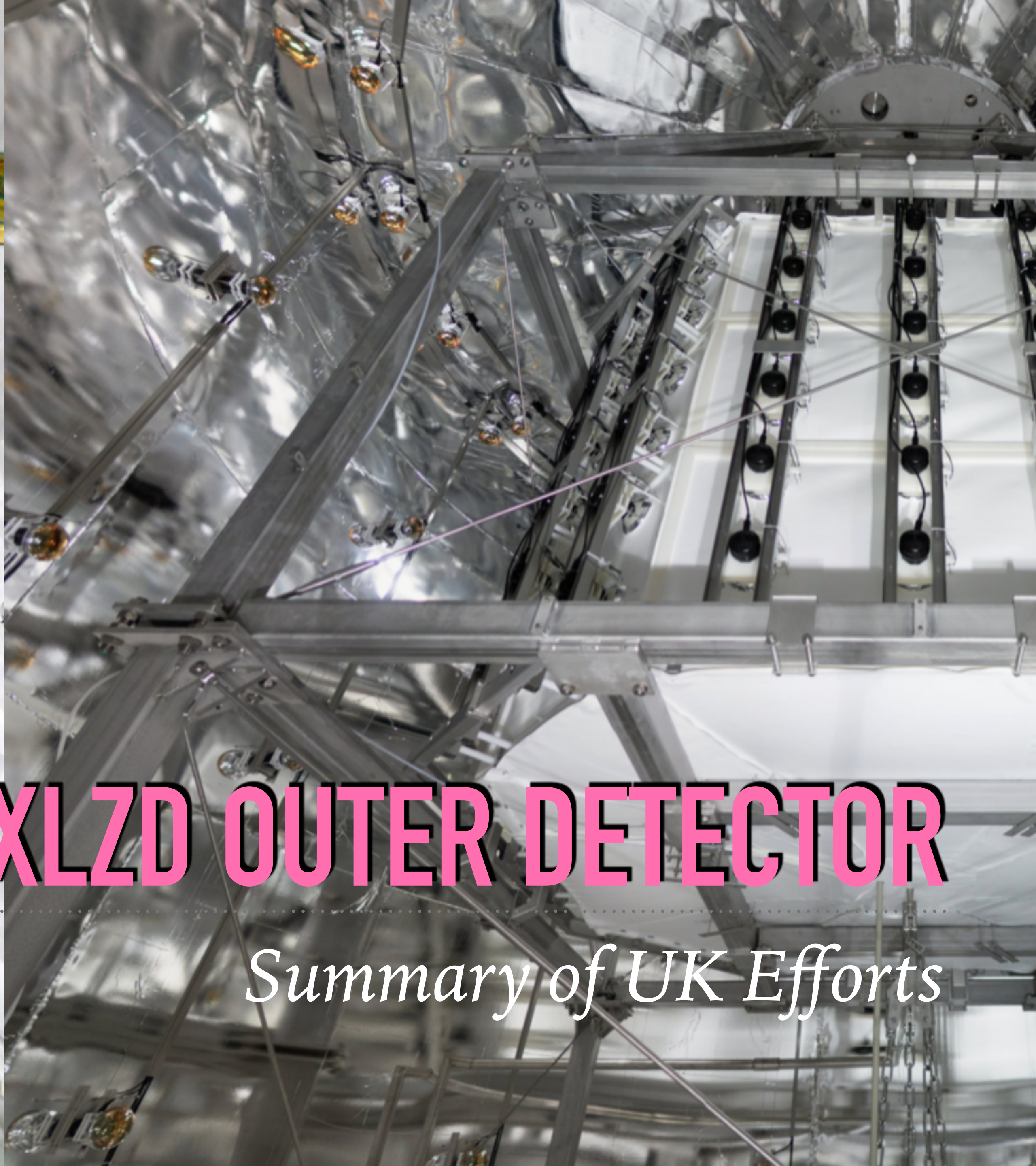




SIMULATIONS OF THE XLZD OUTER DETECTOR

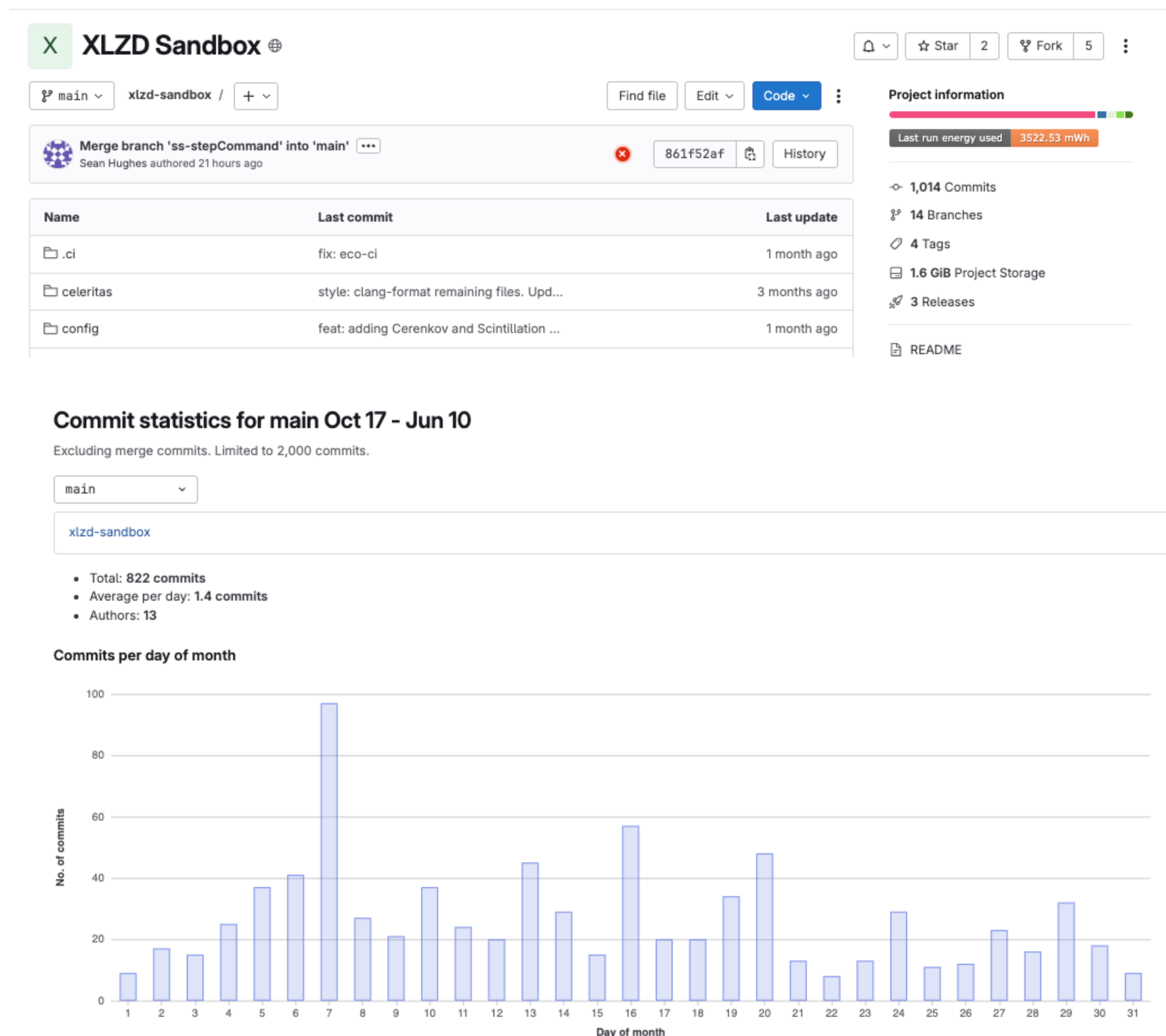
Dr Sally Shaw



Summary of UK Efforts

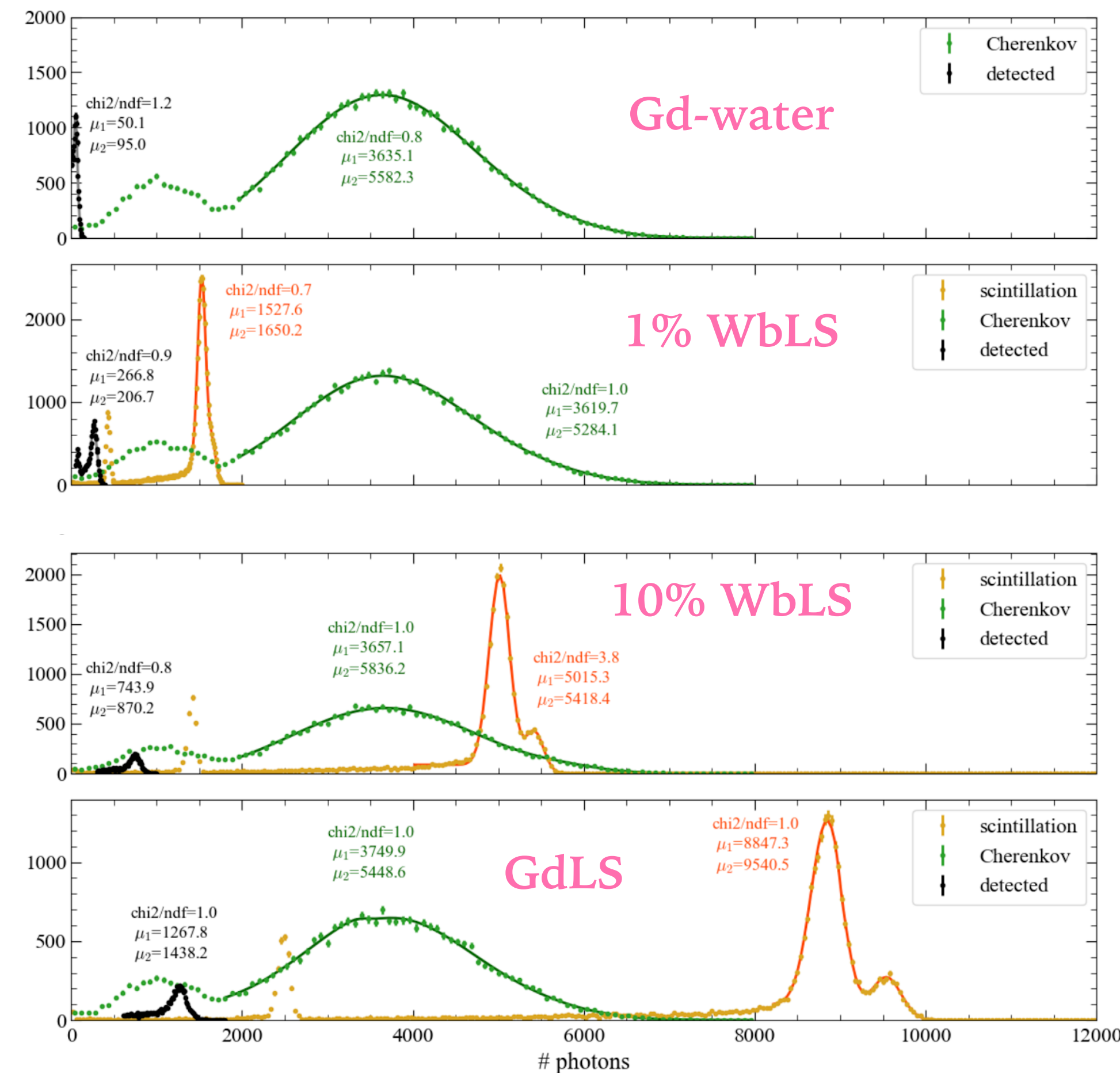
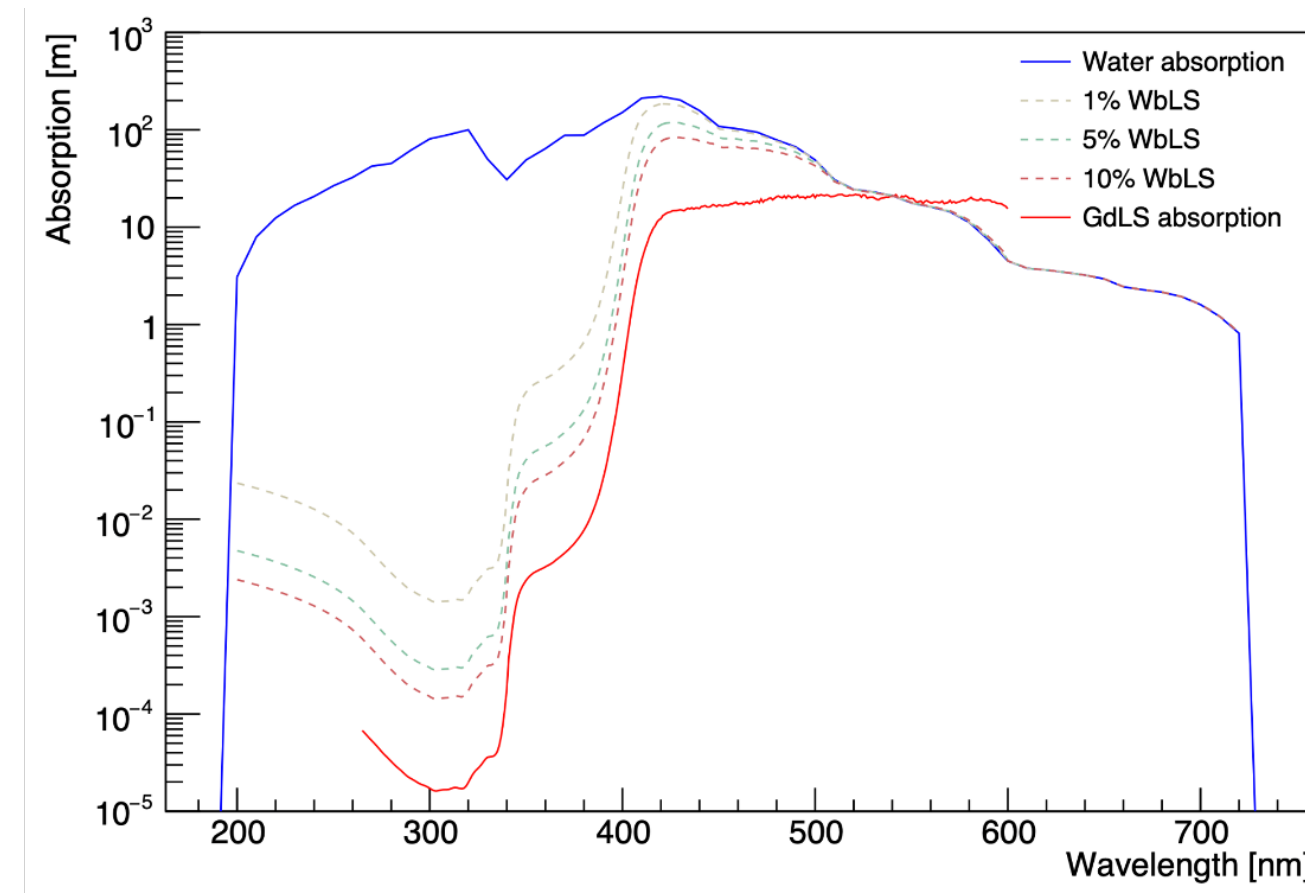
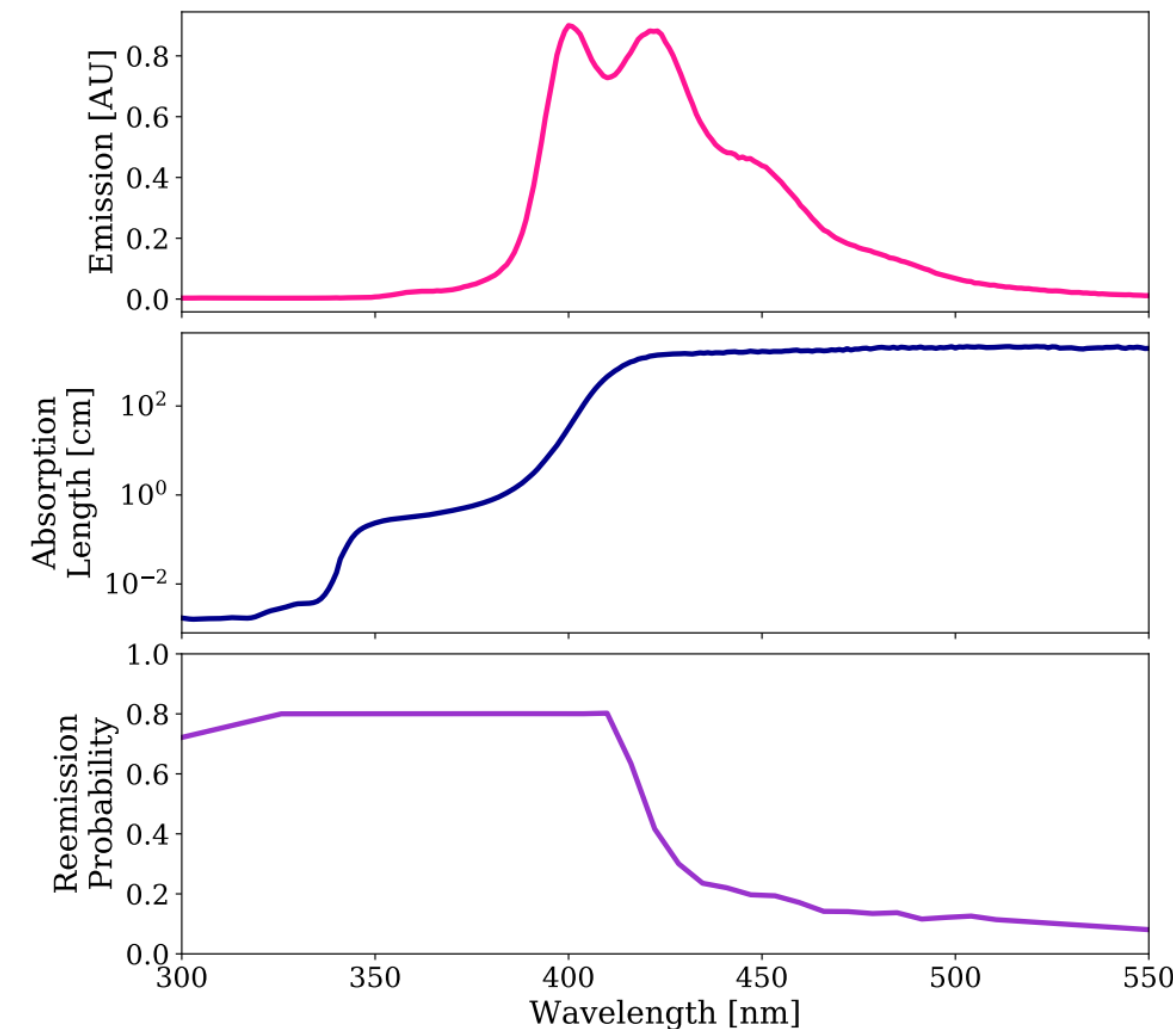
INTRODUCTION & FRAMEWORK

- Standalone Geant4 package - XLZD Sandbox - has been developed to aid design work & early physics studies
 - Open to all to use - [GitLab](#)
- Draws physics list from LZ's BACCARAT
 - [\[Simulations of Events for the LZ Dark Matter Experiment\]](#)
 - G4EMLivermorePhysics
 - G4HadronPhysicsQGSP_BIC_HP_Gd, includes the DICEBOX neutron capture gamma cascade modeling used in LZ
 - Bound-state scattering of thermal neutrons is turned on for hydrogenous materials
- Much of the work in these slides is by **Dr Sean Hughes** (Liverpool), **Dr Alberto Uson** (Edinburgh), **Dr Sam Woodford** (Edinburgh) and **Dr Steve Jones** (Sheffield, left for industry!)



OPTICAL PHYSICS

- For GdLS, LZ's BACCARAT "G4ScintillationMod" code is used (adopted from Daya Bay and modified for LZ), including remission of photons
- WbLS: absorptions of Gd-LS and water using the Beer-Lambert law using the concentrations/densities of both Gd-LS and water (M. Yeh confirmed was a good approximation!)
- Gd-water: Geant4 Cherenkov



See poster "Preliminary Simulations of the XLZD Outer Detector" by Dr Sean Hughes

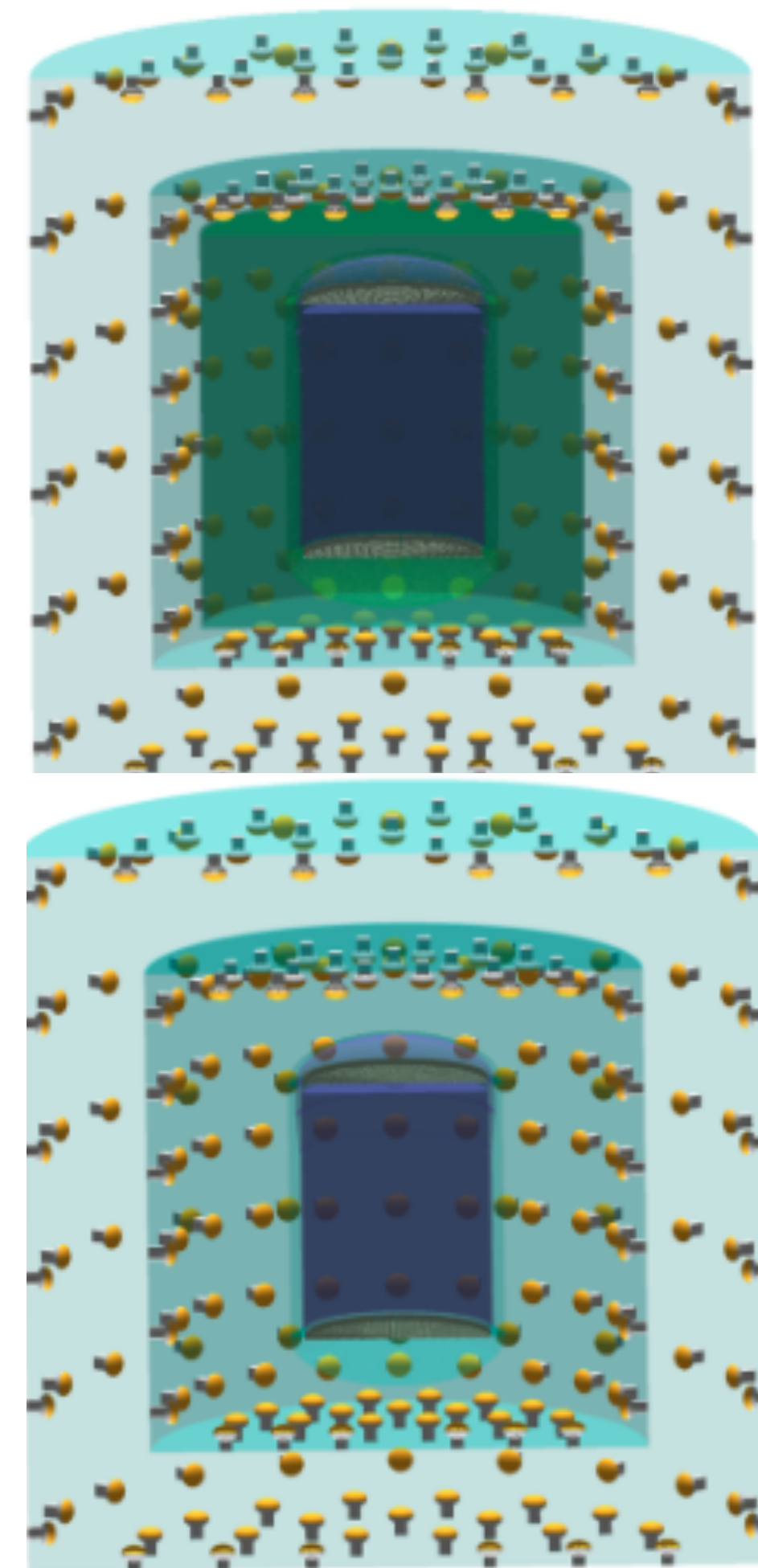
OD OPTIONS AND GEOMETRY

- Modified easily with an input JSON file
- Medium options:
 - Gd-water, no containment
 - 1-10% Gd-WbLS, option for with or without containment
 - GdLS, with containment
- Currently using UK cryostat CAD model - has set initial OD size (if contained) to be about 1m thick on all sides
 - This should be optimised with a study
 - Also based on discussion with acrylic companies - 1m gap to work on both sides of acrylic for feedthroughs, maybe not an issue with paneled designs
- For contained options, nominal stand-off between PMTs 80cm

```

1 {
2   "outerDetector": {
3     "Height": 12,
4     "Radius": 6,
5     "SteelShell": {
6       "Status": true,
7       "Thickness": 0.05
8     },
9     "GdPercent": 0.1,
10    "Medium_options": {
11      "0": "No LAB",
12      "1": "WbLS with 1% concentration of LAB",
13      "2": "WbLS with 5% concentration of LAB",
14      "3": "WbLS with 10% concentration of LAB"
15    },
16    "WbLS_option": 1,
17    "Medium": {
18      "DopedLABGd": false,
19      "DopedWater": true
20    },
21    "PMT": {
22      "Type_options": {
23        "0": "8 inch",
24        "1": "10 inch",
25        "2": "20 inch"
26      },
27      "Type": 0,
28      "Status": true,
29      "Total": 20,
30      "Ladders": 6,
31      "Radius": 6,
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33      "RoofPMTStatus": true,
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36      "Width": 0.2,
37      "Length": 0.25
38    },
39    "OSV": {
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42      "Radius": 4,
43      "PMT": {

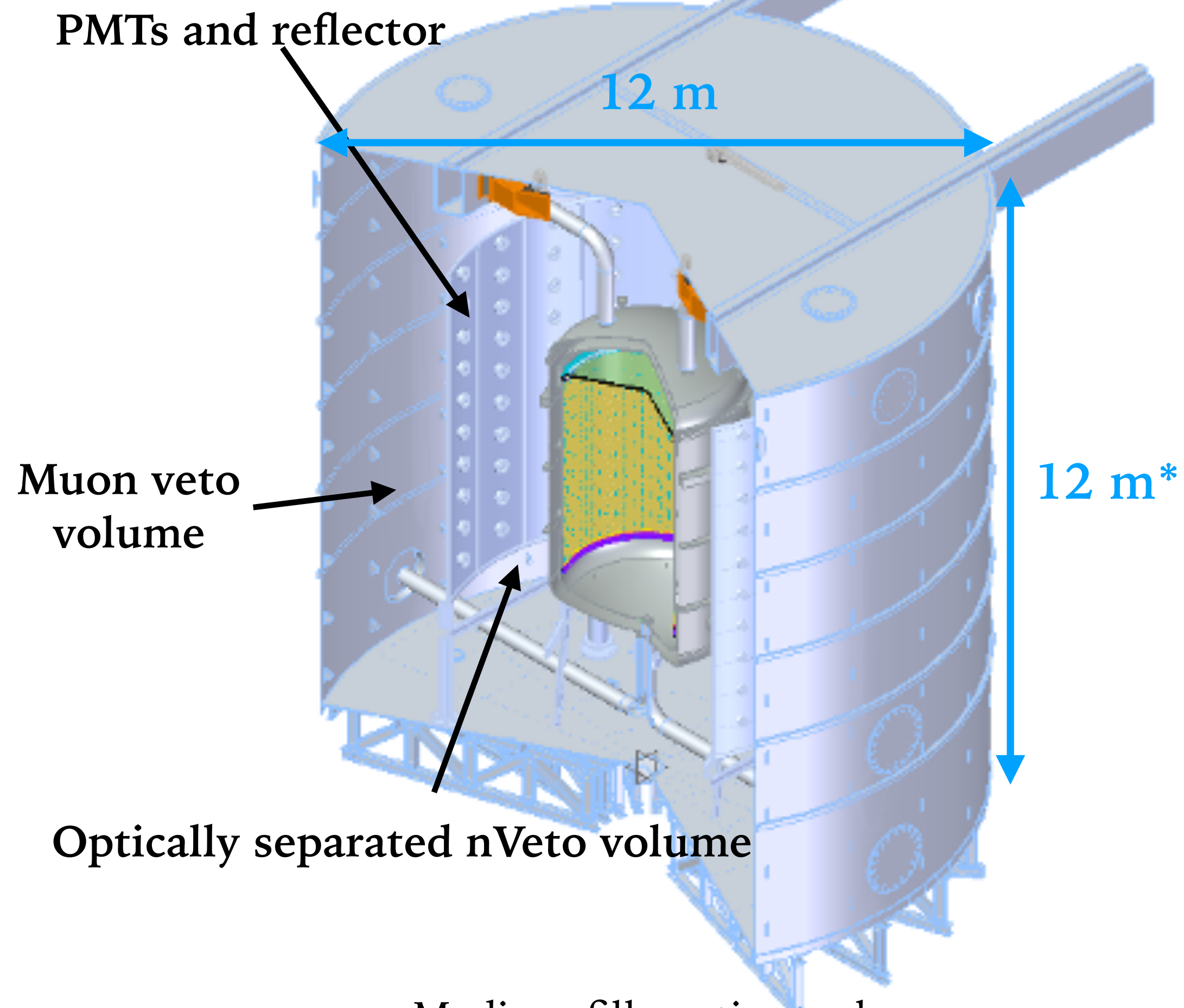
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See poster “*Preliminary Simulations of the XLZD Outer Detector*” by Dr Sean Hughes

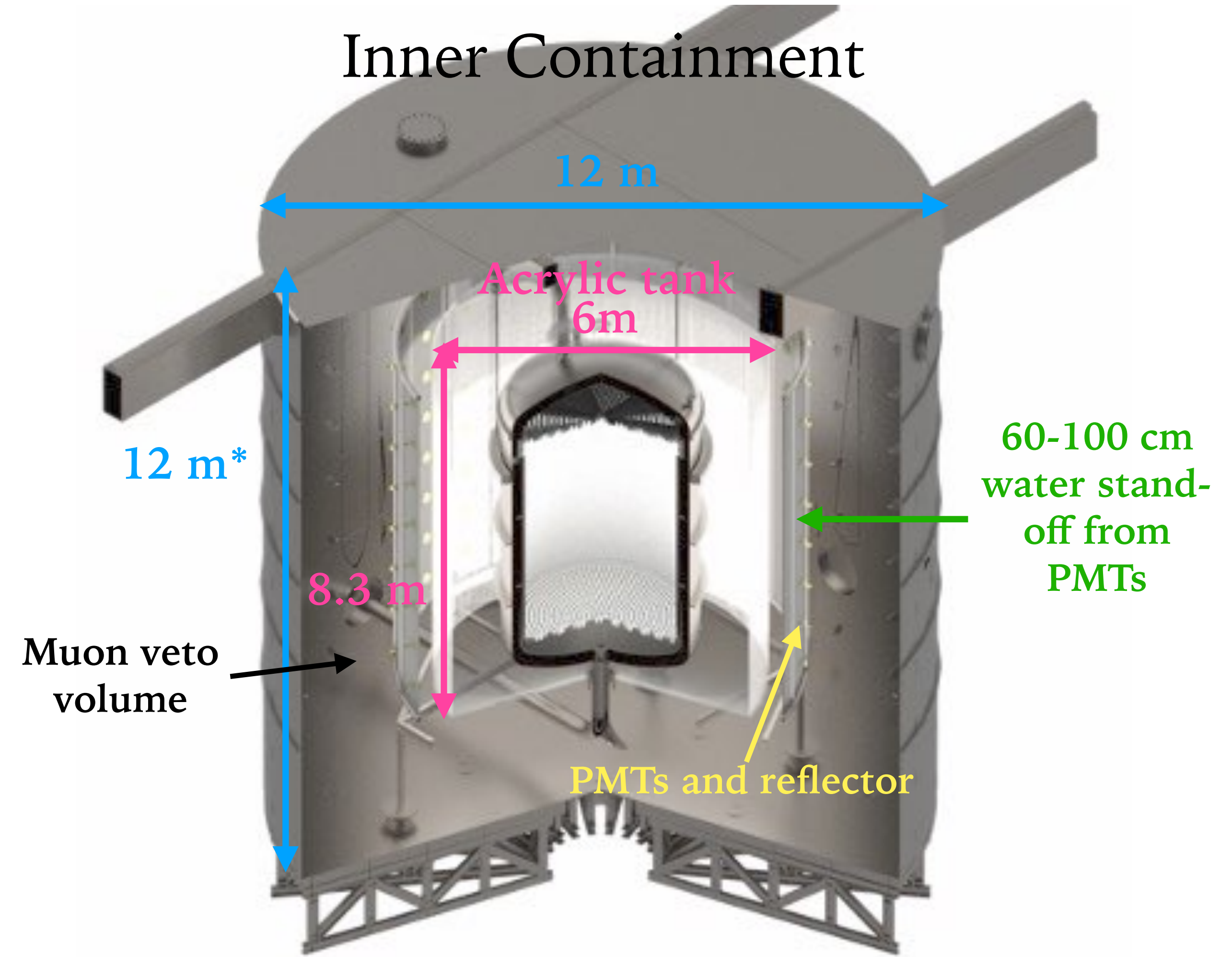
OD OPTIONS AND GEOMETRY

No Inner Containment



Medium fills entire tank
Gd-water, Gd-WbLS, (GdLS?)

Inner Containment



Acrylic tank filled with GdLS or Gd-WbLS
Outside filled with water

STUDIES OF BACKGROUND RATE

- So far, considered a few key backgrounds and considered a 600μs window, max rate for 5% dead time is ~86 Hz:

- **Cavern gammas**

- Scaled from paper [<https://arxiv.org/abs/2504.11613>] - expect 6 Hz if tank can be taller for **Boulby** polyhalite flux (similar for all labs, see backup slides)

- If tank is 12m and OD is ~7m tall - 200 Hz!

- Important initial conclusion: **water tank needs to be taller**

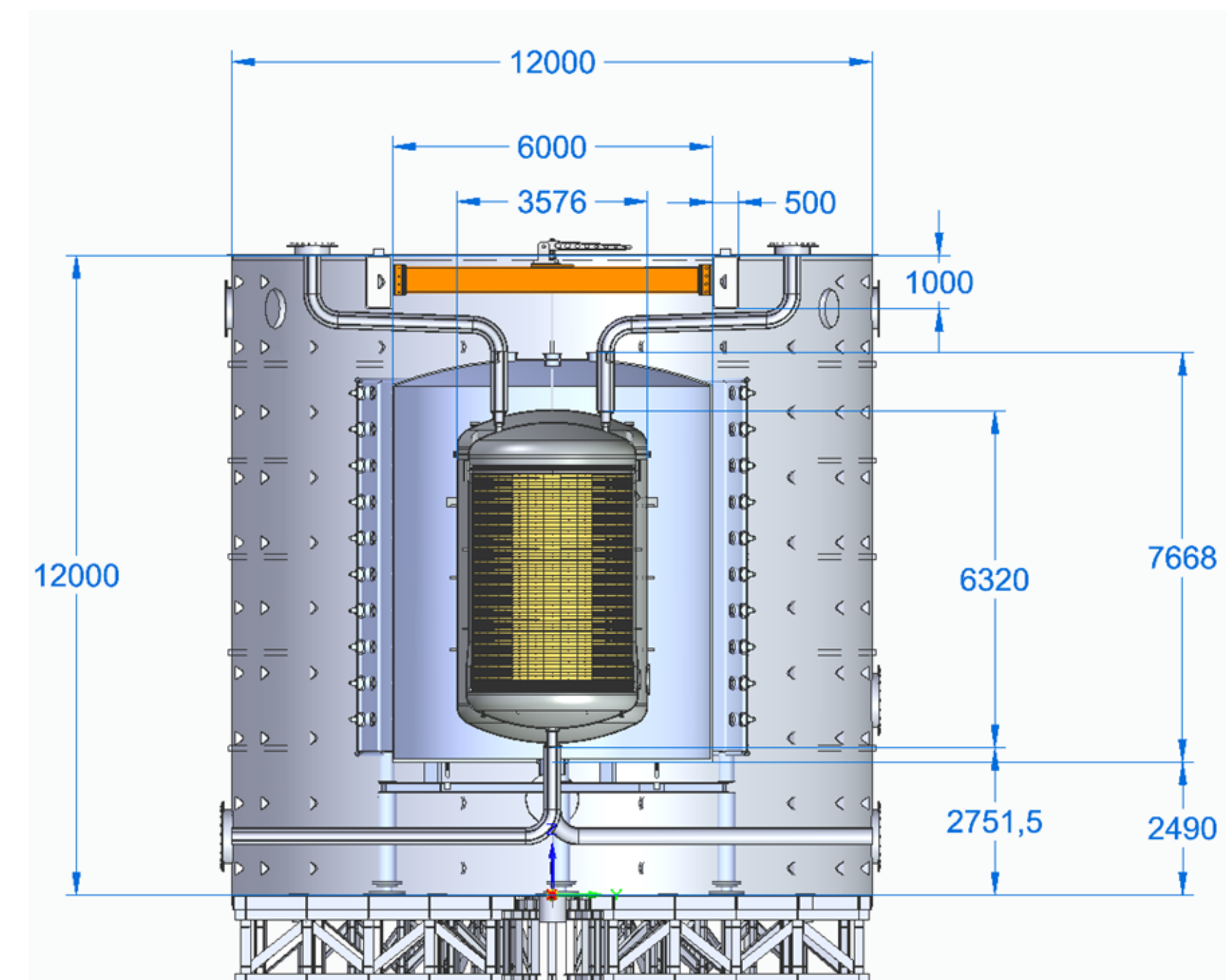
- **Internal medium contaminants**

- Scaled up from LZ OD: pessimistic (GdLS is highest BG, no reduction in LZ radiopurity): 68 Hz above 200 keV

- **Cryostat**

- Assume LZ Ti radioactivities [<https://arxiv.org/abs/1702.02646>]
 - I estimated ~25 Hz from cryostat at 0 keV threshold - Sean's simulation says 30 Hz, dropping to 3 Hz at 100 keV, 2 Hz at 200 keV

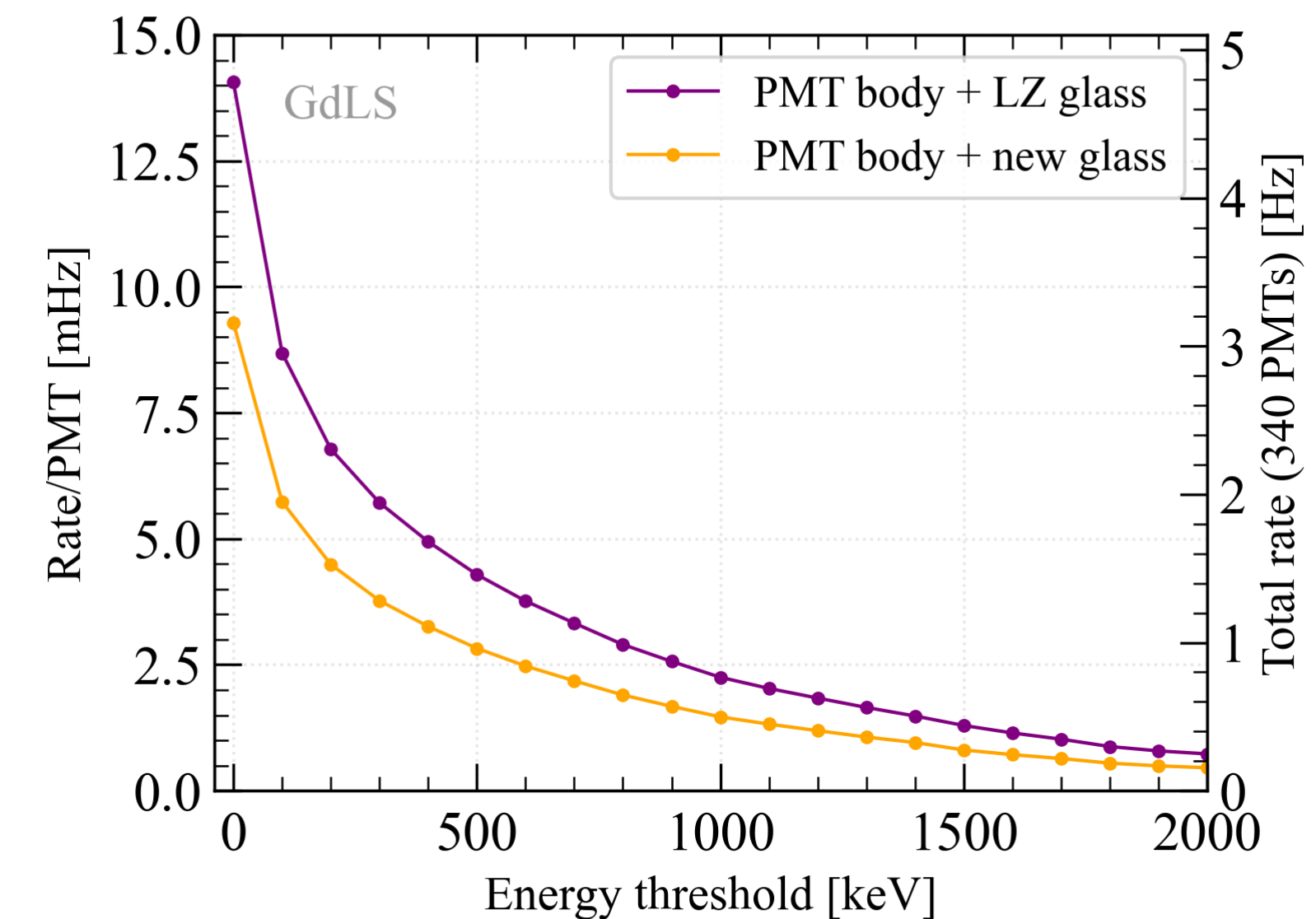
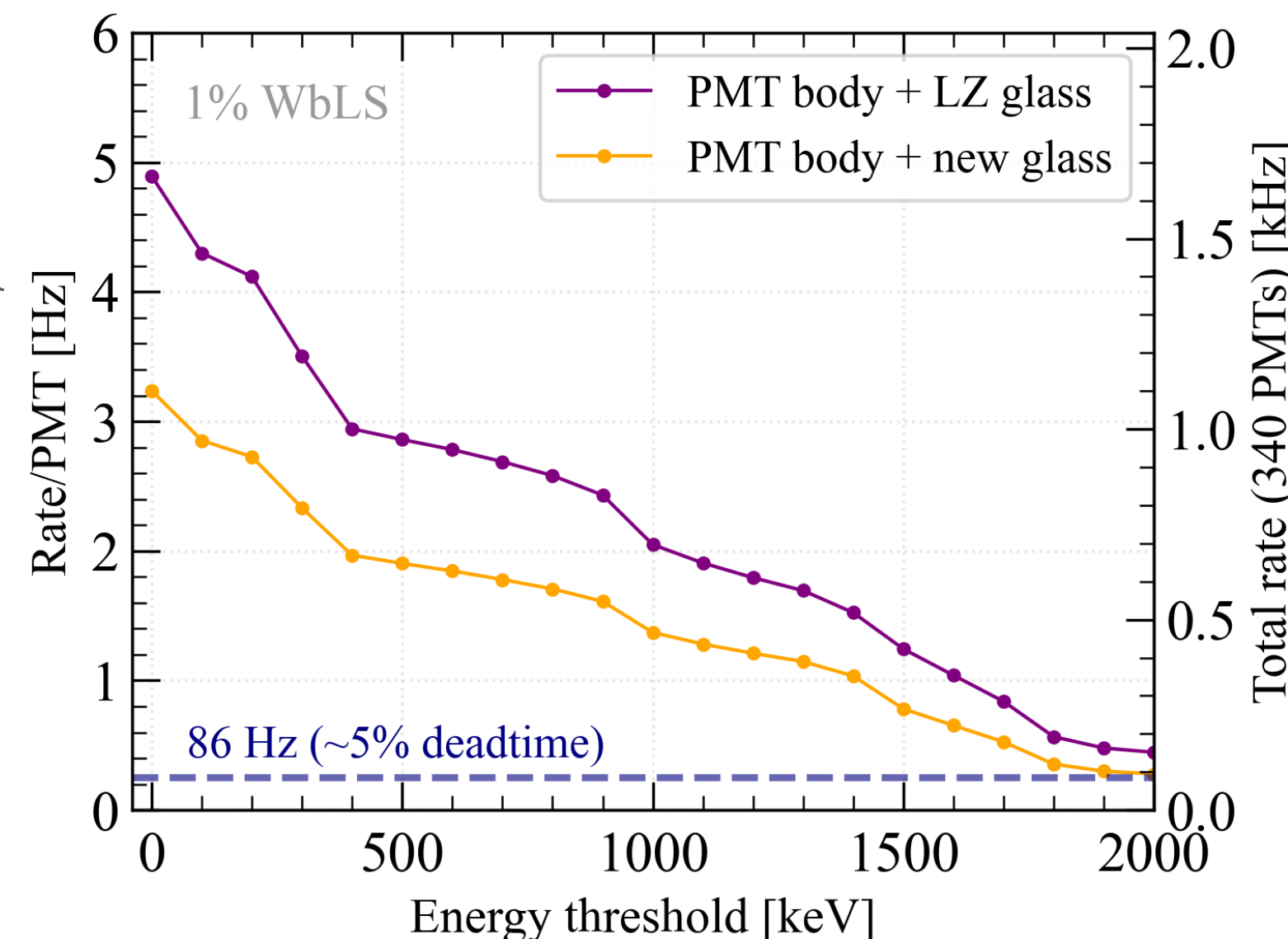
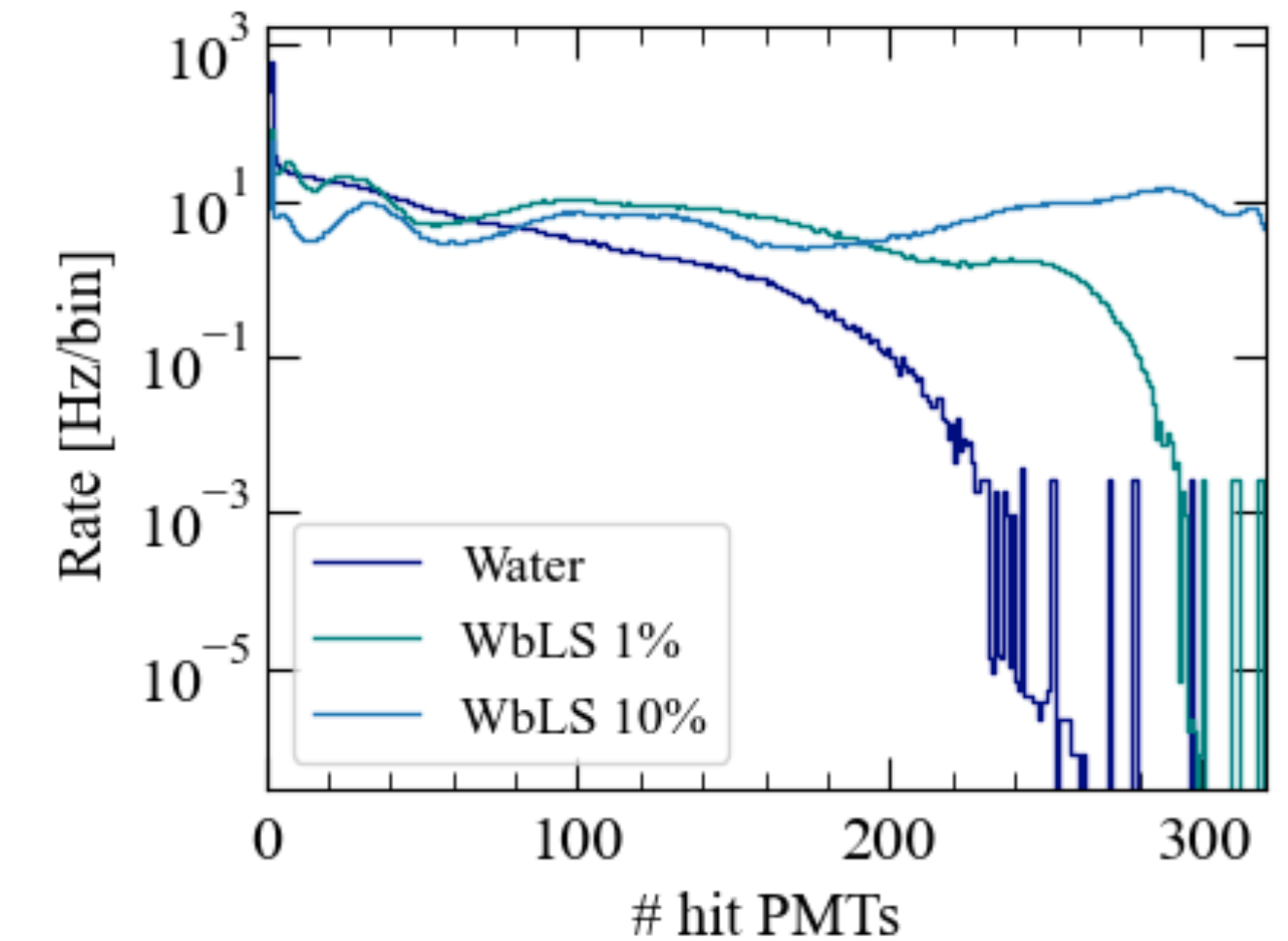
- **OD PMTs** - see next slide



OD PMT SIMULATIONS

- Placing PMTs directly in scintillator medium produces a significant rate
- Plots use LZ PMT radioassay + data from Hamamatsu on a new, low R glass
- Placing PMTs directly in even 1% WbLS is very challenging - need to raise threshold to ~ 2 MeV minimum
 - Potential to mitigate with position reconstruction, but this doesn't avoid trigger rate/occupancy
- With 80cm water gap, rates are reduced significantly to a few Hz at low threshold across 340 PMTs

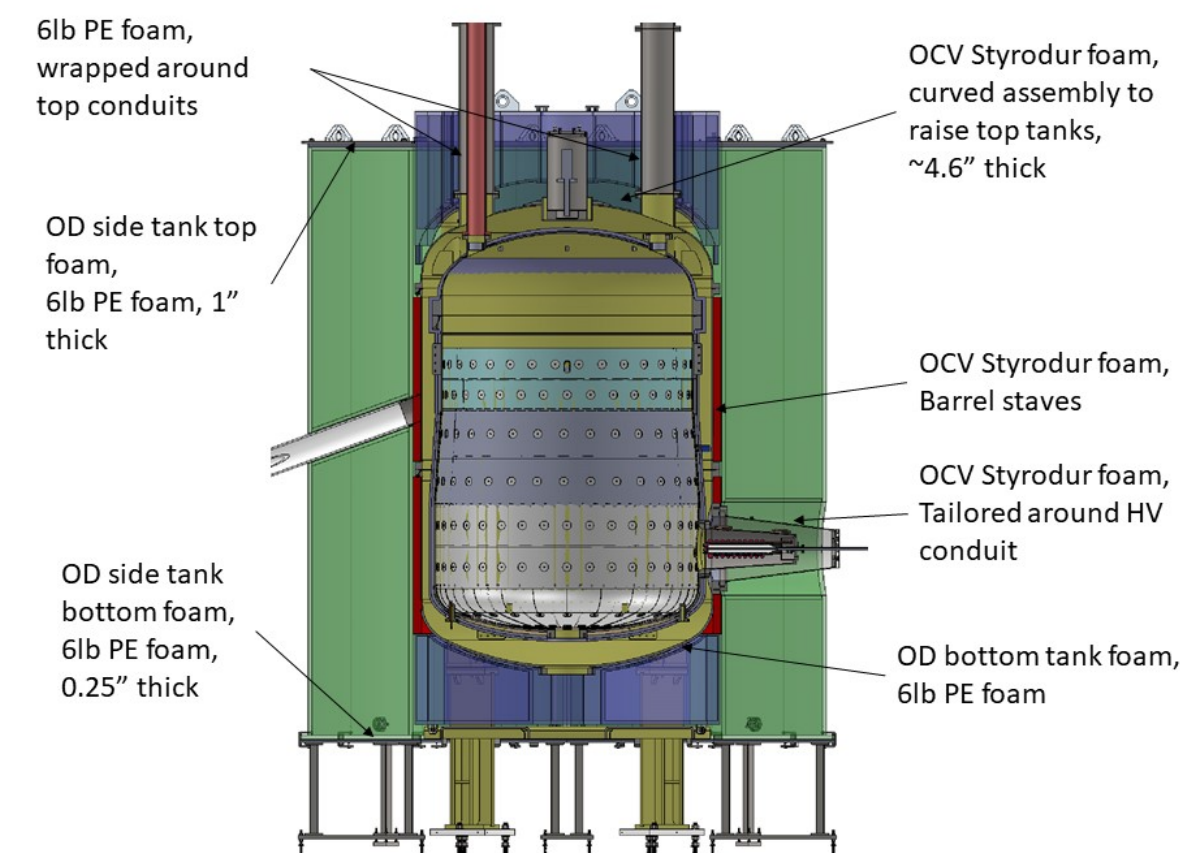
		Hamamatsu		
		U (Bq/PMT)	Th (Bq/PMT)	K (Bq/PMT)
R5912 Full PMT	XENONnT	1.3	1.6	2.3
	LZ Low Rad	1.54	1.04	1.62
	LZ High Rad	4.1	5	7.3
R5912 Glass Only	Standard Glass	3.4	4.4	6.6
	Low-R Glass	0.84	0.44	0.91
	New Low-R Glass	0.03	0.02	0.99
WbLS0-proof 10" R16367		2.56	1.61	15.87



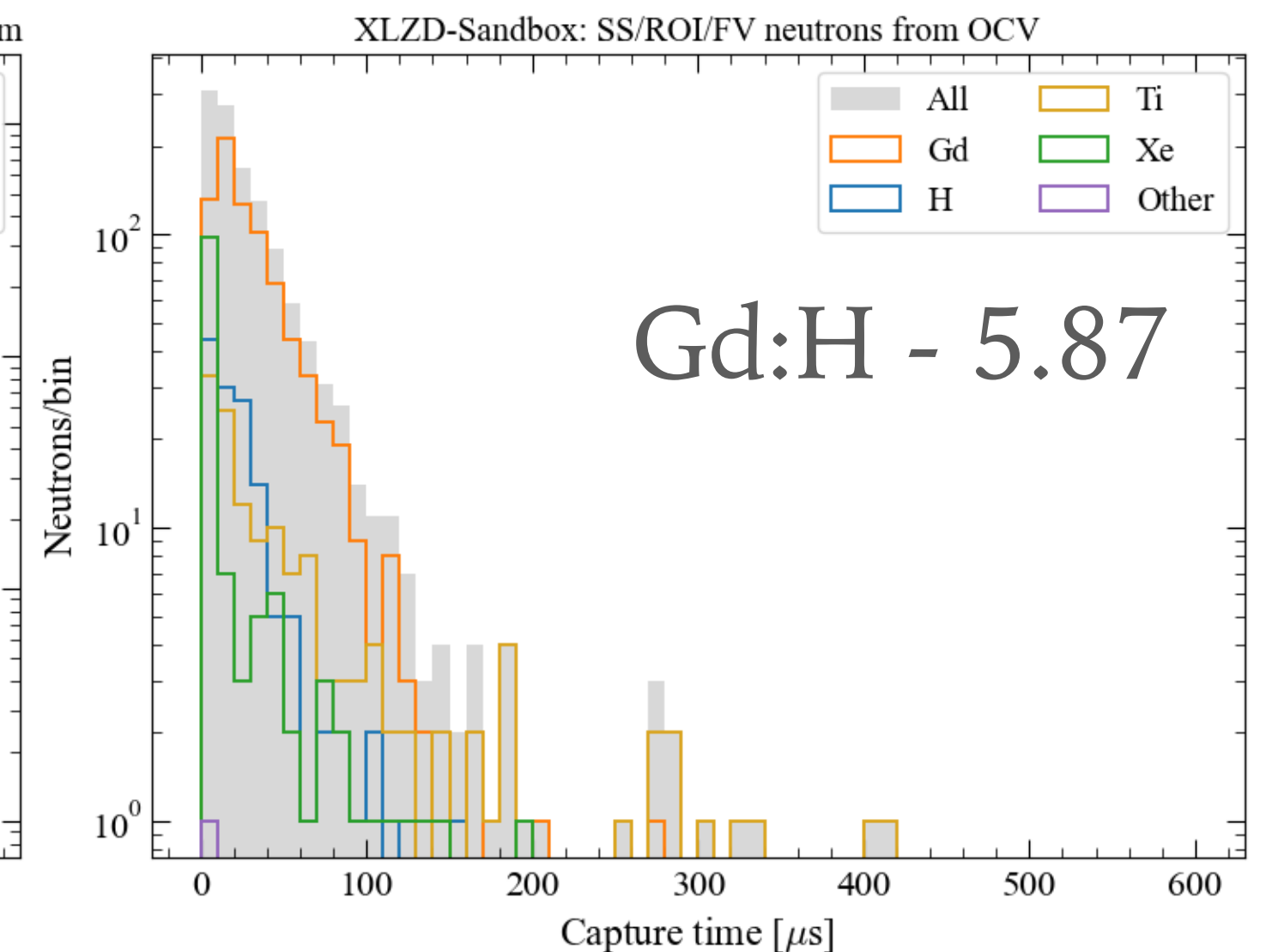
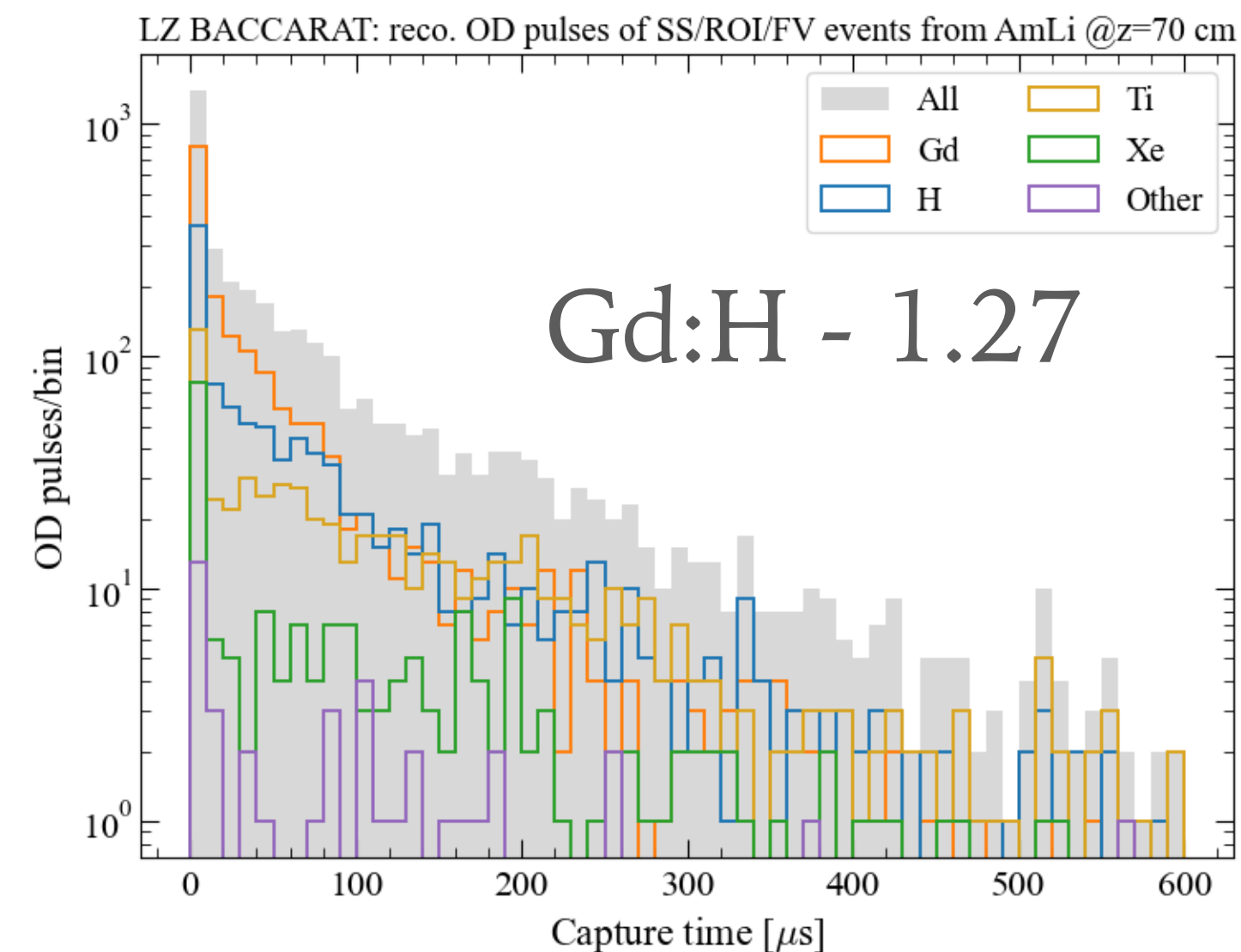
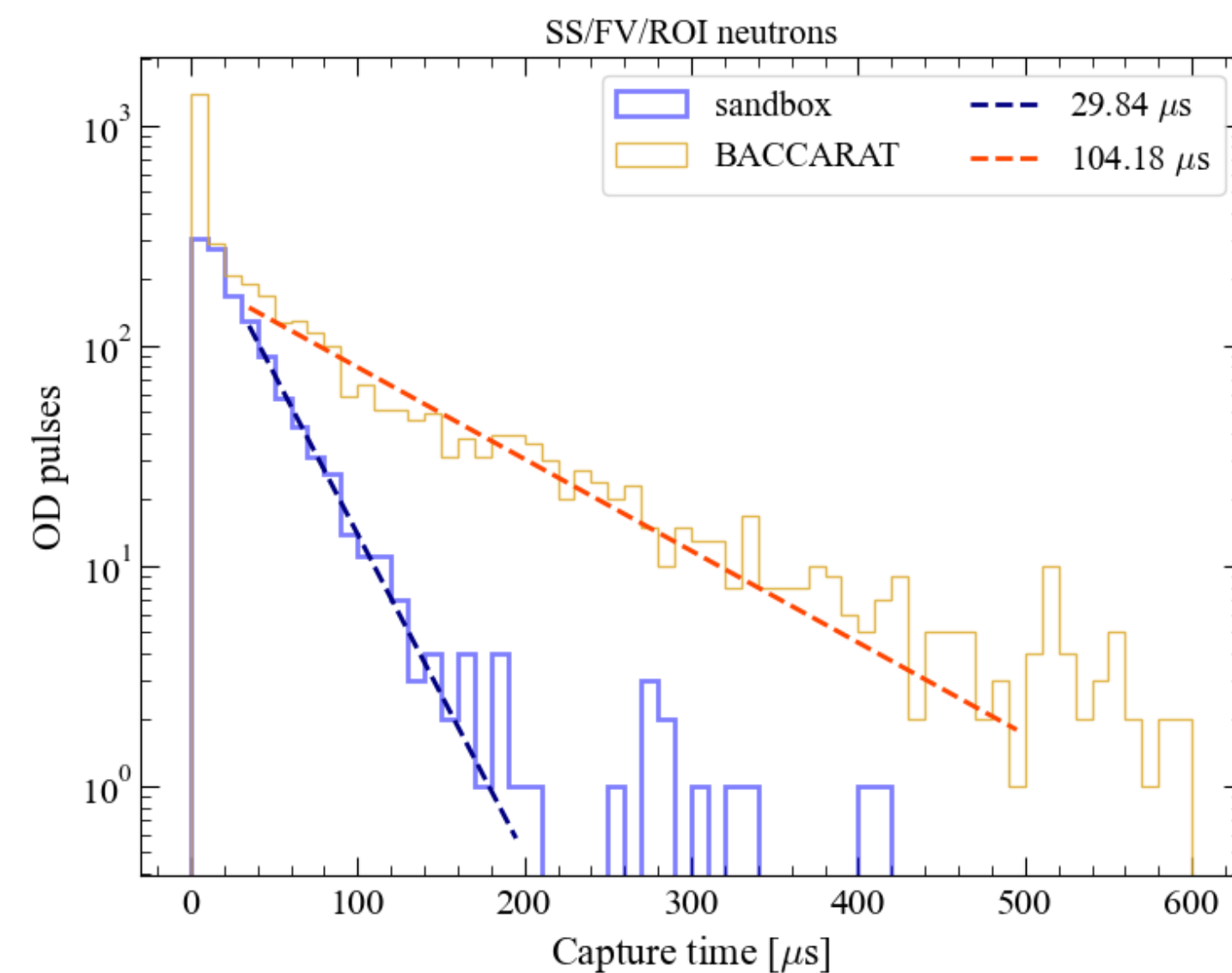
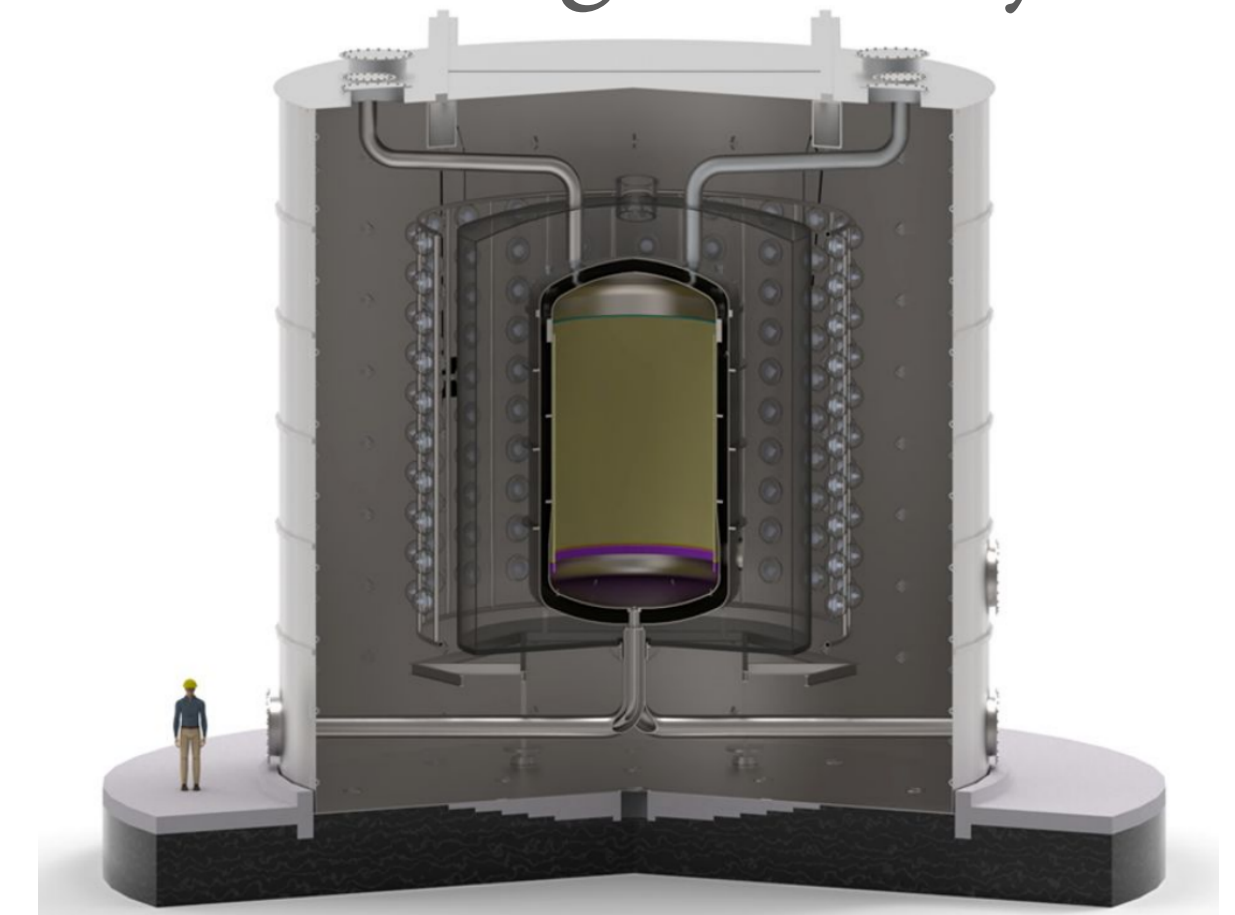
NEUTRON THERMALISATION

- Broad agreement we want no material between the cryostat and the OD medium
- Aim to avoid issue in LZ with long capture times due to hydrogenous materials close to cryostat - foam, water, acrylic
- The efficiency simulations later in this talk used a $600\mu\text{s}$ window - overkill, needs optimising

LZ geometry

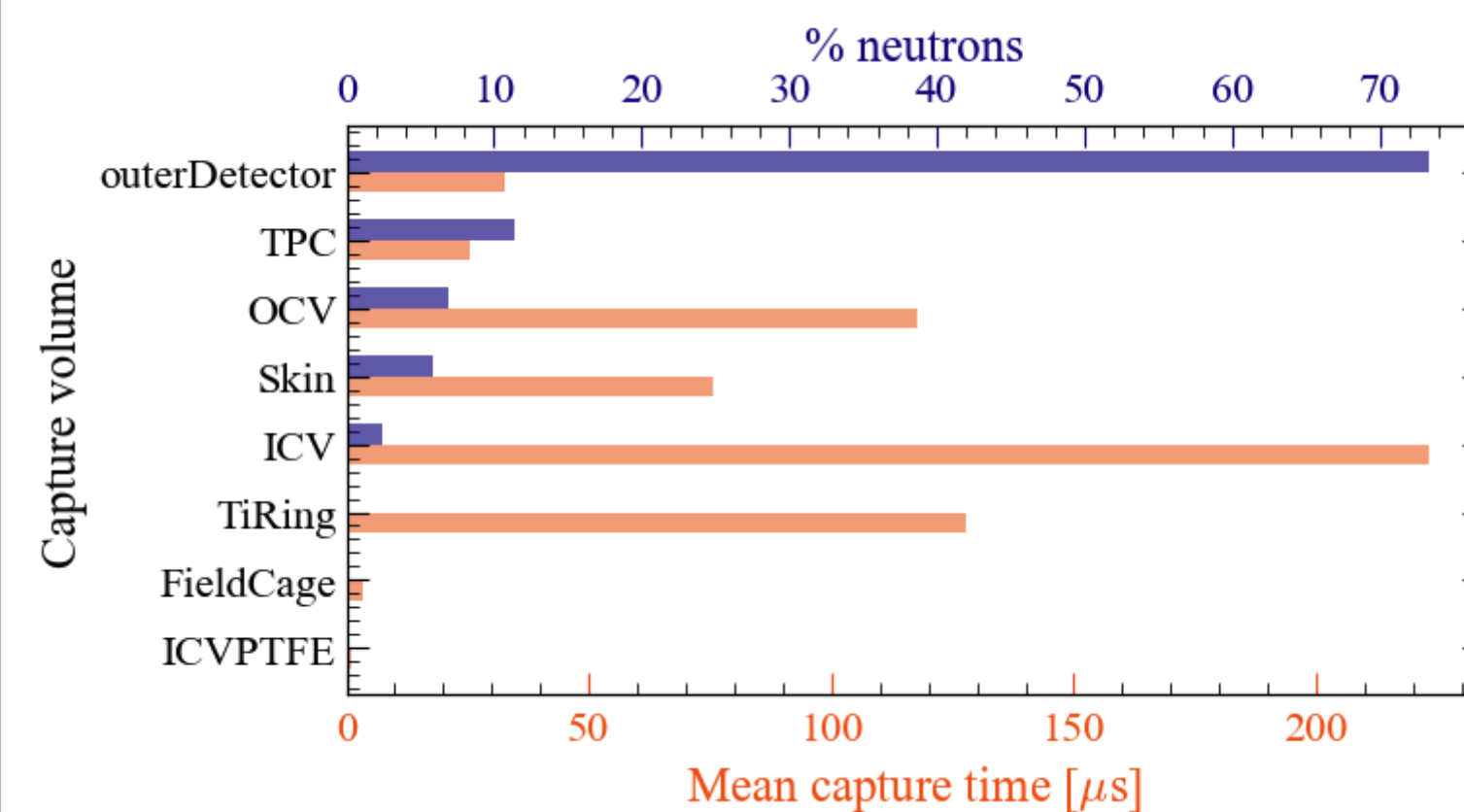
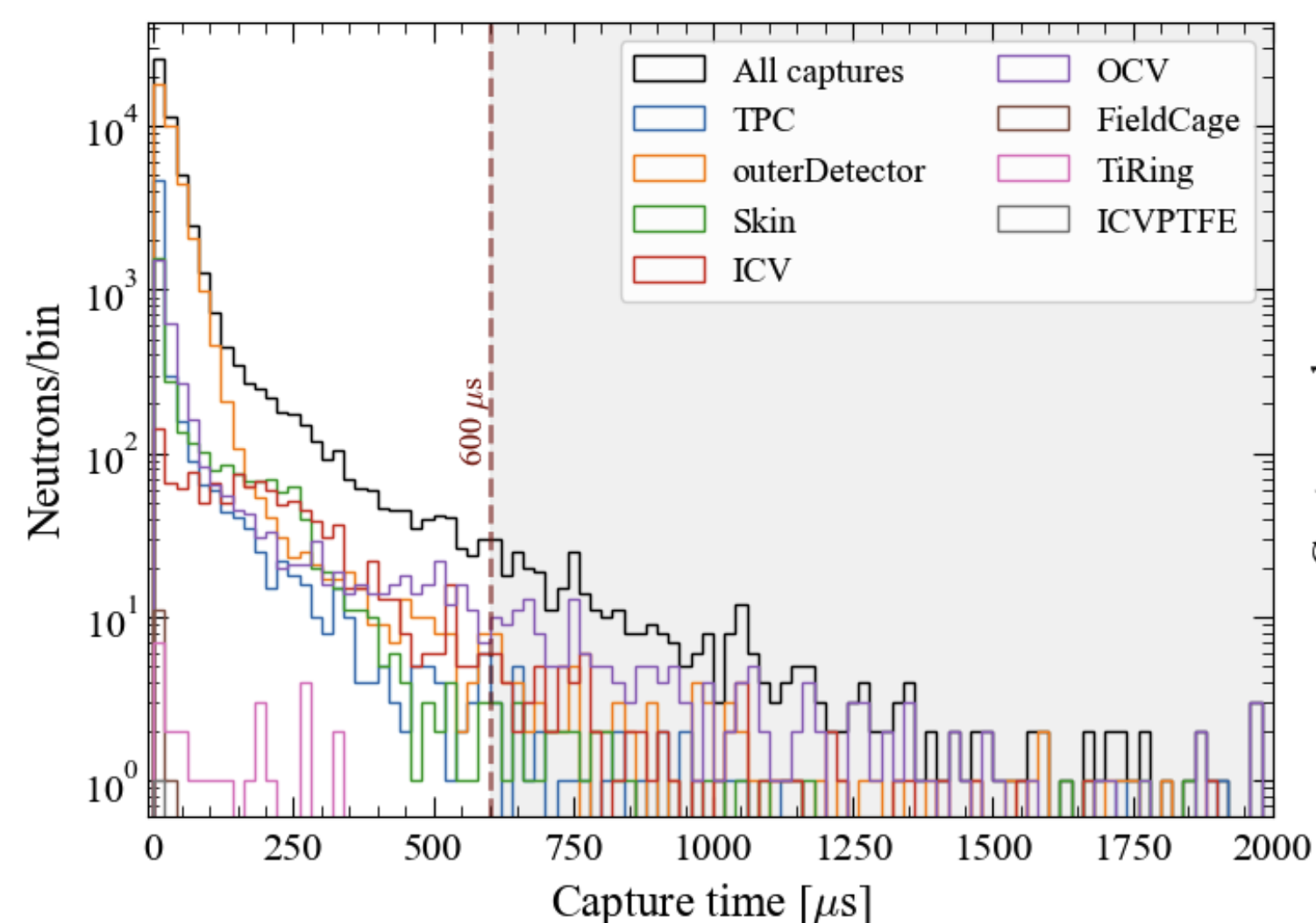
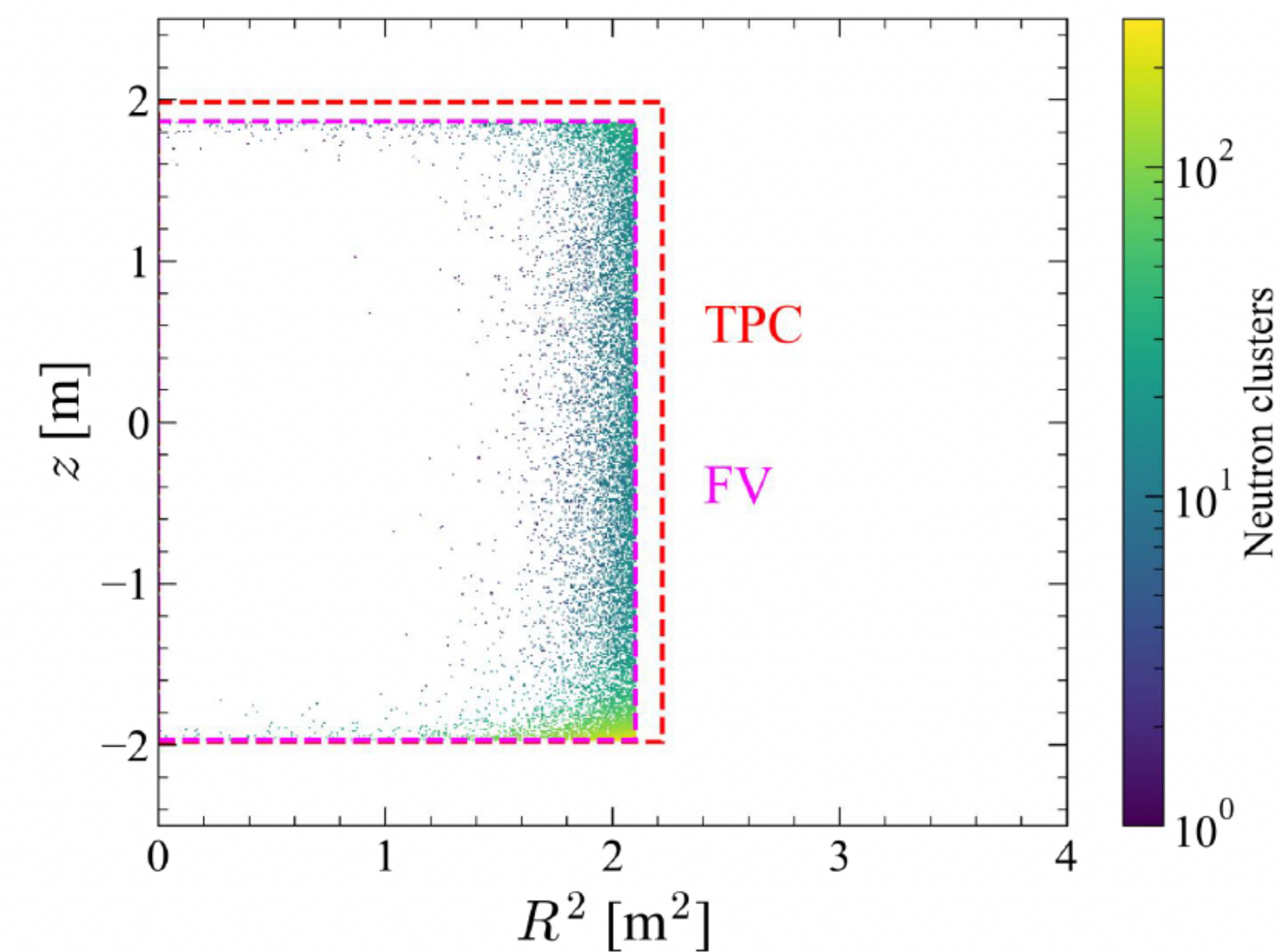
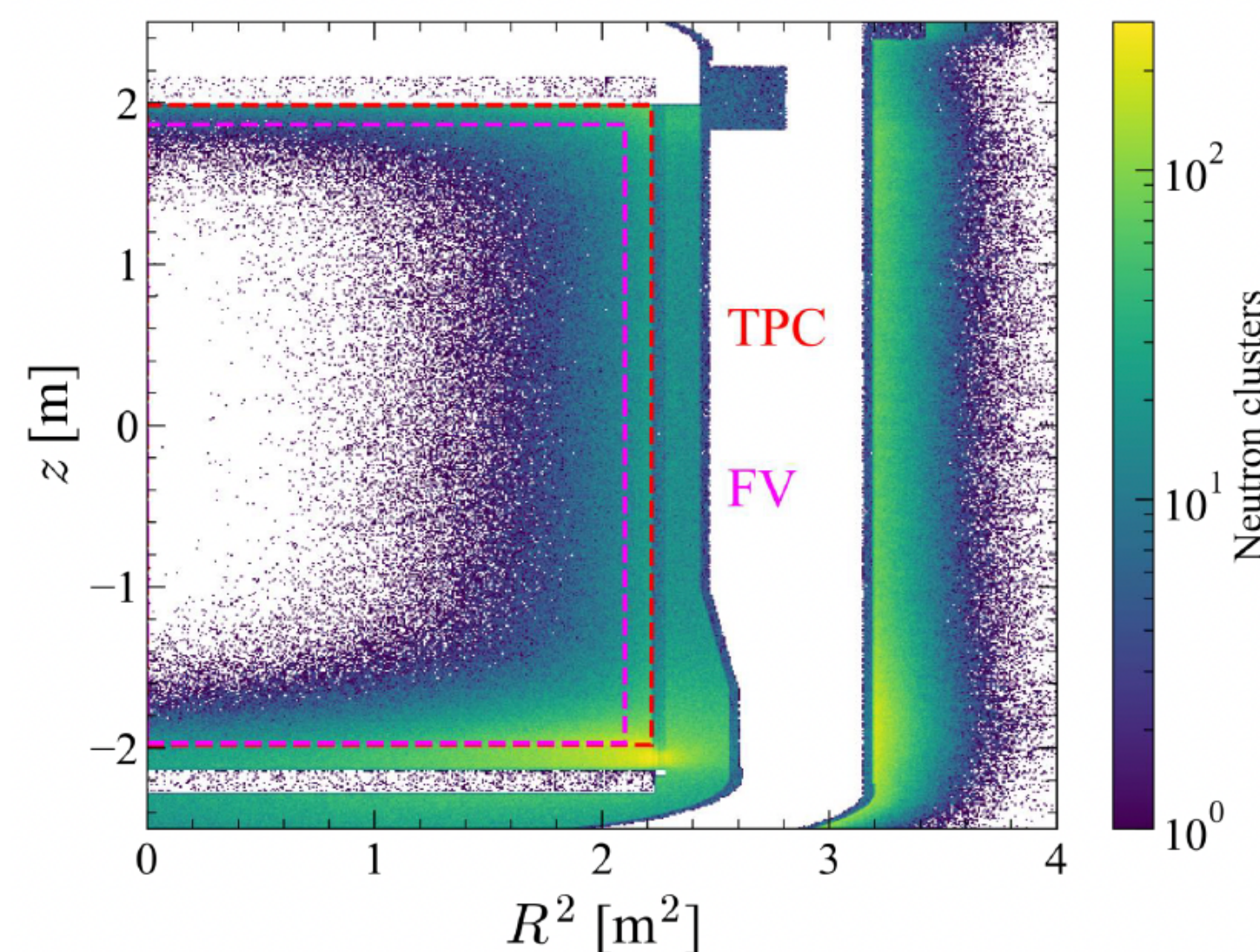


XLZD geometry



NEUTRON SIMULATIONS

- Key background sources simulated
 - Cryostat
 - PMTs
 - PTFE
 - Resistors
- SOURCES4a (,n) neutron spectra from LZ
- Neutron energy deposits are clustered using:
 - $R = 30$ mm
 - $z = 2$ mm
 - $t = 100$ ns



NEUTRON VETO EFFICIENCY

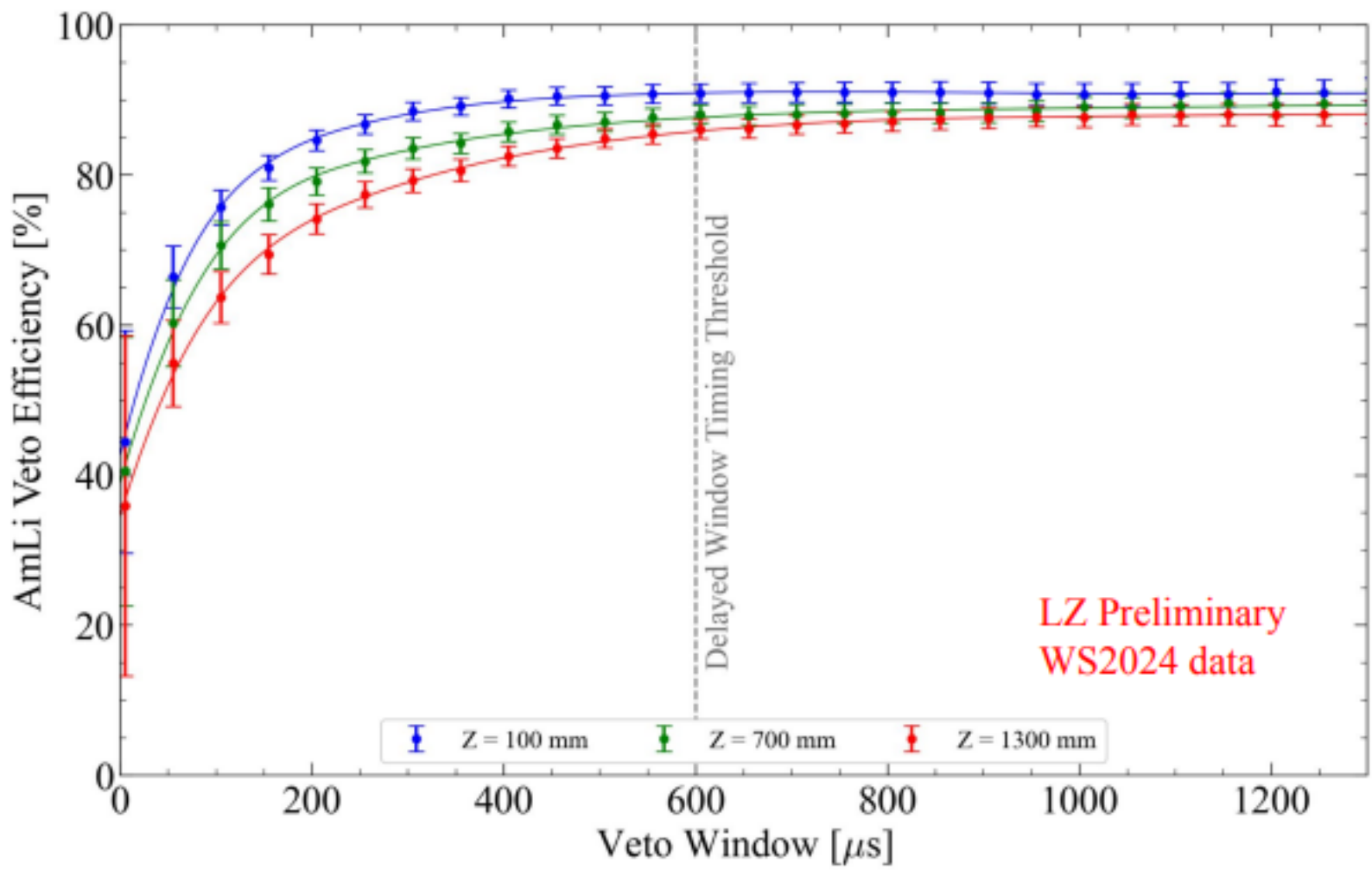
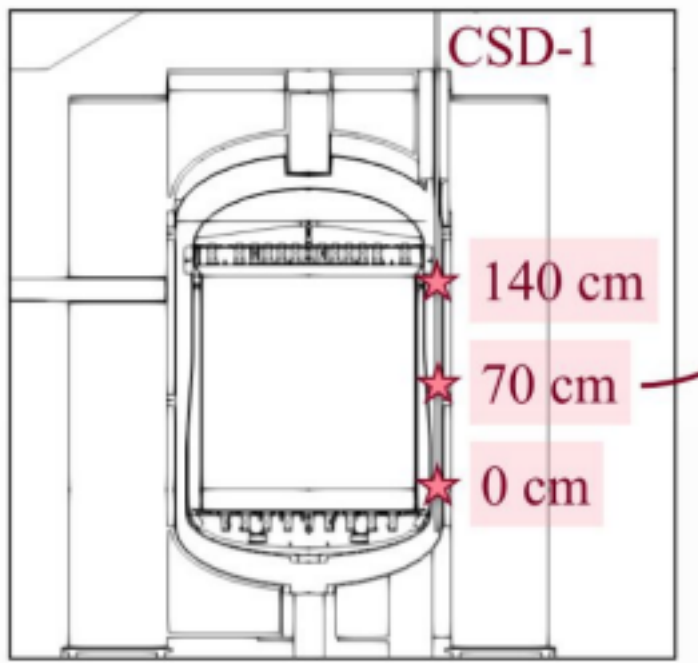
- From requirements task force:
 - Neutron NR rate <10% of CEvNS
 - 0.0046 - 0.0064 counts t-y
 - We have aimed for < 1 count in 10 years
- Simulations of the key NR backgrounds indicate a rate of ~ 1.1 NR/year, resulting in a required veto efficiency of >91%
- We have conservatively raised this to >95%
 - Accounts for 4% systematic observed in LZ across all calibration sources (higher in sim than data)

Parameter	Units	Proposed Requirement	Comment
WIMP cross-section 5σ sensitivity at 2800 GeV/c ²	cm ²	$< 2 \times 10^{-47}$	Observation of Majorana triplet model and higher mass EW multiplet models
WIMP cross-section 90% exclusion at 60 GeV/c ²	cm ²	$< 2 \times 10^{-49}$	Exclusion of majority of Higgs portal models
Fiducial exposure	t-y	> 500 – 650	Range corresponds to LNGS – Boulby/SNL/SURF
Analysis threshold	pe	≤ 4	i.e. no worse than a 4-fold coincidence requirement. FIXED
Neutron NR background	cnts/t-y	< 0.0046-0.0064	Aim for rate <10% of CEvNS NR. Range corresponds to LNGS – Boulby/SNL/SURF
Pb-214 activity	μBq/kg	< 0.1	Aim for rate < solar ER (and < CEvNS NR after discrimination)
Kr-85 concentration	ppt	< 0.1	Aim for rate < solar ER (and < CEvNS NR after discrimination)
Active mass	tonne	> 60	FIXED
ER leakage @50% NR acc	%	< 0.5	
Single electron efficiency	%	XXX	TBD. Derived in FlameNEST.
LCE	%	> 50	Averaged absolute LCE
Drift field	V/cm	> 80	
TPC PMT QE	%	> 31	FIXED
Gas field	kV/cm	> 6.75	
Electron lifetime	ms	> 10	FIXED

Preliminary Draft -- for Discussion

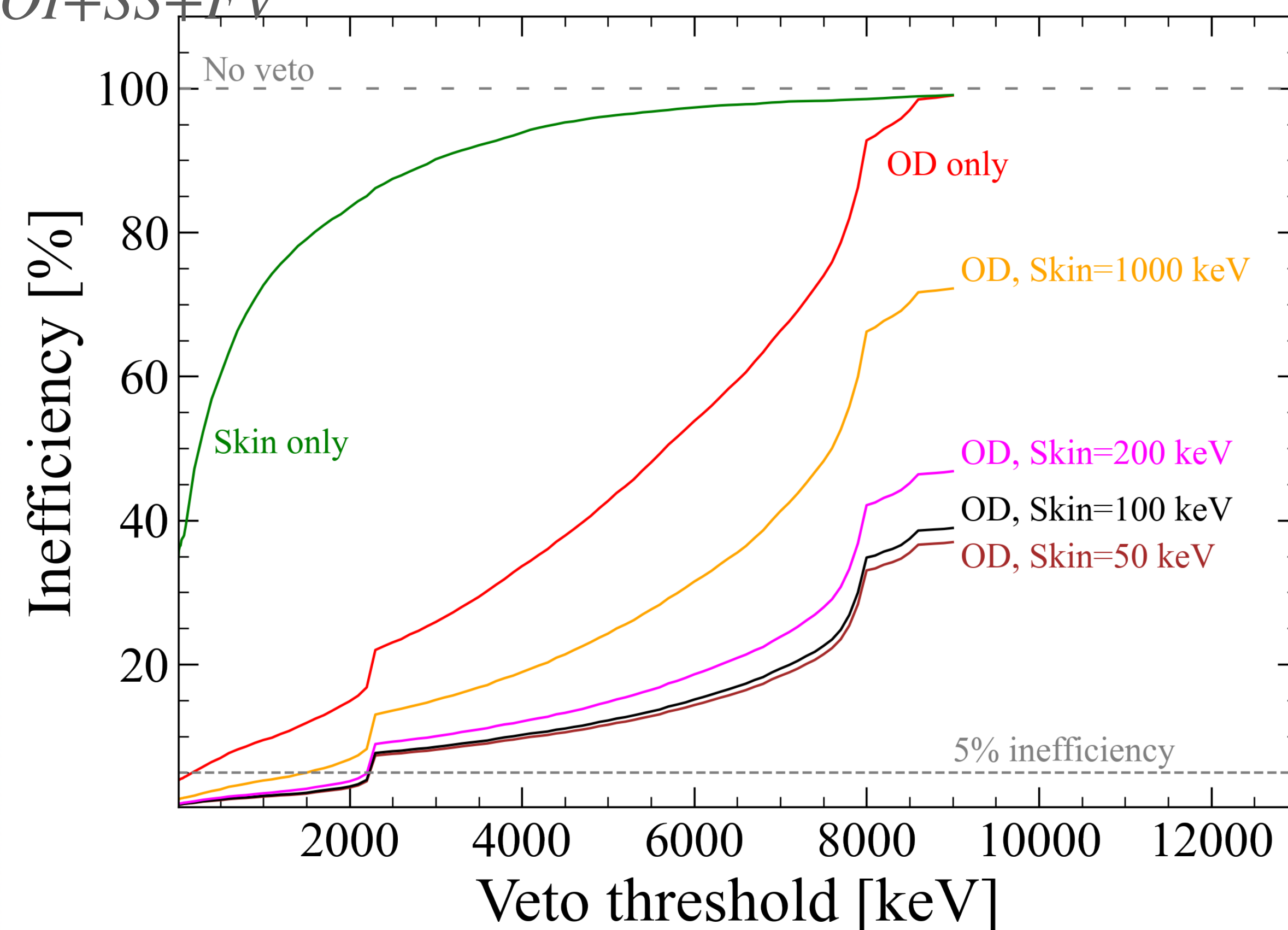
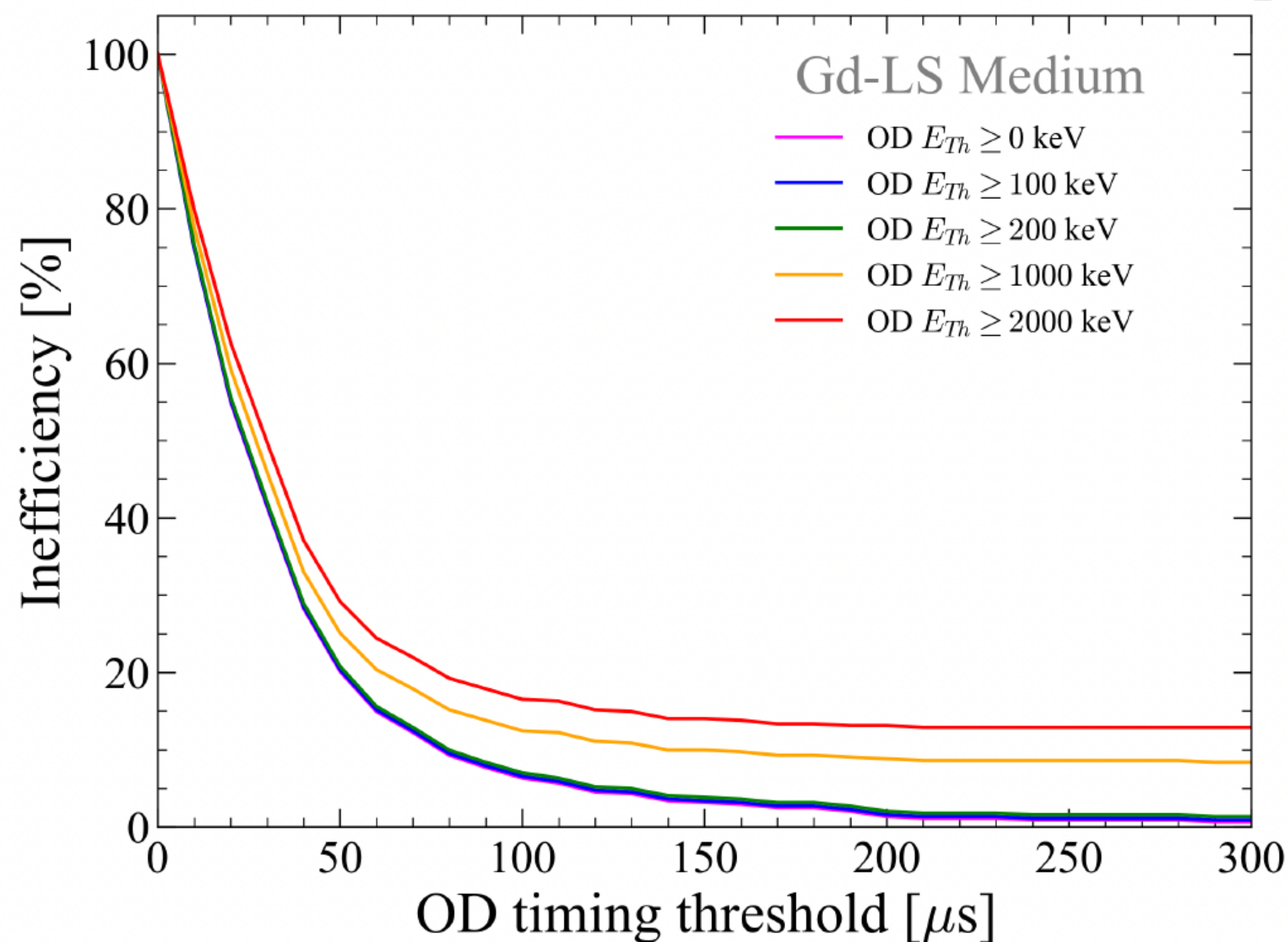
11

LZ AmLi data



NEUTRON VETO EFFICIENCY

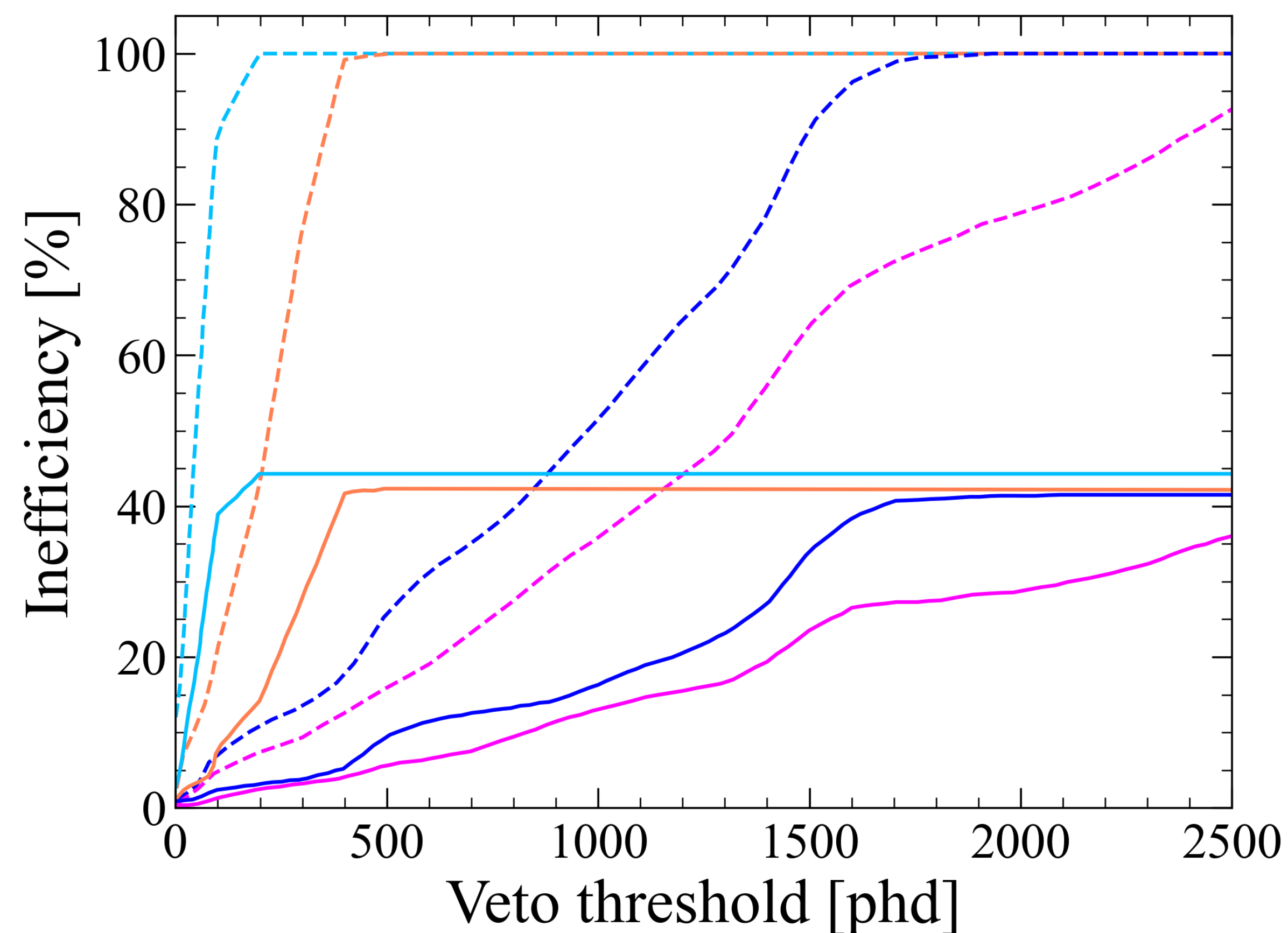
$$\epsilon = \frac{N_{ROI+SS+FV+(OD(E_{th},\Delta T)||Skin(E_{th},\Delta T))}{N_{ROI+SS+FV}}$$



See poster “XLZD Outer Detector: Neutron Veto Efficiency” by Dr Sam Woodford

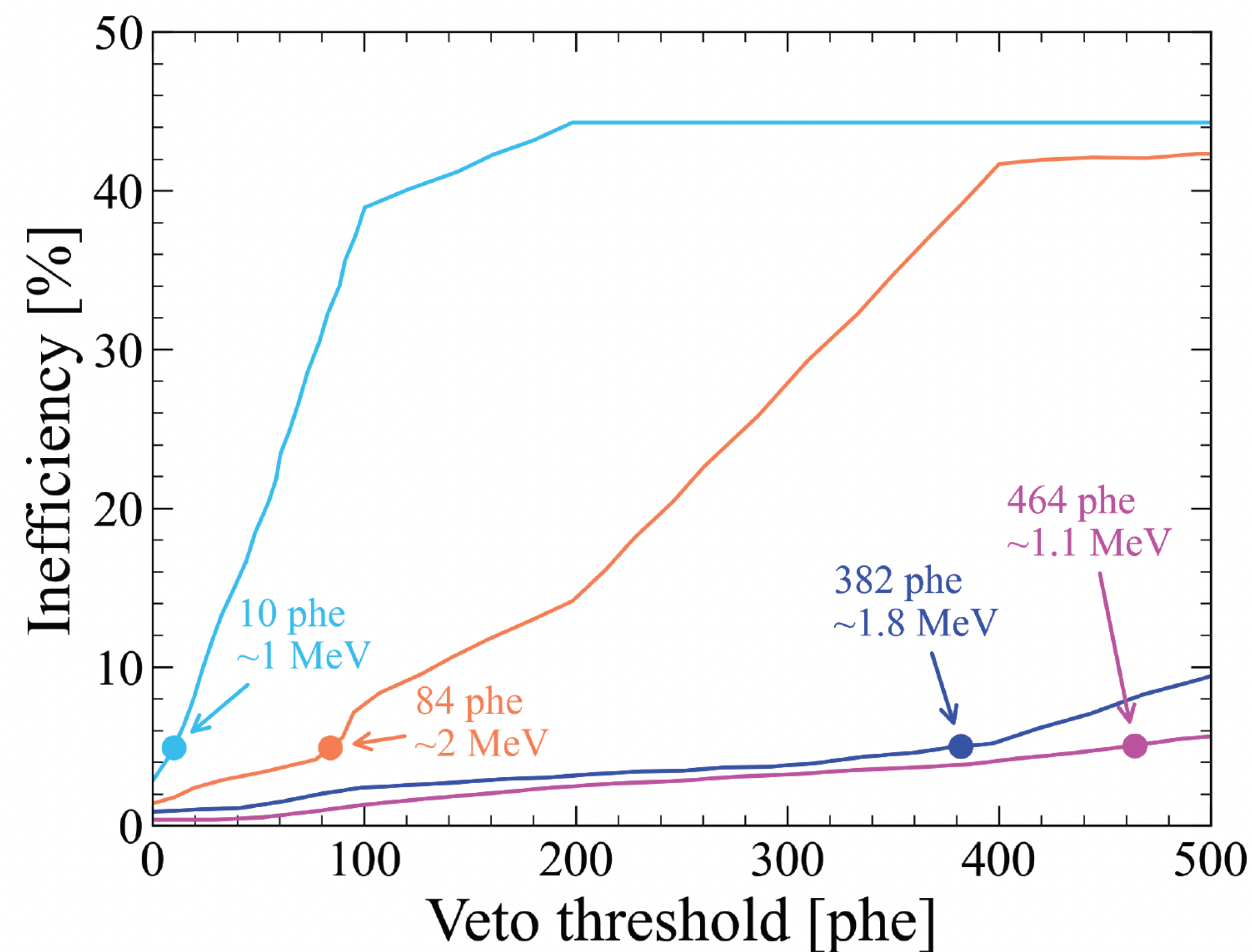
NEUTRON VETO EFFICIENCY

- Gd-Water OD Only
- Gd-WbLS (1%) OD Only
- Gd-WbLS (10%) OD Only
- Gd-LS OD Only
- Gd-Water OD or Skin > 100 keV
- Gd-WbLS (1%) OD or Skin > 100 keV
- Gd-WbLS (10%) OD or Skin > 100 keV
- Gd-LS OD or Skin > 100 keV



Only combined efficiencies, zoomed in

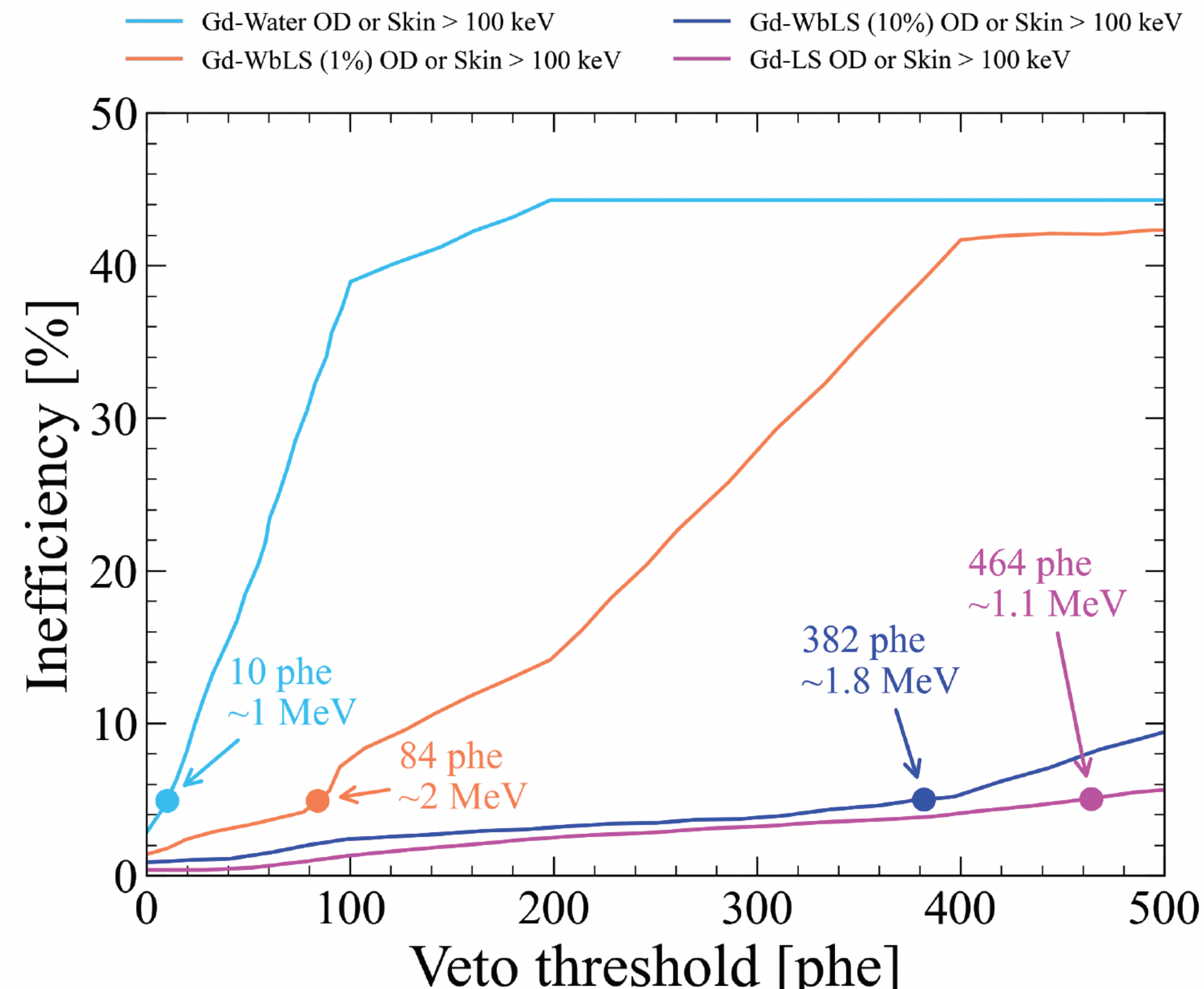
- Gd-Water OD or Skin > 100 keV
- Gd-WbLS (1%) OD or Skin > 100 keV
- Gd-WbLS (10%) OD or Skin > 100 keV
- Gd-LS OD or Skin > 100 keV



See poster “XLZD Outer Detector: Neutron Veto Efficiency” by Dr Sam Woodford

NEUTRON VETO EFFICIENCY

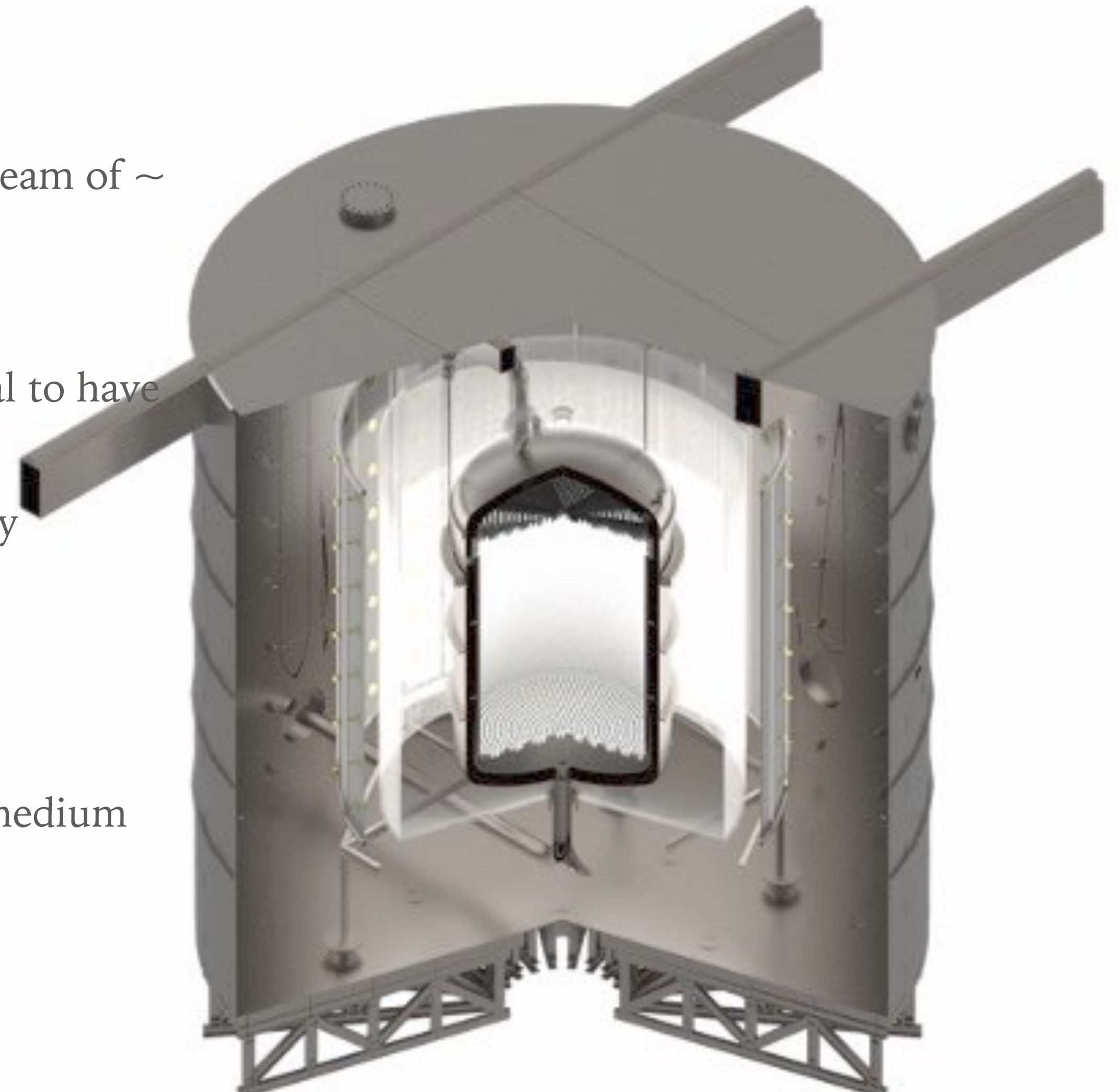
- Full optical simulations
- Preliminary results, caveats:
 - These are expected to be optimistic for WbLS (LY with no Gd-loading used, may drop to 50%)
 - 120 PMTs used - PMT array optimization studies are still immature
- Low threshold is readily be achieved with GdLS



See poster “XLZD Outer Detector: Neutron Veto Efficiency” by Dr Sam Woodford

CONCLUSIONS

- There has been a huge effort in the UK to establish a Geant4 simulation framework to be used for Outer Detector design and performance studies
 - XLZD-Sandbox recently expanded for whole UK project, now with a team of ~ 15 PIs, postdocs & students contributing
 - Very happy for others to use - please let me know!
 - Will work closely with simulations task force going forward - potential to have this package as part of official XLZD framework
- Preliminary simulations of the OD suggest that the neutron veto efficiency requirement is most readily achieved with GdLS
- Key further work needed:
 - Expand **neutron background modeling** to more components
 - Investigate **mitigation of high rate caused by PMTs submerged in medium**
 - **Optimisation** of OD size and PMT arrangement
 - Expand studies of **OD backgrounds**
 - **Validate WbLS optics/LY** when more data available for Gd-loaded
 - ...

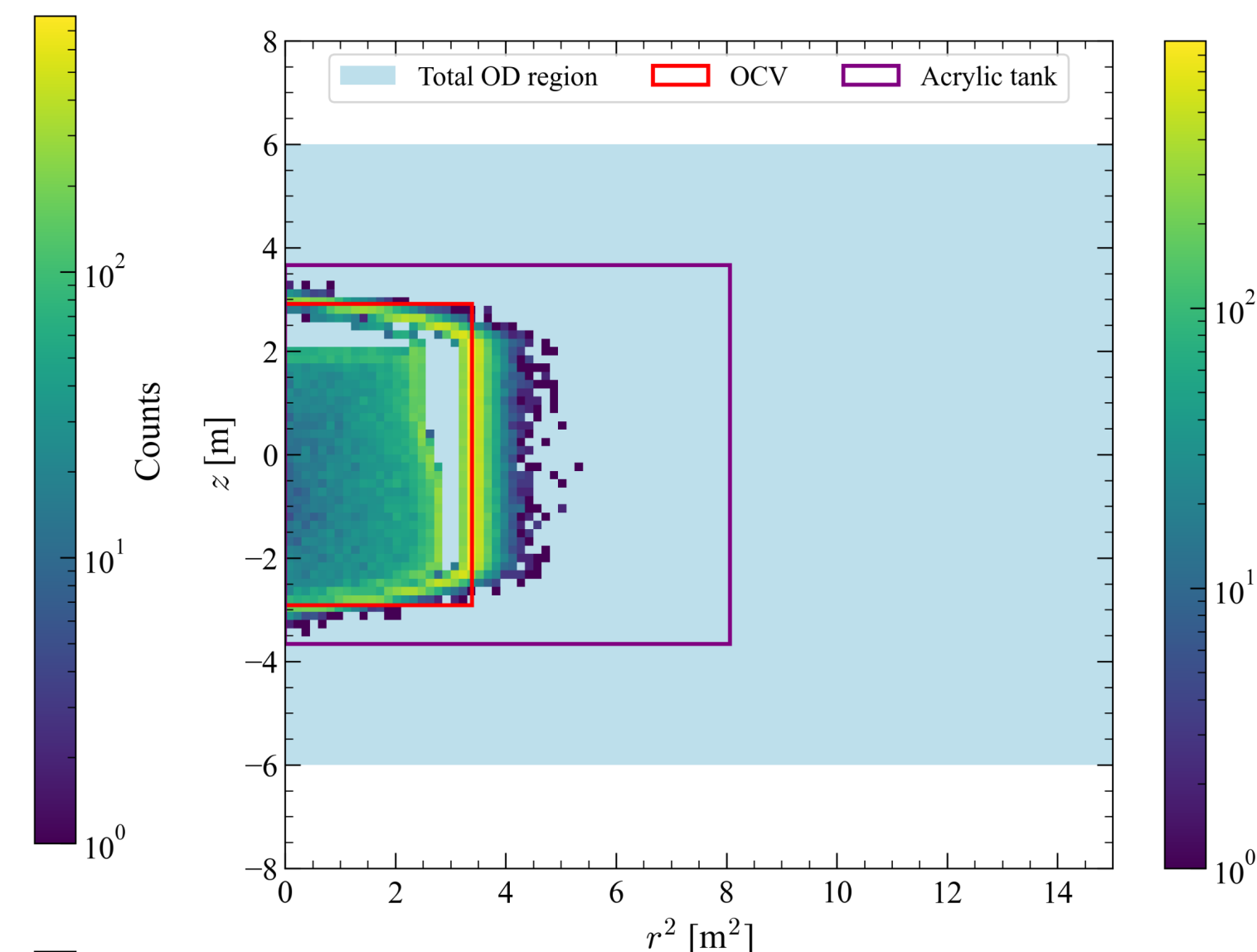
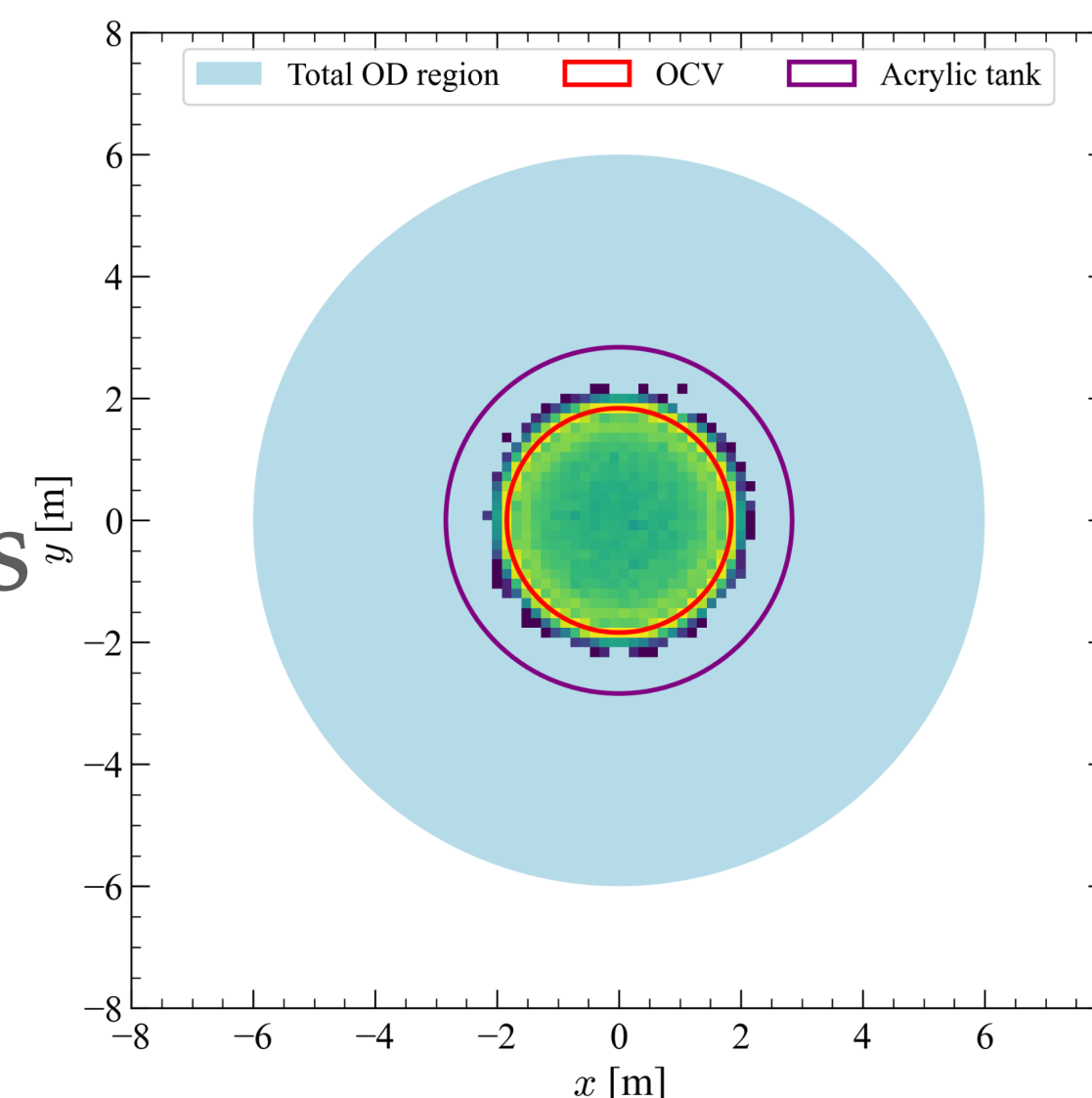


BACKUP SLIDES

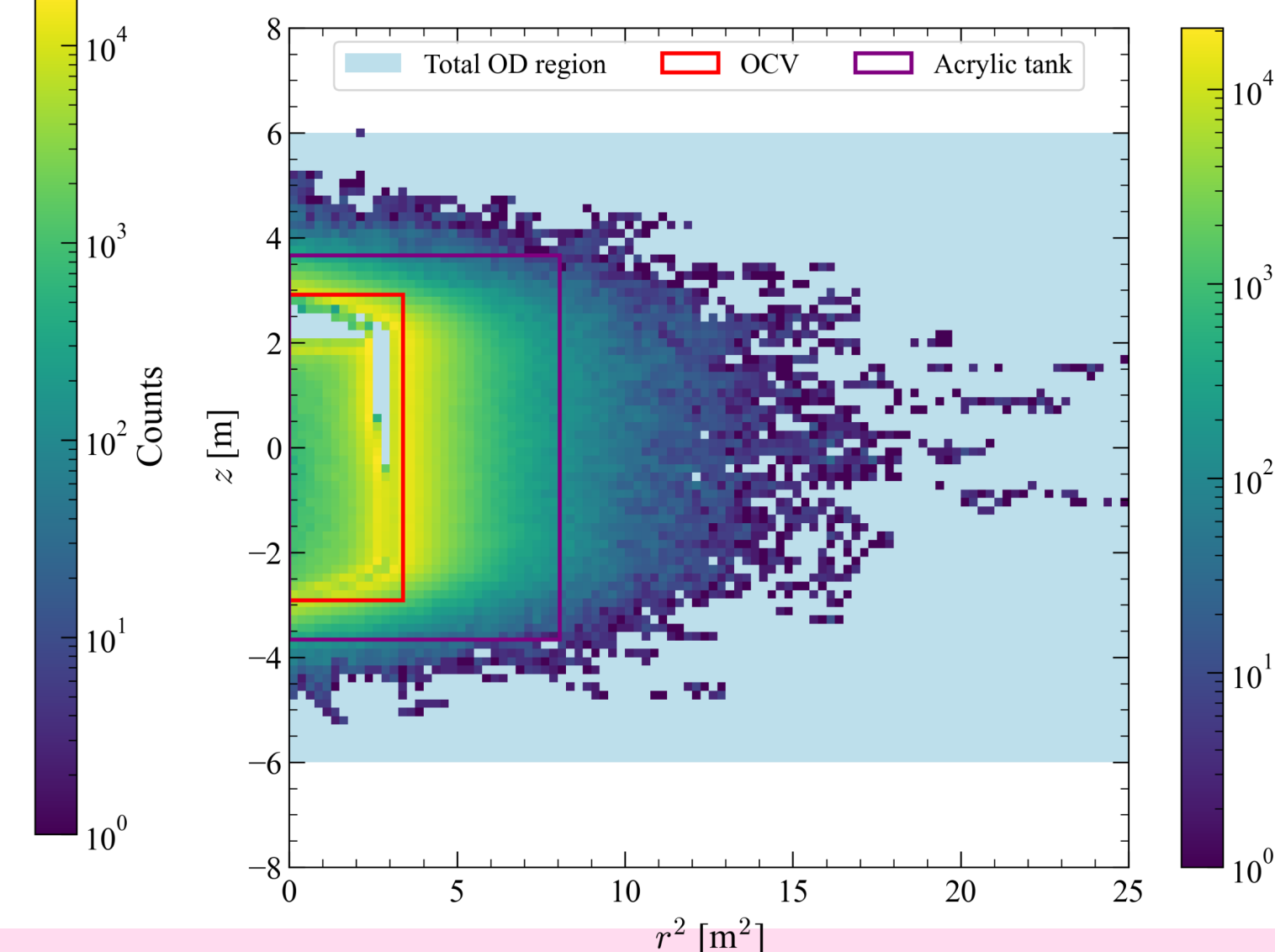
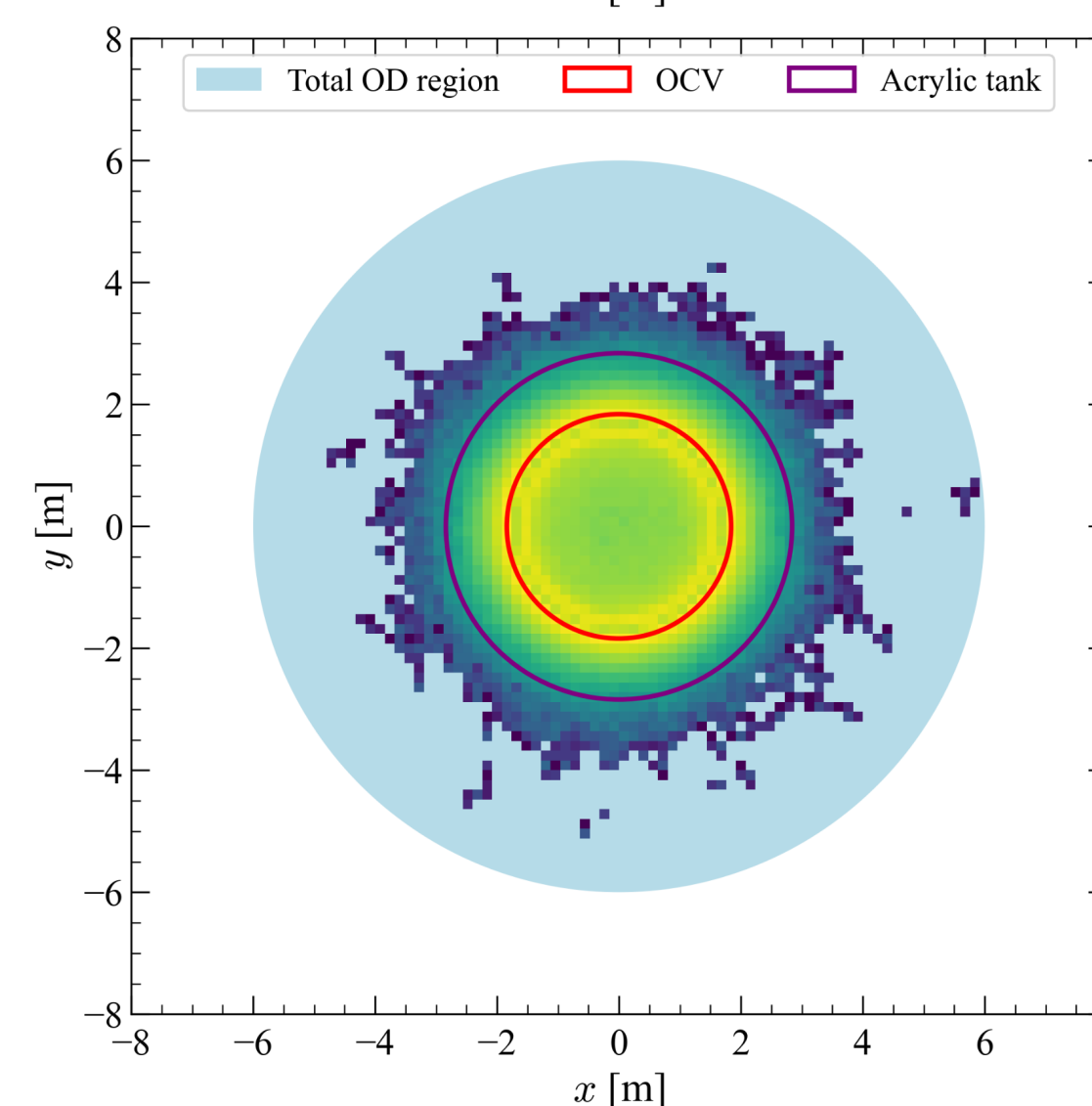
NEUTRON CAPTURES AND GAMMA RANGE

- 1m gap on all sides for acrylic vessel contains all nCaptures as expected
- Aim to avoid neutrons in hydrogenous materials which slows down neutron capture

Neutrons



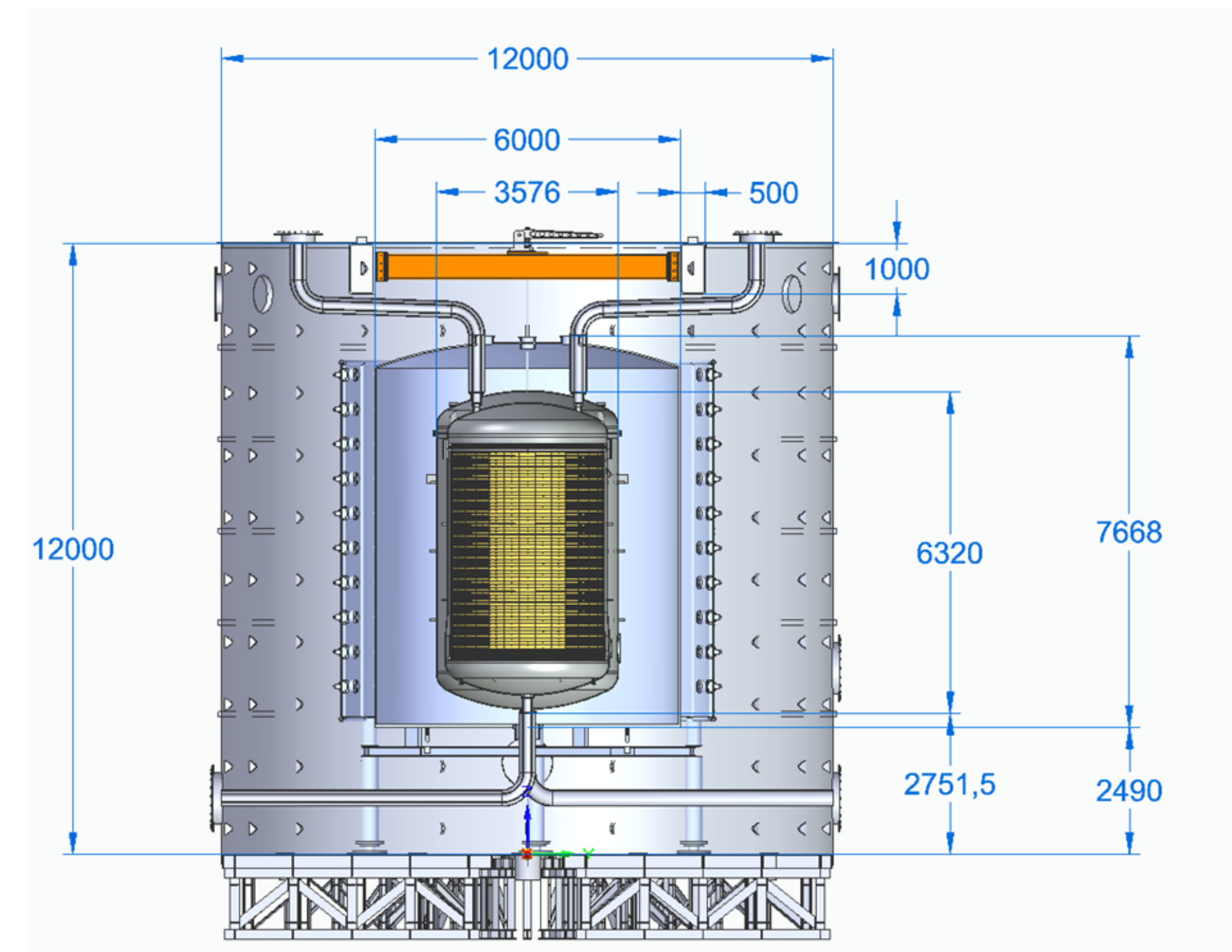
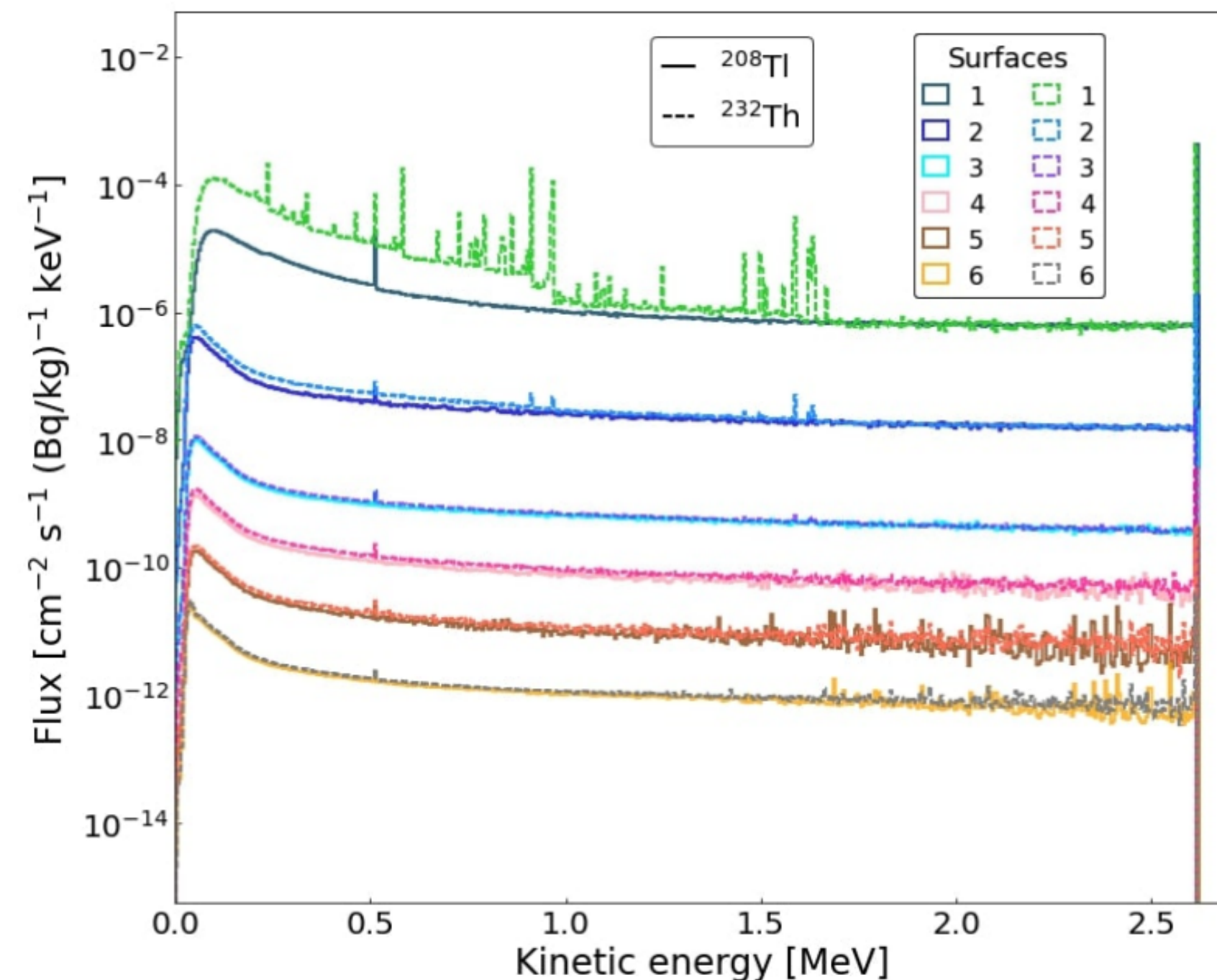
Gammas



PRELIMINARY CAVERN RATE

- Paper [\[https://arxiv.org/abs/2504.11613\]](https://arxiv.org/abs/2504.11613) considered a smaller OD (and smaller cryostat)
- Use flux at 3rd surface as closer to OD dimensions and scale accordingly using attenuation lengths for key gammas ray energies

Volume	Height [m]	Diameter [m]	Distance from WT [m]	
			Top & sides	Base
1st surface	11.14	12.10	-0.10	-0.10
WT	10.94	11.90	0	0
2nd surface	8.94	9.90	1.00	1.00
3rd surface	7.54	7.90	2.00	1.40
4th surface	6.74	6.40	2.75	1.45
5th surface	5.96	4.92	3.49	1.49
GdLS	5.94	4.90	3.50	1.50
6th surface	4.96	3.92	3.99	1.99
OCV	4.94	3.90	4.00	2.00



LABORATORY CAVERN BACKGROUNDS

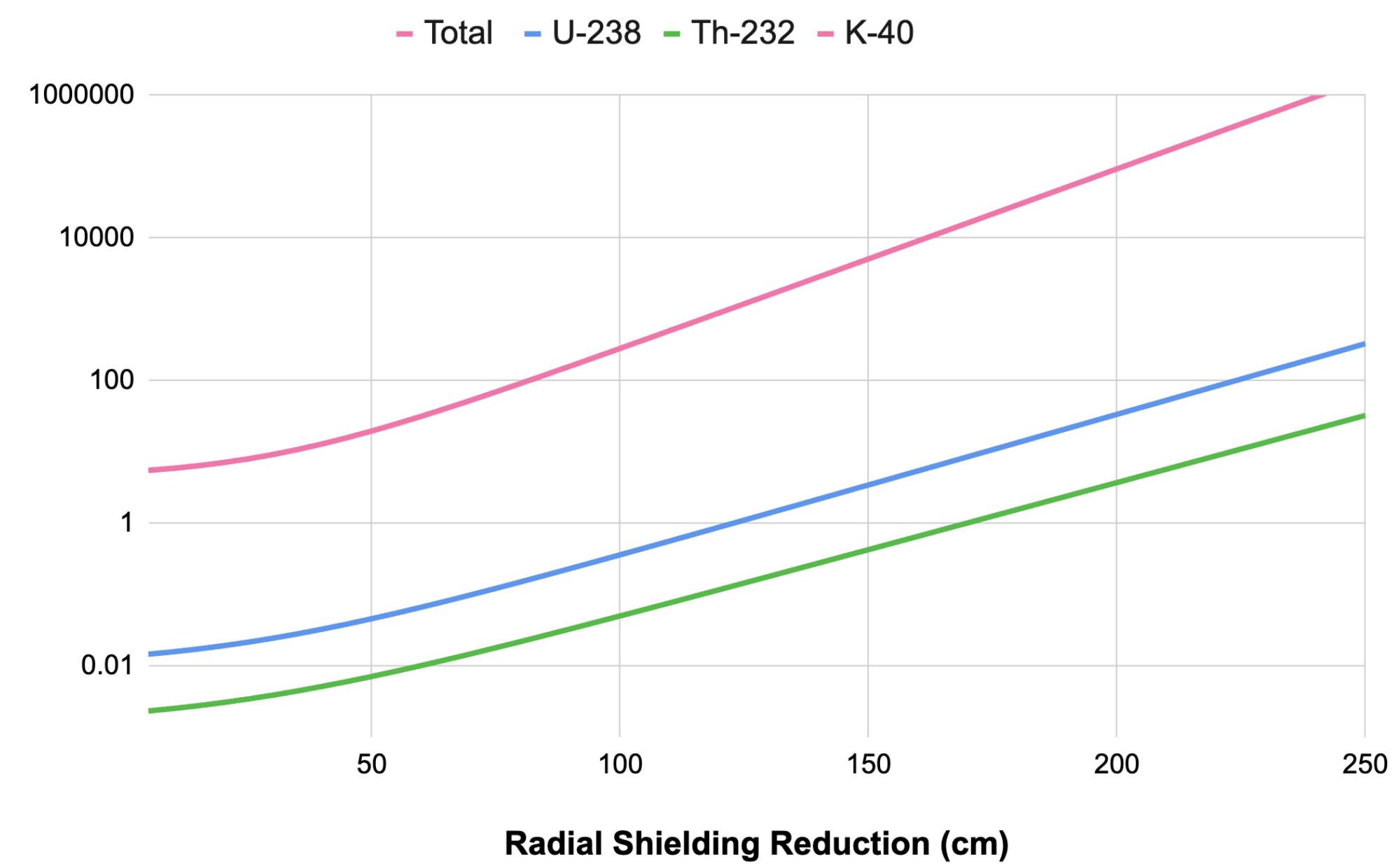
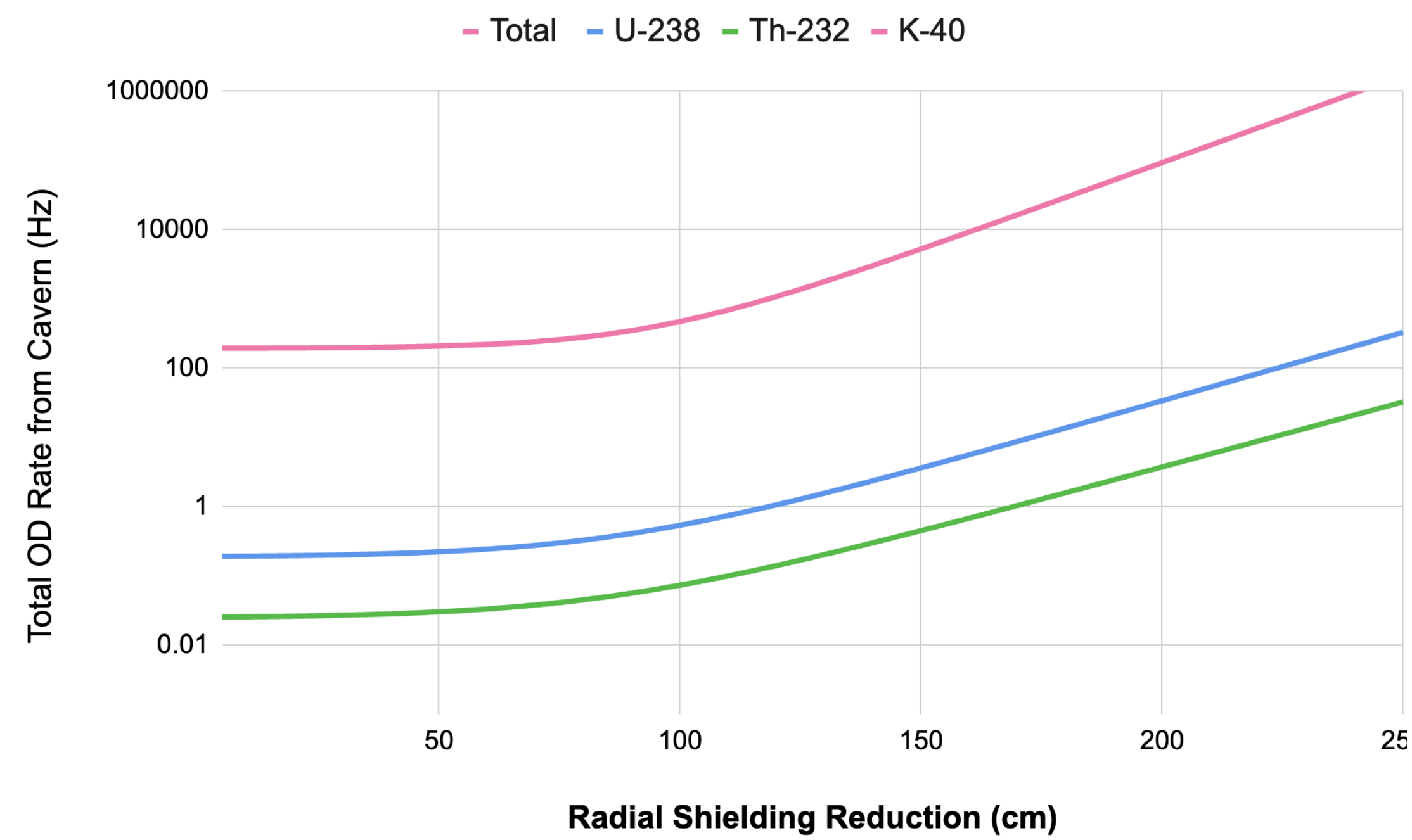
Laboratory	K (Bq/kg)	U (Bq/kg)	Th (Bq/kg)	Dominant Source	Total Rate (Hz)
Boulby, UK* - POLYHALITE	2500 ± 126	0.354 ± 0.042	$(1.14 \pm 0.37) \times 10^{-2}$	polyhalite	5.57
Boulby, UK* - Current lab	112 ± 2	1.63 ± 0.06	1.88 ± 0.06	mudstone & halite	0.70
Gran Sasso, Italy*	70 ± 2	9.5 ± 0.3	3.7 ± 0.2	concrete	1.27
Snolab, Canada	240 ± 10	15 ± 2	9.7 ± 0.2	shotcrete	3.09
SURF, USA	220 ± 60	29 ± 15	13 ± 3	shotcrete	4.24

➤ THIS ASSUMES A 13.5 m TALL WATER TANK AND A STEEL PLATE BENEATH!

PRELIMINARY CAVERN RATE

- With 1.8m water shielding at top rate is vastly dominated by K40 from the top (194 out of 198 Hz!
- By increasing water shielding on top to be 2.5m, total rate is ~6 Hz

Chain/ Isotope	Polyhalite Activity (Bq/kg)	Rate of Gammas Entering OD (Hz)	
		Total	Total with extra shielding at top
U-238	0.356	0.193	0.015
Th-232	0.0114	0.026	0.002
K-40	2500	196	5.55



CRYOSTAT BACKGROUND

- Cryostat submerged in medium - could produce significant rate
- Use LZ Ti radioassay results to estimate cryostat rate
 - Calculate maximum possible rate by calculating decays/s, multiplying by number of gammas/betas in the chains and accounting for $\sim 50\%$ going outwards: ~ 30 Hz
- Simulation result agrees: 30 Hz at low threshold, dropping to 3 Hz at 100 keV, 2 Hz at 200 keV
- This does not taking into account many components! Welds, support structures, etc

Experiment	Type	Mass (kg)	^{238}U (mBq/kg)	^{232}Th (mBq/kg)	^{60}Co (mBq/kg)	^{40}K (mBq/kg)	^{46}Sc (mBq/kg)
DarkSide50 [29]	SS	175	<1	<1	13.1 ± 1	-	-
XENON100 [27]	SS	74	<1.8	<0.03	5.4 ± 0.5	<9	-
XENON1T [30]	SS	870	2.4 ± 0.7	0.21 ± 0.06	<0.36	9.7 ± 0.8	2.7
ZEPLIN-III [31]	Cu	400	<6.22	<2.03	-	<0.32	-
EXO-200 [32]	Cu	5,901	<0.01	<0.003	-	<0.01	-
GERDA [33]	Cu	16,000	0.017 ± 0.005	0.014 ± 0.005	0.018 ± 0.005	<0.049	-
	SS	25,000	<1.2	<1.2	19	<2.9	-
MJD [34]	Cu	1,297	<0.0003	<0.0003	-	-	-
LUX [11]	Ti	230	<0.25	<0.2	-	<1.2	2.5
LZ (this work)	Ti	1,827	$U_e < 1.6$ $U_l < 0.09$	$Th_e: 0.28 \pm 0.03$ $Th_l: 0.23 \pm 0.02$	<0.02	<0.54	2.0 ± 0.1

