

Minesweeper modeling in the n^+ layer of HPGeS



Feriozzi Rita XXXX cycle

Supervisor : Natalia di Marco

Co-supervisors: Valentina Biancacci, Riccardo Biondi

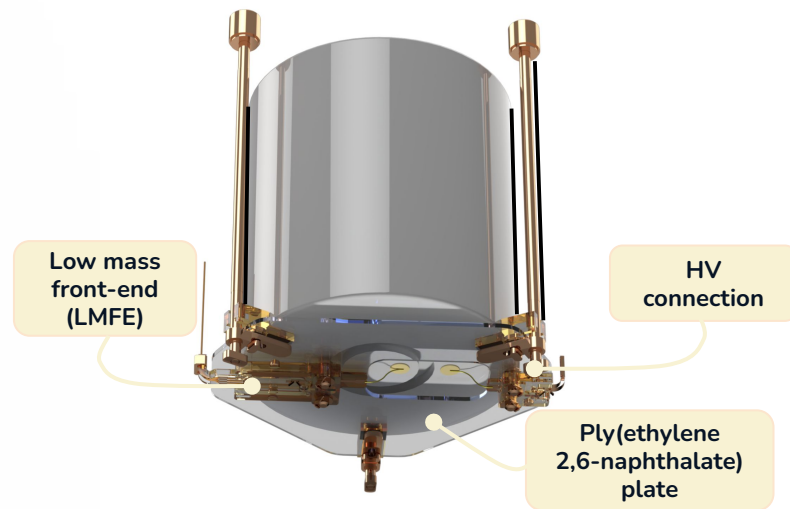
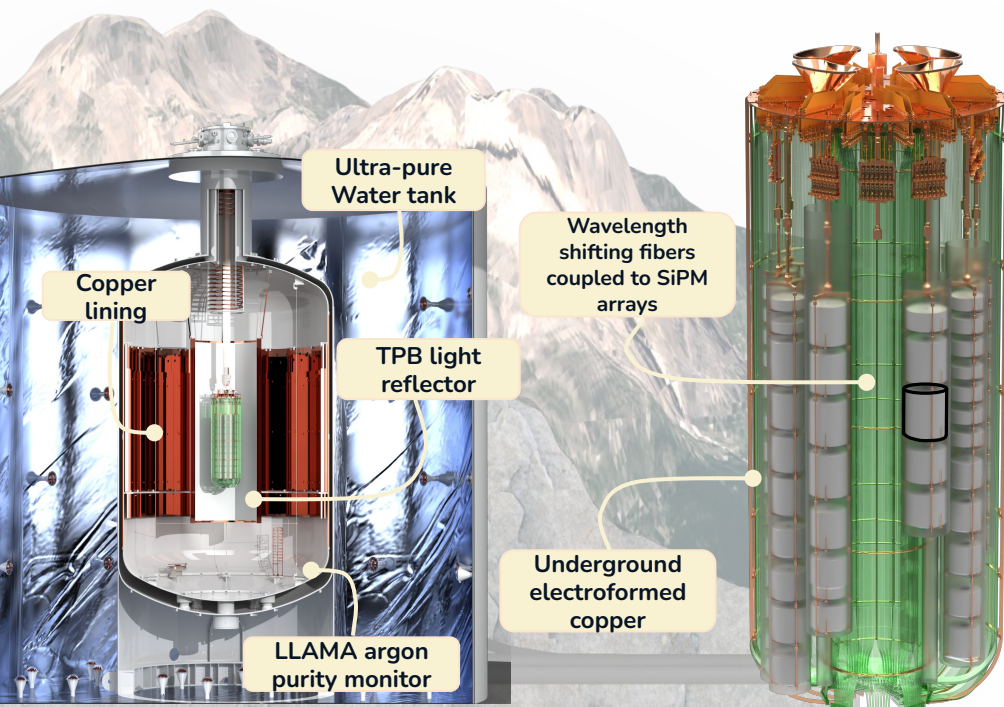
Passage of the year 2025/2026, 14th October 2026

LEGEND - 200

- 90 tons of liquid Ar, 200 kg of enriched Ge
- Data taking started in March 2023
- Background index goal of 2×10^{-4} cts/(keV kg yr)

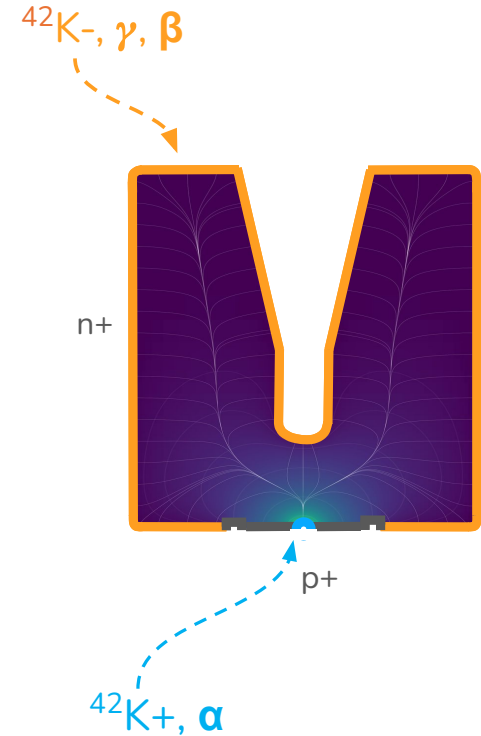
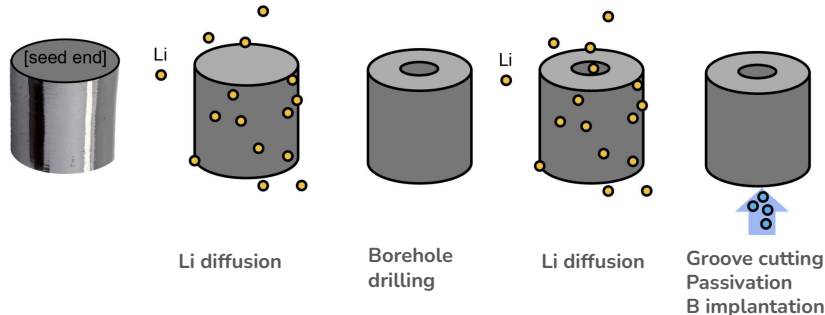
$$T_{(1/2)}^{0\nu\beta\beta} > 10^{27} \text{ yr @ 90\% CL}$$

(5 yrs)



High Purity Germanium detectors (HPGe)

- **p+ doping** → boron implantation
 - **Thin contact** O(0.1-1 μm)
 - **Excellent** segmentation capabilities
- **n+ doping** → lithium diffusion
 - **Thick contact** O(1 mm)
 - Robust, blocks **alphas**
 - **Cannot** be segmented reliably

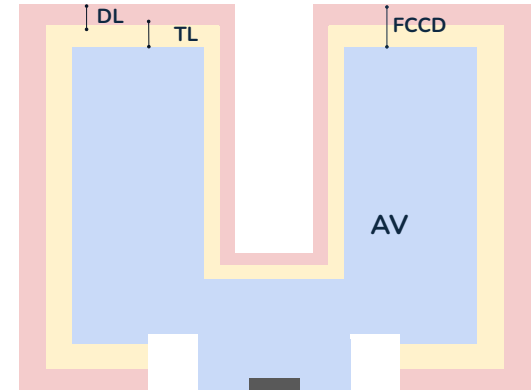
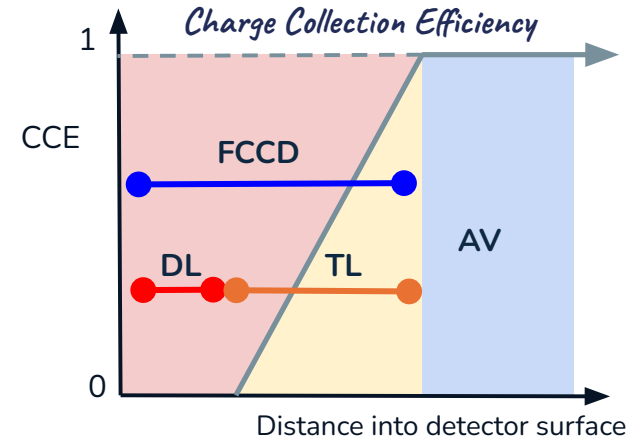


The Reduced Charge Collection Layer (RCC)

HPGe detectors have a dead layer:

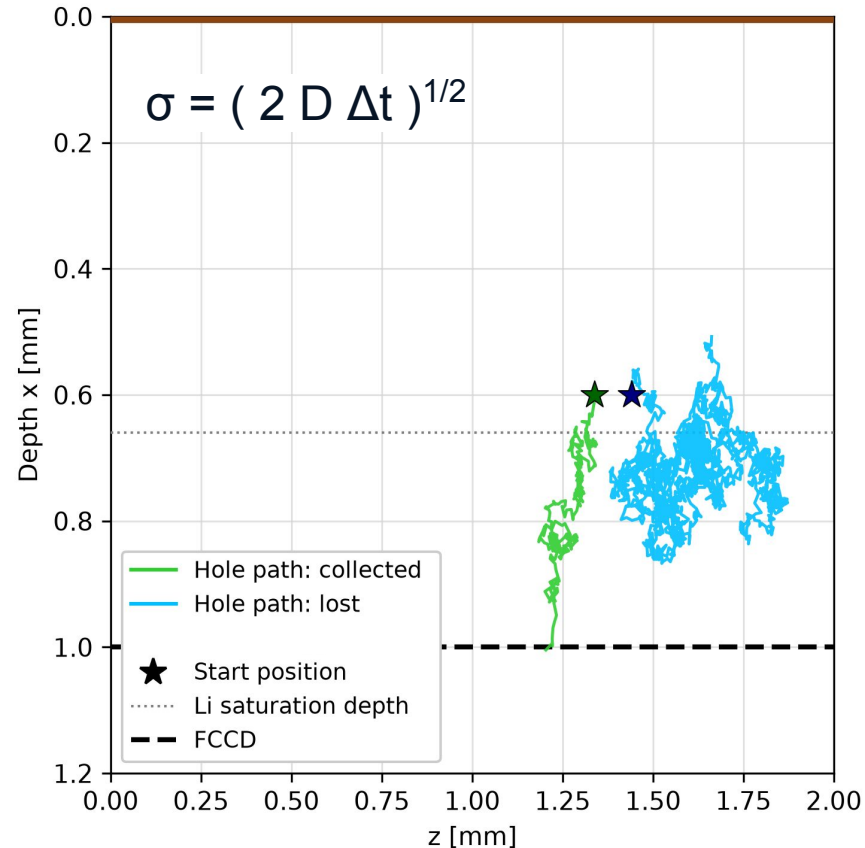
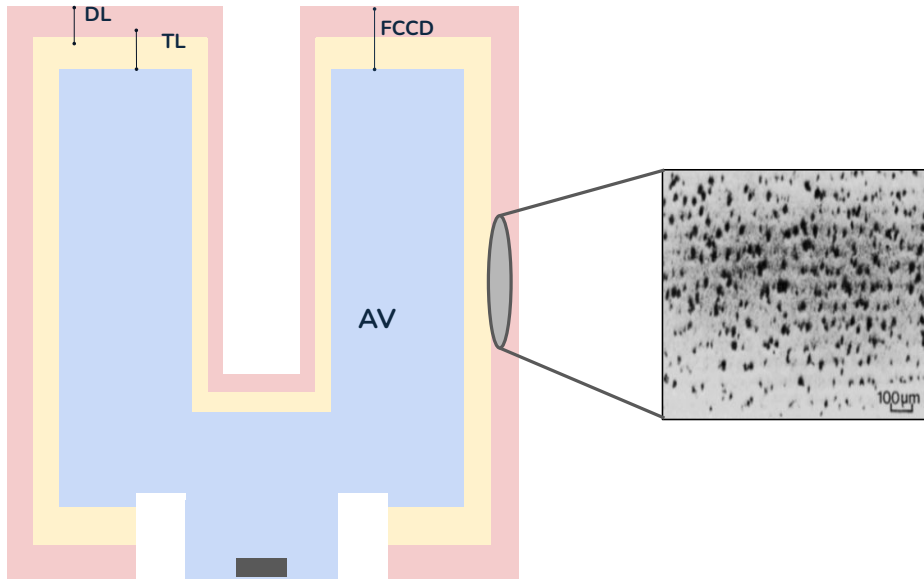
- **Dead Layer (DL)** = region of NO charge collection on the surface of semiconductor detectors. A conductive layer, created by Lithium diffusion
- **Transition Layer (TL)** = partial charge collection
- **Full Charge Collection Depth (FCCD)** = TL + DL

We estimate the FCCD empirically by comparing characterization data of detectors exposed to known radioactive sources with MC simulations



The dead layer : why do we lose carriers?

- Holes that diffuse on a Li precipitate → **LOST**
- Holes that reaches the FCCD → **COLLECTED**

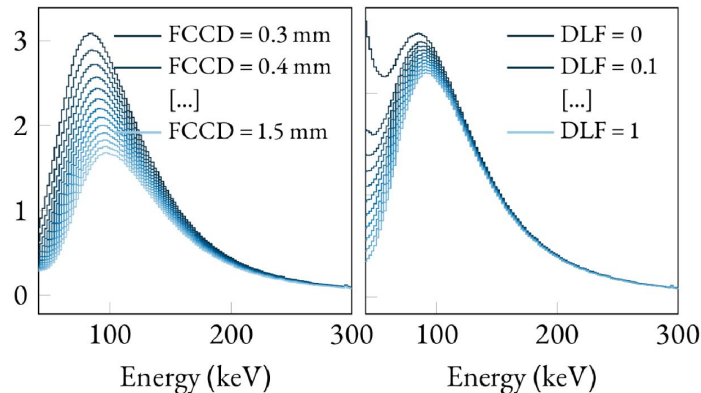


Why do we care?

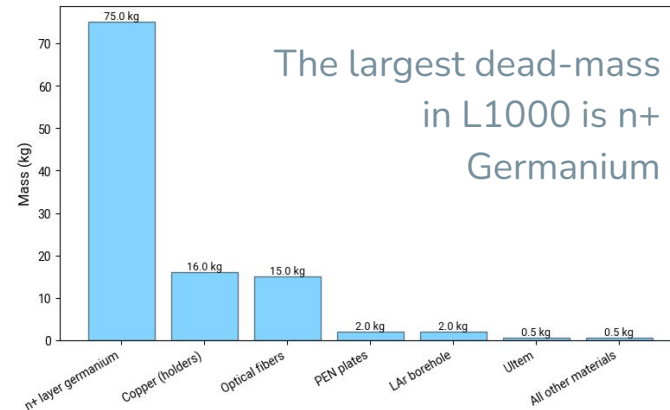
The correct active volume determination is important because:

- The $0\nu\beta\beta$ half-life is a function of active mass.
- Degraded events could mimic $0\nu\beta\beta$ signature.
- Major systematic uncertainty comes from AV fraction that impacts **detection efficiency of $2\nu\beta\beta$ (absence of FCCD growth model → 86% total uncertainty)**
- It is a crucial task for precision measurements in LEGEND

Credit to V. Biancacci



Credit to T. Dixon



Model lithium precipitation

1

Lithium precipitates
extraction and spatial
distribution

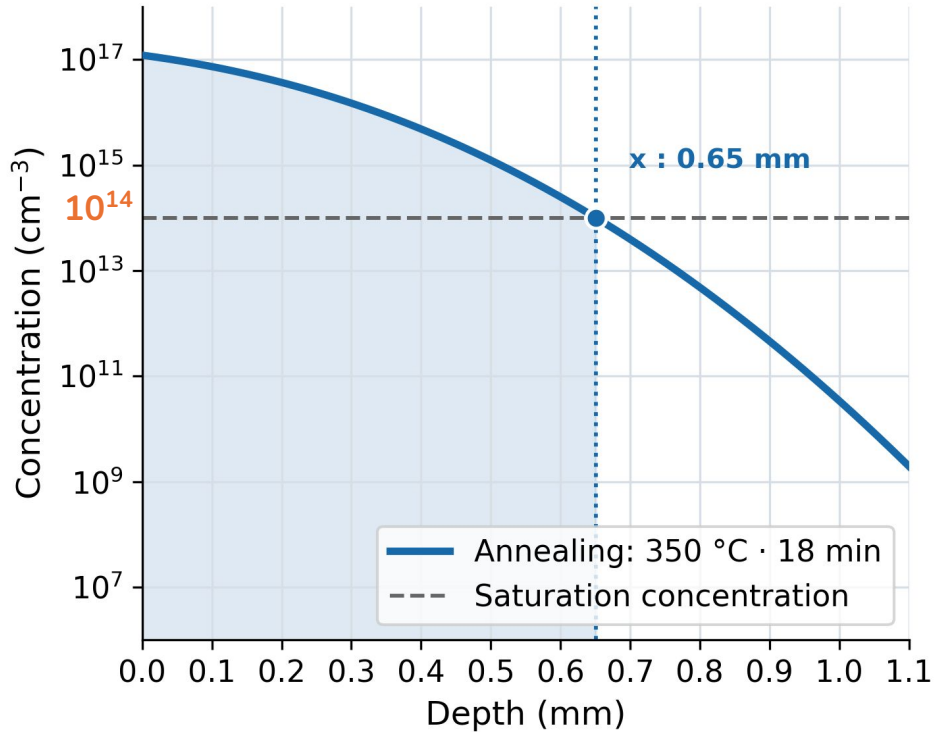
2

Radius distribution and
volume conservation

3

Fix lithium position

Model lithium precipitation (1)



diffusion equation

$$\frac{\delta C(x, t)}{\delta t} = D \cdot \frac{\delta^2 C(x, t)}{\delta x^2}$$

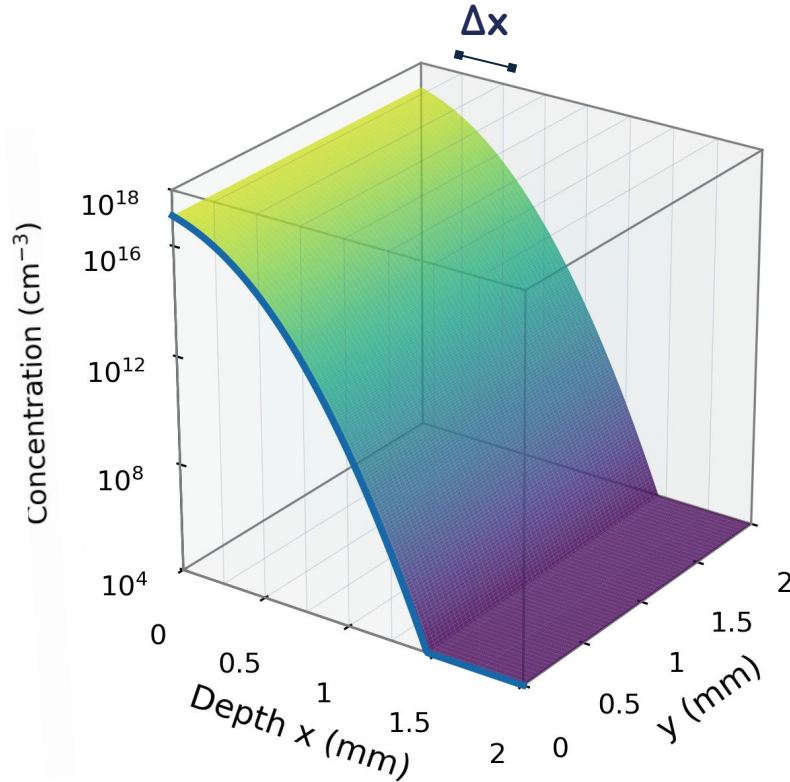
$C(0, t) = \text{const}$

Lithium concentration profile

$$C(x, t) = C_s \cdot \operatorname{erfc} \left(\frac{x}{2 \cdot \sqrt{D \cdot t}} \right)$$

Shape controlled by the **Temperature** and **time** of annealing

Model lithium precipitation (1)



CONCENTRATION OF RECOMBINATION SITES IN Δx

$$\lambda_i = \alpha * (C_d(x_i) - C_s) * \Delta x * L_y * L_z$$

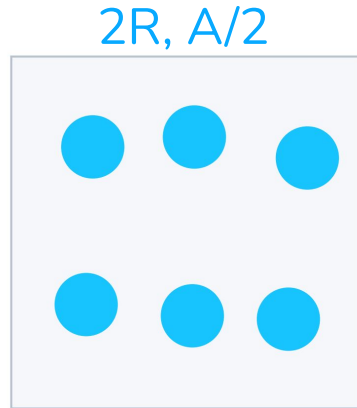
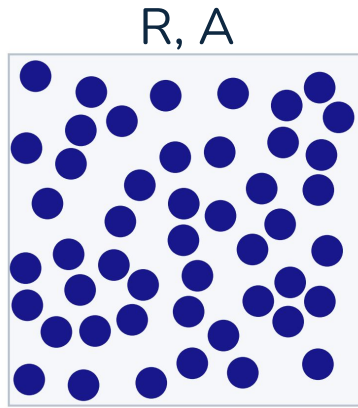
How much lithium is converted into a precipitate

HP : minimum size of Li to be considered a precipitate is **20 μm** ^[*]

$$N_{20}(x) = \text{Poissonian}(\lambda_i)$$

Radius distribution (2)

- Very high density region $\rightarrow$ precipitates can rearrange with bigger radius



Same lithium volume



Different covered area

- The covered area is the key parameter affecting the **CCE**.
- Charge-carrier loss depends on the **lithium cross-sectional area**.

Radius distribution (2)

1. Conserve Lithium volume

Larger spheres $\rightarrow$ fewer spheres

$$N_R(x) = N_{20}(x) (r_0 / R)^3$$

2. Keep at least 6 spheres per slice

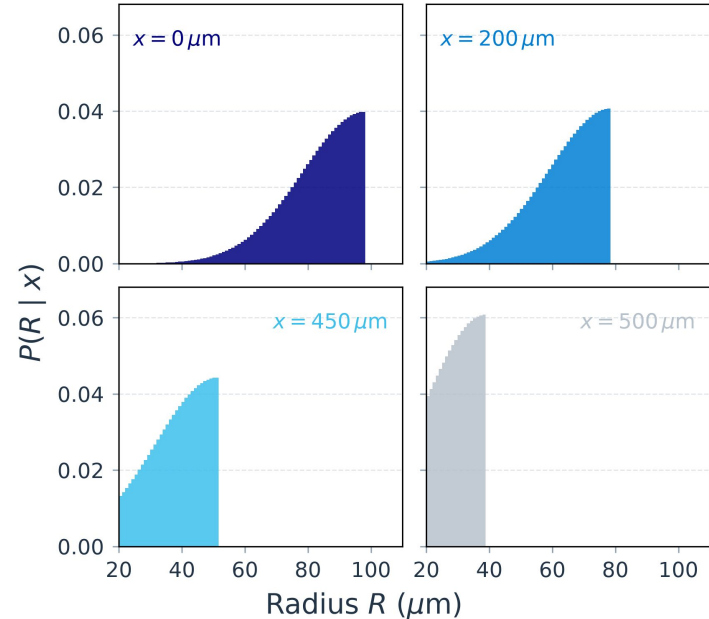
Avoiding concentrating lithium into too few large precipitates.

$$R_{\max}(x) = r_0 (N_{20}(x) / 6)^{1/3}$$

3. Apply gaussian preference

$$\omega(R|x) = \exp \left(- \frac{1}{2} (R - R_{\max}(x))^2 / \sigma^2 \right)$$

$$P(R_i|x) = \omega(R_i|x) / \sum_k \omega(R_k|x)$$



The remaining volume is represented by precipitates of radius r_0 , randomly positioned in the slice.

Radius distribution (2)

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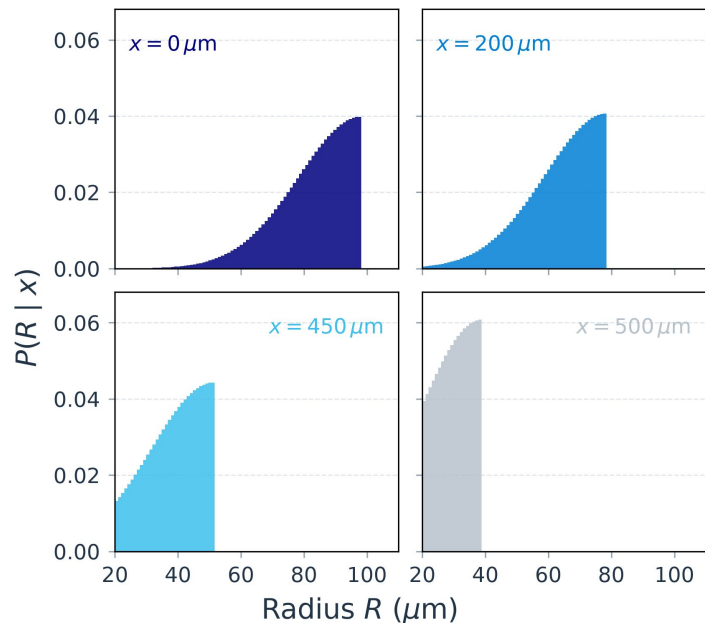
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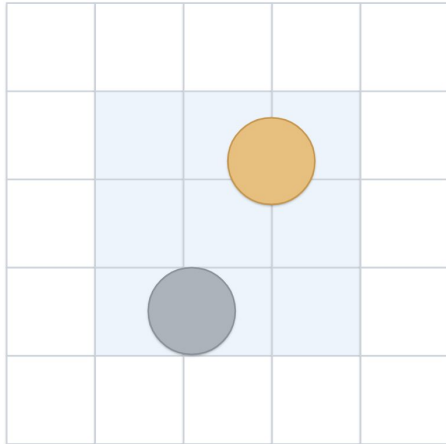
The parameters have been tuned to not have any systematic in the CCE simulation

Fix the lithium (3)

1. Divide the volume into cubic cells of side 240 μm
2. Sample a position; check its cells and the 26 neighbouring cells.
3. No overlap : ACCEPT. Overlap : sample a new position

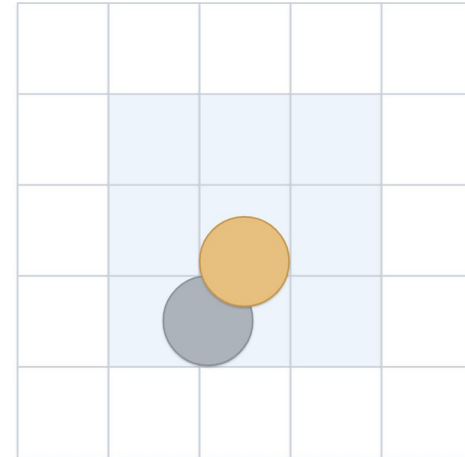
$$\text{Overlap if : } (x_{i+1} - x_i)^2 + (y_{i+1} - y_i)^2 + (z_{i+1} - z_i)^2 < (R_{i+1} + R_i)^2$$

NO OVERLAP $\rightarrow$ ACCEPT



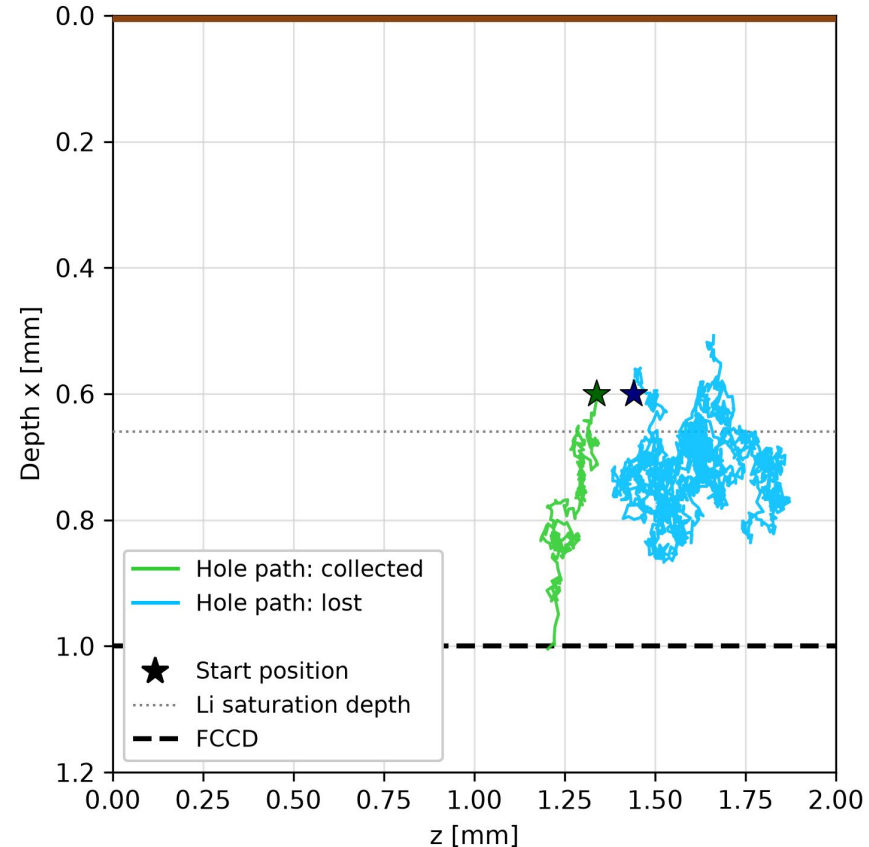
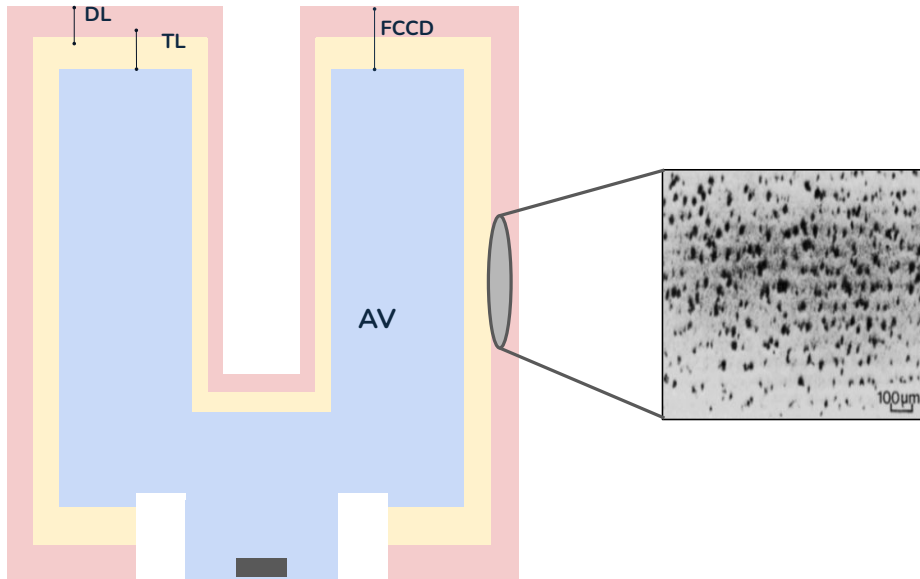
- Candidate
- Prev. placed

OVERLAP $\rightarrow$ RESAMPLE



The dead layer

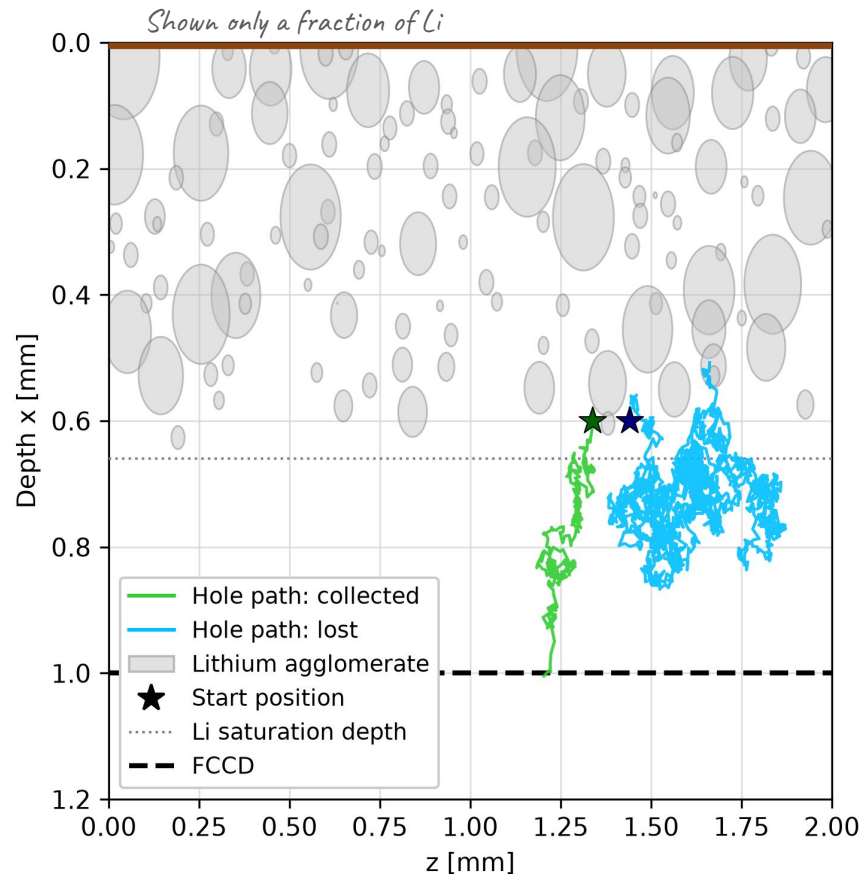
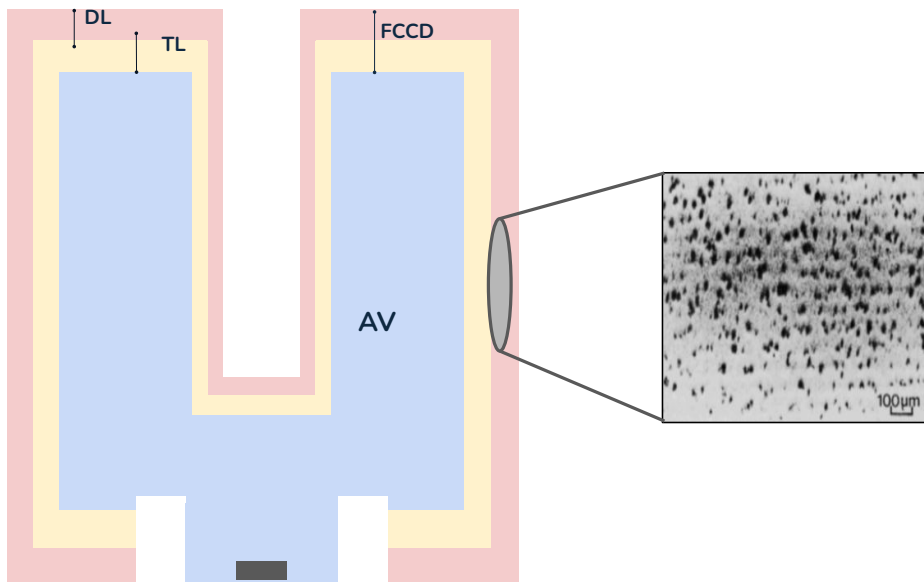
- Holes that diffuse on a Li precipitate → **LOST**
- Holes that reaches the FCCD → **COLLECTED**



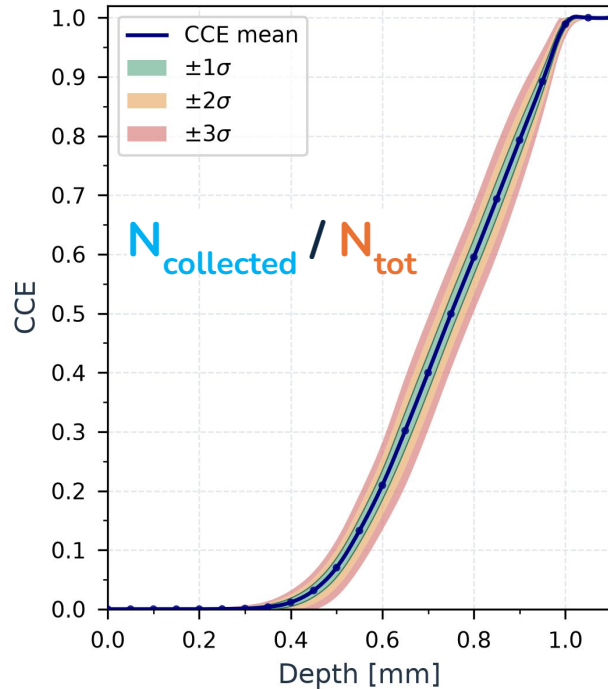
The dead layer



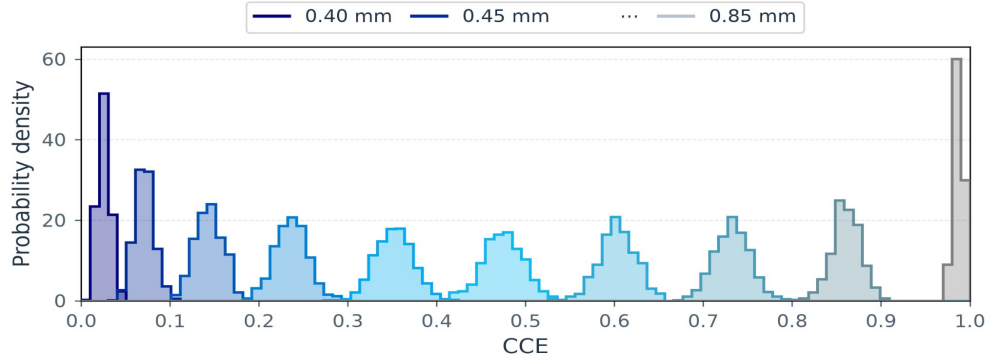
- Holes that diffuse on a Li precipitate → **LOST**
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CCE curves



- Simulate **independently** N_{tot} holes located at (x_0, y_0, z_0)
- **Random** walk (no E field)
- Count the holes that reaches FCCD (E field) $\rightarrow N_{\text{collected}}$

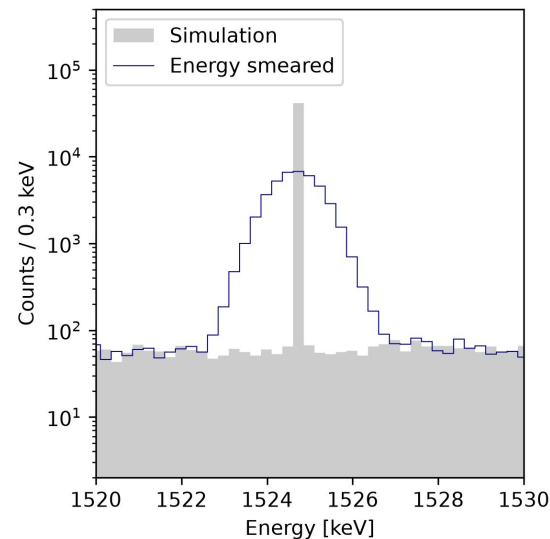
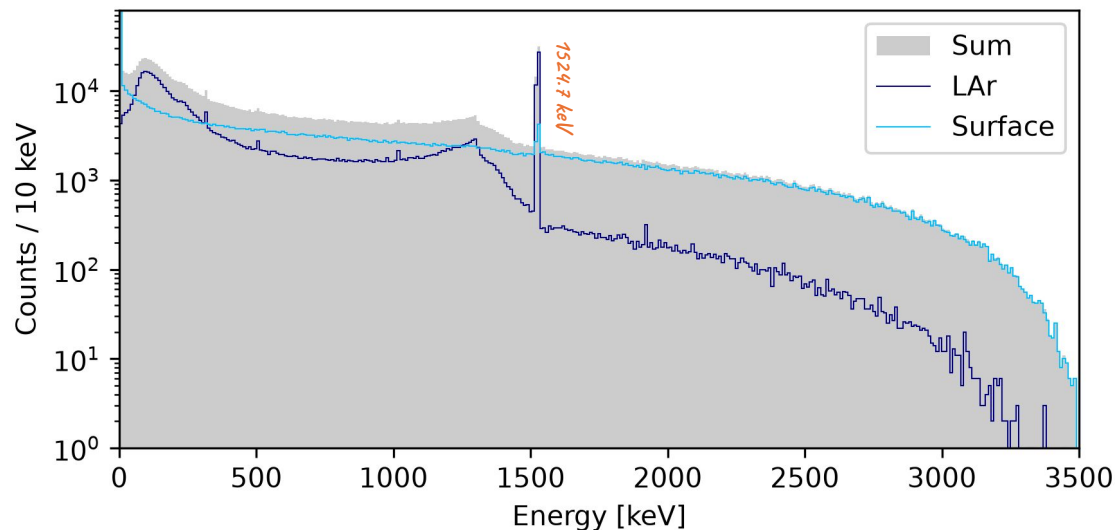
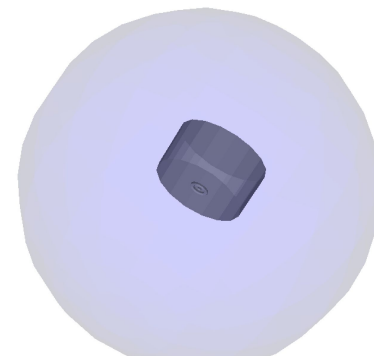
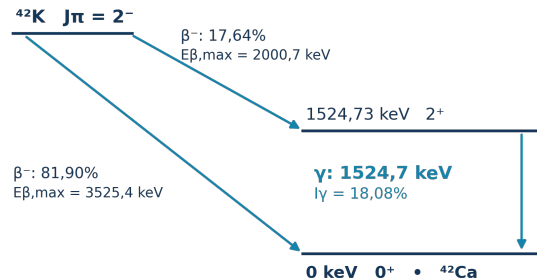


Probabilistic nature of the collection (and loss) of the carriers.

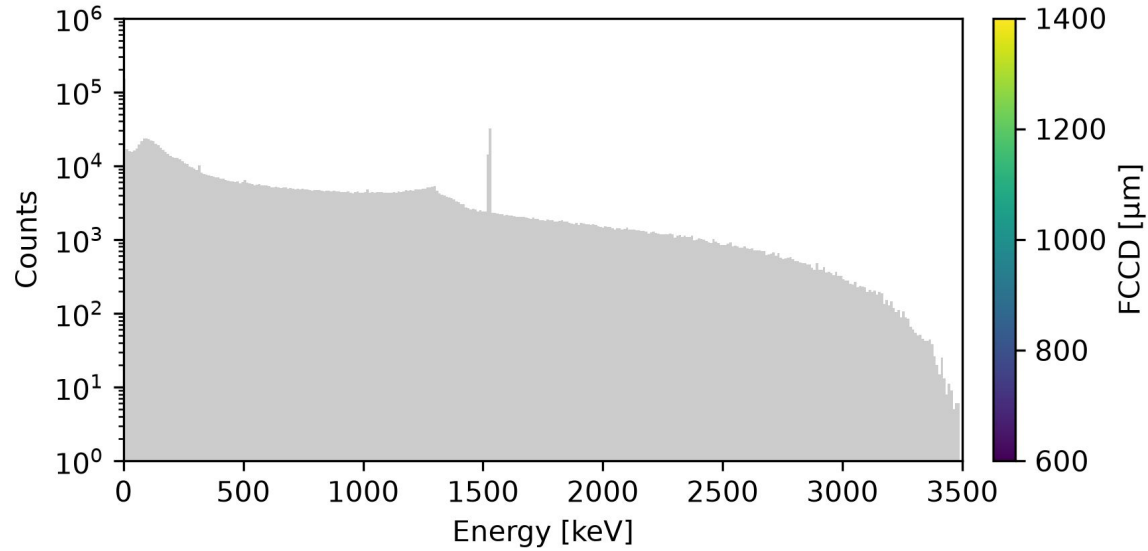
CCE effect on the spectrum

- Bege in a LAr spherical volume
- ^{42}K can decay:
 - In the LAr
 - On n^+ surface ($^{42}\text{K}_+$)

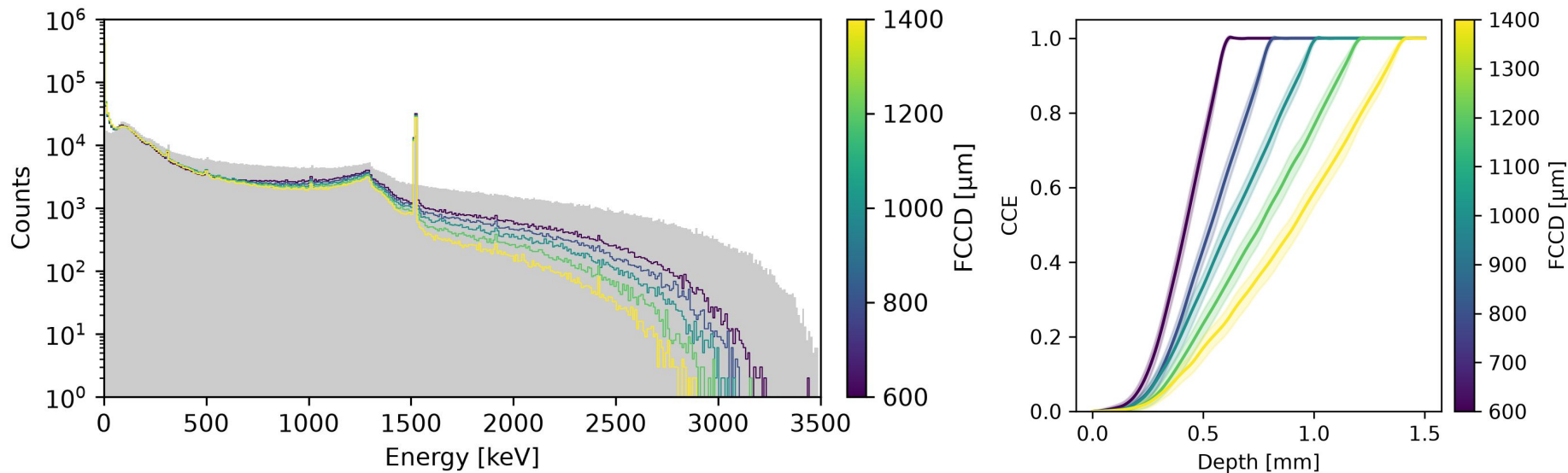
$T_{1/2} = 12,360(3) \text{ h}$ | $Q\beta = 3525,4 \text{ keV}$



CCE effect on the spectrum



CCE effect on the spectrum



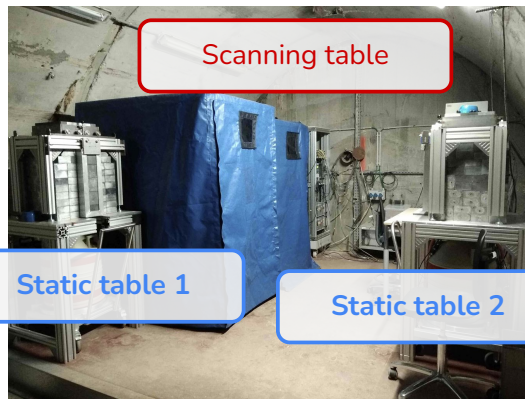
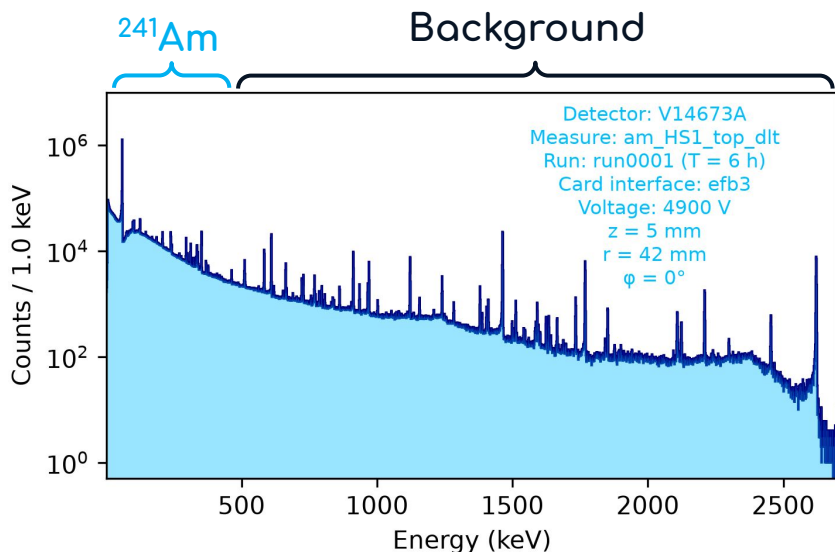
Known the energy deposition coordinates

$$E(x) = E_0(x) \cdot CCE(x)$$

$$\text{with } CCE(x) = \mu(x) \pm \mathcal{G}(\mu, \sigma)$$

Not only modelling : HADES data comparison

- HADES is an underground laboratory managed by the Belgian research program EURIDICE
- $\phi_\mu \sim 0.1 \text{ m}^{-2}\text{s}^{-1}$



^{60}Co : depletion voltage

^{228}Th : calibrating PSD and validate simulations

^{241}Am : FCCD measurements

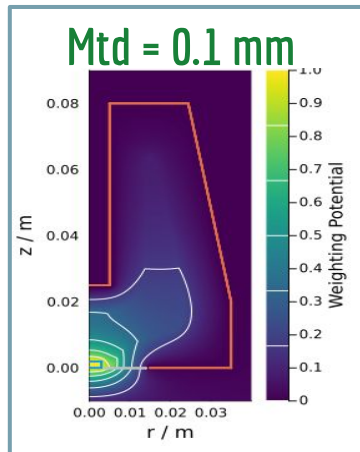
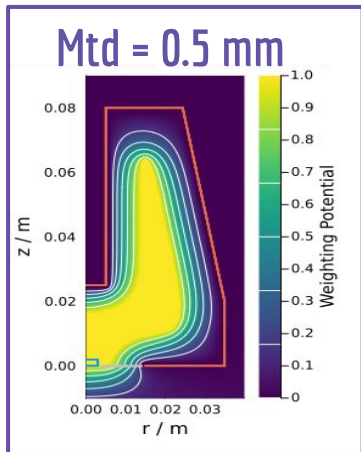
^{133}Ba : FCCD measurements

Background run

Weighting Potential convergence

The weighting potential (WP) is highly sensitive to **grid resolution** near the p^+ electrode, where **steep gradients occur**.

Mtd = grid resolution

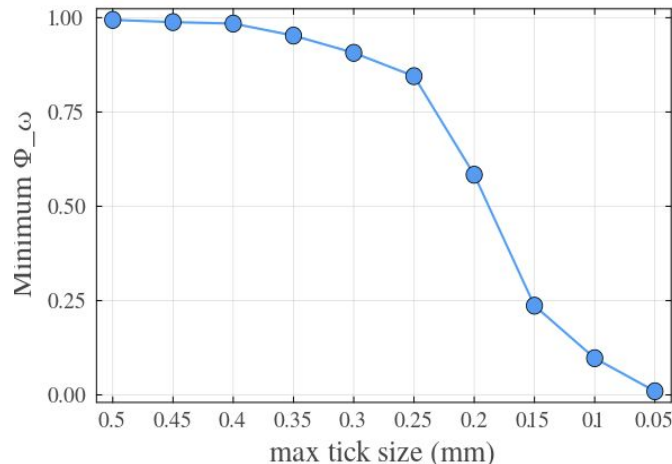
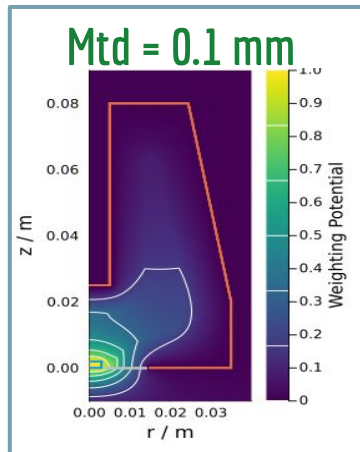
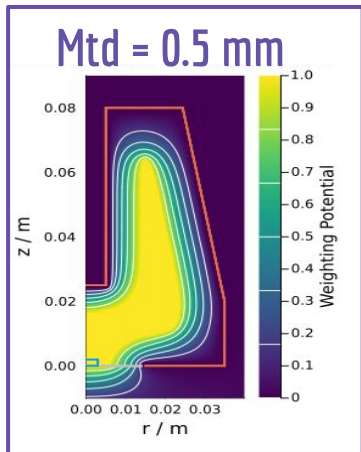


Controlling the WP at very small scales is fundamental to understanding how the signal is formed in the n^+ layer $O(1 \text{ mm})$
Need to use way smaller grid resolutions

Weighting Potential convergence

The weighting potential (WP) is highly sensitive to **grid resolution** near the p^+ electrode, where **steep gradients occur**.

Mtd = grid resolution

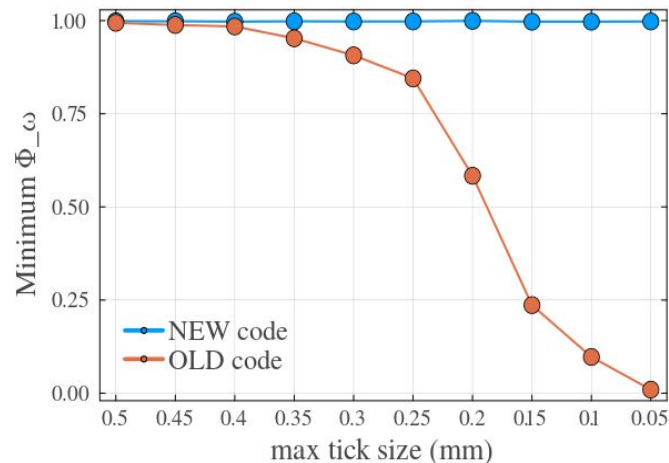
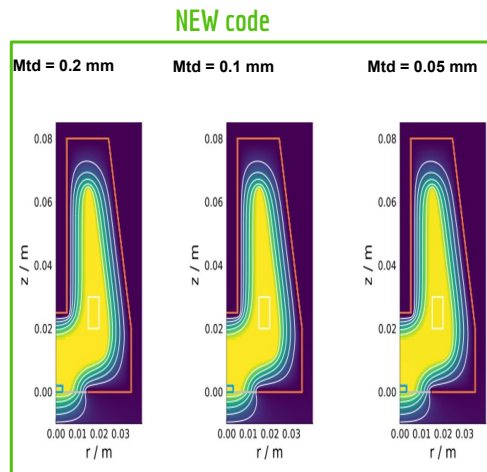
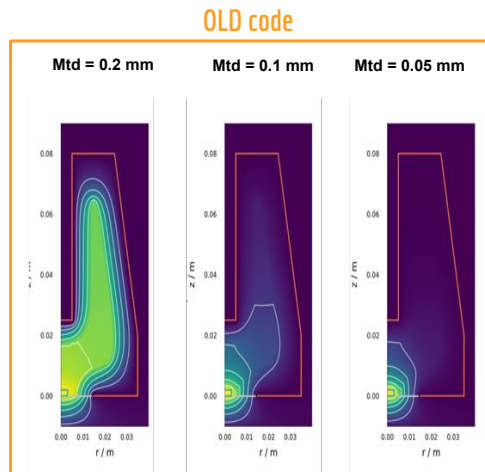


Check the **minimum** of the WP

Direct contact with the p^+ electrode $\rightarrow$ behaving like a **conductive material** (undepleted $\rightarrow$ no charge density), the weighting potential must be equal to 1.

Weighting Potential convergence

SOLVED : instead of applying the initial state directly to a fine grid, the simulation is **initialised on a coarse grid** and an **initial** convergence is computed.



When the initial grid is **too dense**, the algorithm gets stuck around an **incorrect solution**, and continues to **oscillate** around it until the iteration stops when maximum of the residual of the **weighting potential** is smaller than a **certain convergence limit** (default 10^{-7}).

Quality cuts @ $E < 500$ keV

The study of the performance of quality cuts below 500 keV plays a key role in all analyses operating in the **low-energy region**.

This includes:

- **Trinucleon analyses**
- **Bosonic Dark matter** searches
- Studies of the **^{39}Ar spectrum**
- ...

Therefore, this work enables low-energy analyses using cuts that:

- already perform **well** and are **validated**

OR

- can be **further optimized**



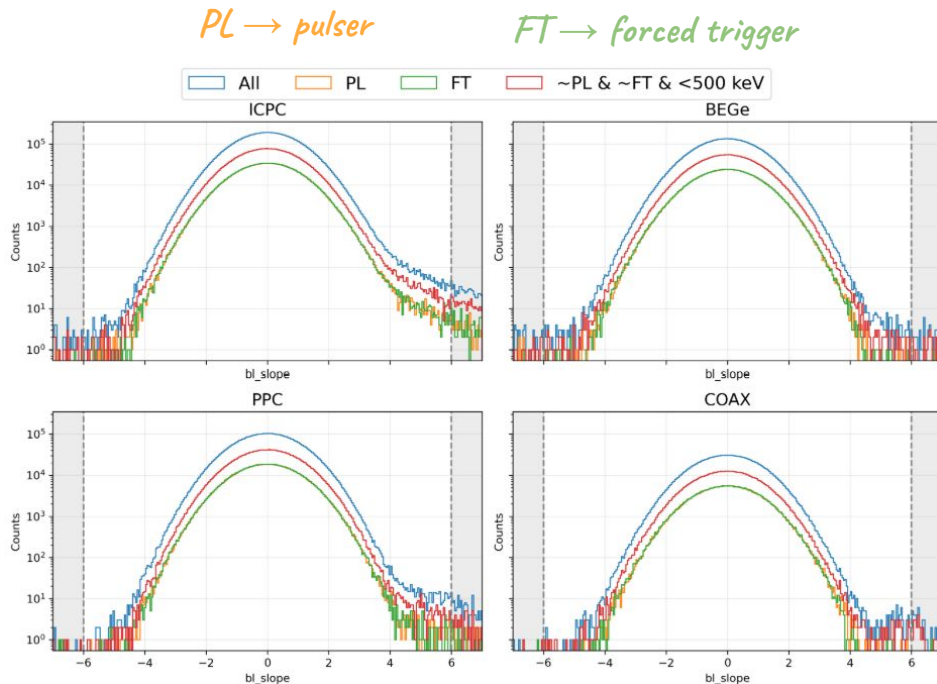
Quality cuts @ $E < 500$ keV

[*] Operational energy threshold

is
positive
polarity
candidate

1. is_valid_slope
2. is_valid_slope_rms
3. is_valid_tail_rms
4. is_not_noise_burst
5. is_valid_cuspEmin
6. is_valid_trap_tpmx
7. is_low_cuspEmax
8. is_valid_cuspEmax

$$\zeta = (x - \mu) / \sigma$$



The **is_positive_polarity_candidate** performs well
also in the energy range (40, 500) keV [*]

Conclusions

- **Motivation:**

Understanding charge collection in the lithium-diffused surface region is essential to improve the modelling of surface backgrounds in LEGEND-200;

- **What we have done so far:**

- **CCE modelling — ongoing:** Developing a model of charge collection efficiency based on the probabilistic description of charge diffusion and loss through recombination.
- **Weighting potential convergence — completed:** Verified that the weighting potential simulation converges at small spatial scales, providing a necessary basis for signal modelling.
- **Quality cuts below 500 keV — completed:** Verified consistent quality-cut behaviour at low energies, supporting analyses in this energy range.

- **Next steps**

Validate the CCE model against HADES measurements with a collimated ^{241}Am source, then extend its application to LEGEND-200 detectors.

Talks, Schools & Publications

Talks

- **IFAE 2026**
“Primi risultati di LEGEND : alla ricerca del doppio decadimento beta senza neutrini”
- **COSMO 2026**
“ Latest results from the LEGEND experiment on the search for Neutrinoless Double Beta Decay ”

Conferences, Collaboration meetings and schools

- **LEGEND collaboration meetings**,
Winter - LNGS | spring - Naples
- **IFAE 2026**, Bologna
- **COSMO 2026**, Leiden
- **ISAAP school 2026**, Munich

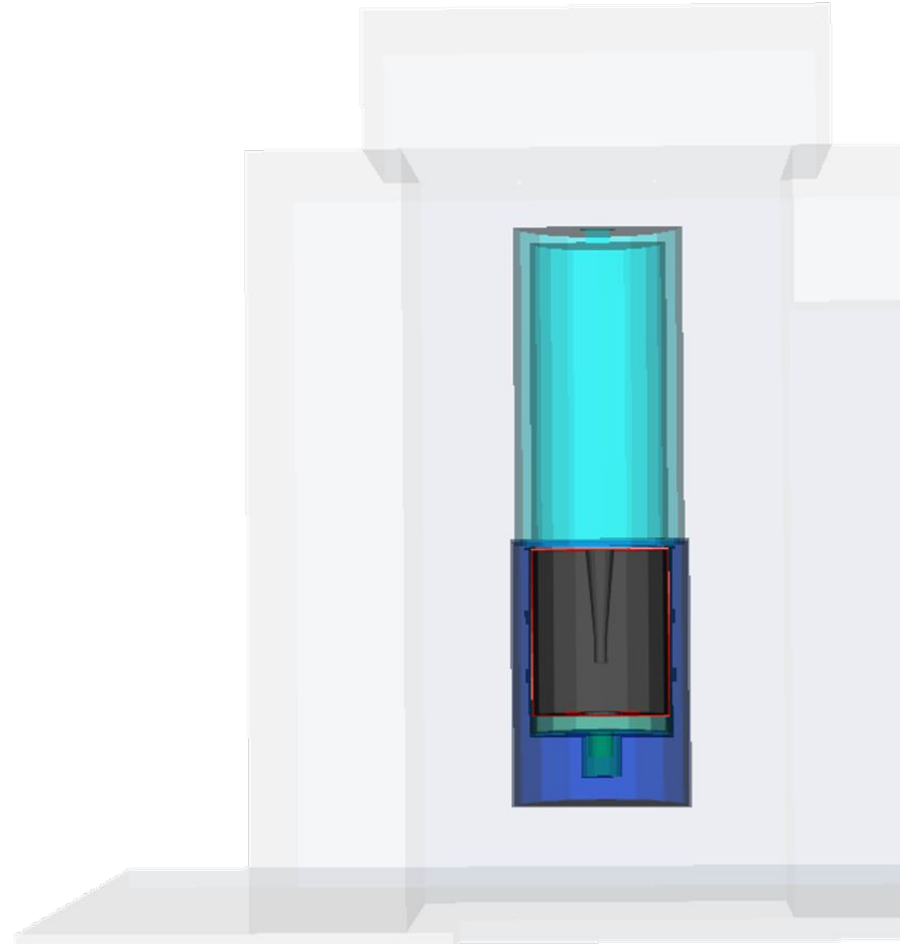
Poster

- **Refining the RCC layer model for SolidStateDetectors.jl new release (v0.11.0) - LEGEND spring collaboration meeting, naples**

Publications

- **Energy Calibration and Performance of HPGe Detectors in the LEGEND-200 Experiment**
arXiv:2605.22479 (2026)
- **New limits on $^{94,96}\text{Zr}$ double beta decay to excited states of $^{94,96}\text{Mo}$**
in preparation
- **Proceeding IF AE**
submitted

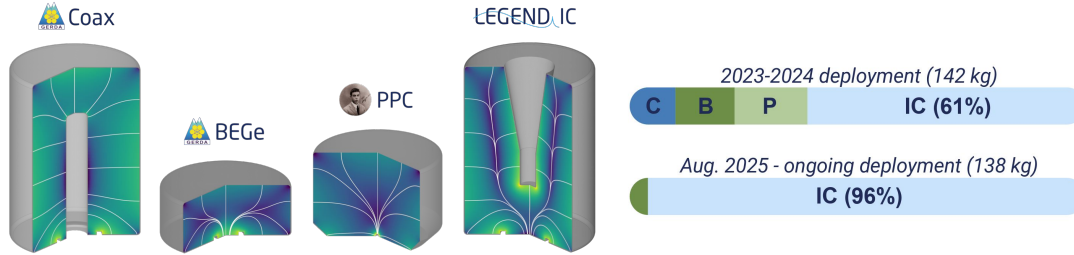
Backup



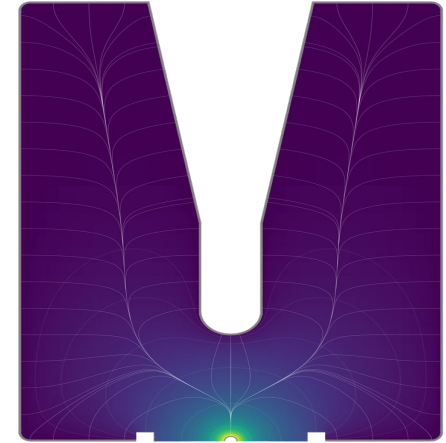
List of content

- 1 LEGEND-200
- 2 High Purity Germanium detectors
- 3 Full Charge Collection Depth
- 4 CCE modelling
- 5 Weighting potential numerical convergence
- 6 Low energy Quality Cuts
- A Side project : New limit on $^{94,96}\text{Zr } 0\nu\beta\beta$ decay

High Purity Germanium detectors (HPGe)



- High detection efficiency (the detector itself is the $\beta\beta$ source)
- Enrichment of the $\beta\beta$ -decaying isotope from 7.7% up to 92%
- Excellent energy resolution at $Q\beta\beta$ (0.12% FWHM)
- Intrinsic radiopurity (the best background/FWHM performance in the field)



Role of the Spatial Grid in Trapping Simulation

- Grid → candidate selection
- Distance → trapping decision

A Li precipitate is **not confined to a cell**

A charge is **not centered in a cell**

} The cell is only a **spatial index**

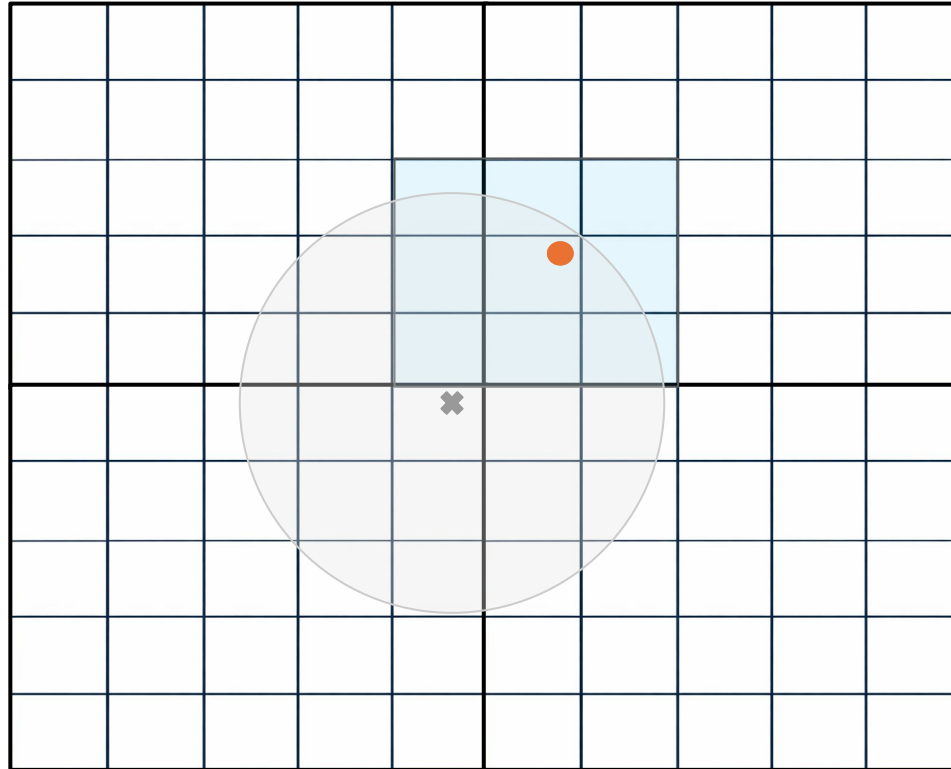
If grid scale $\neq$ physical scale (r_{Li})

→ bias in trapping probability

→ distortion of CCE

Role of the Spatial Grid in Trapping Simulation

Cell size $\ll d_{\text{Li}}$



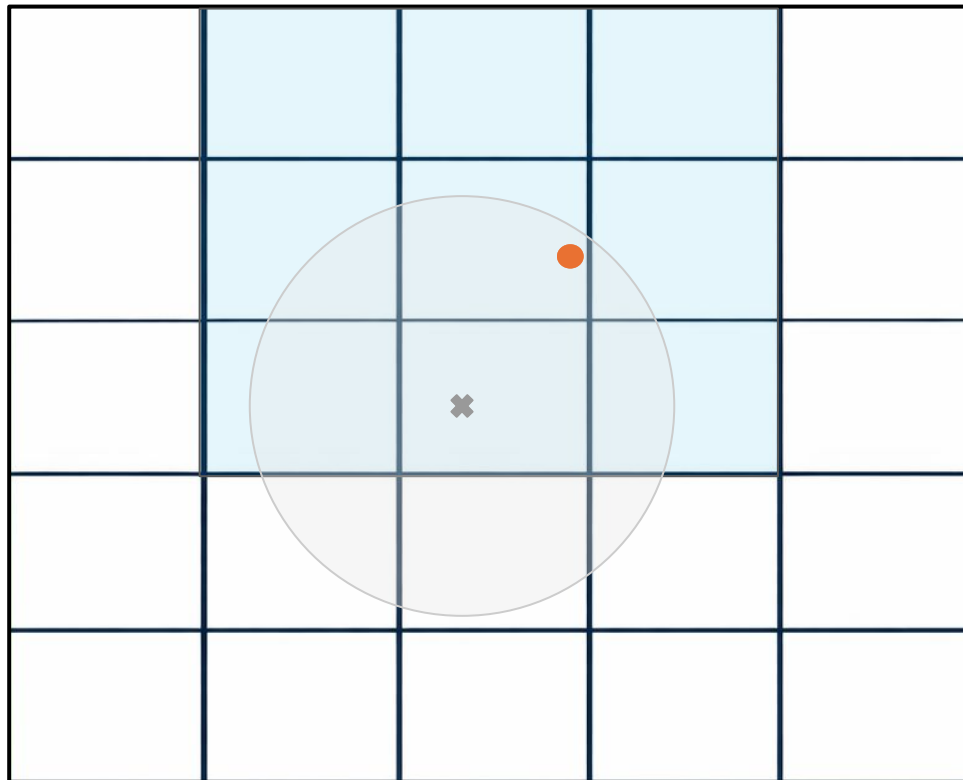
● charge

✕ Li center

In principle the charge is lost!
But the Li is not seen because
the Li center is outside the 26
cells

Role of the Spatial Grid in Trapping Simulation

Cell size == d_{Li}

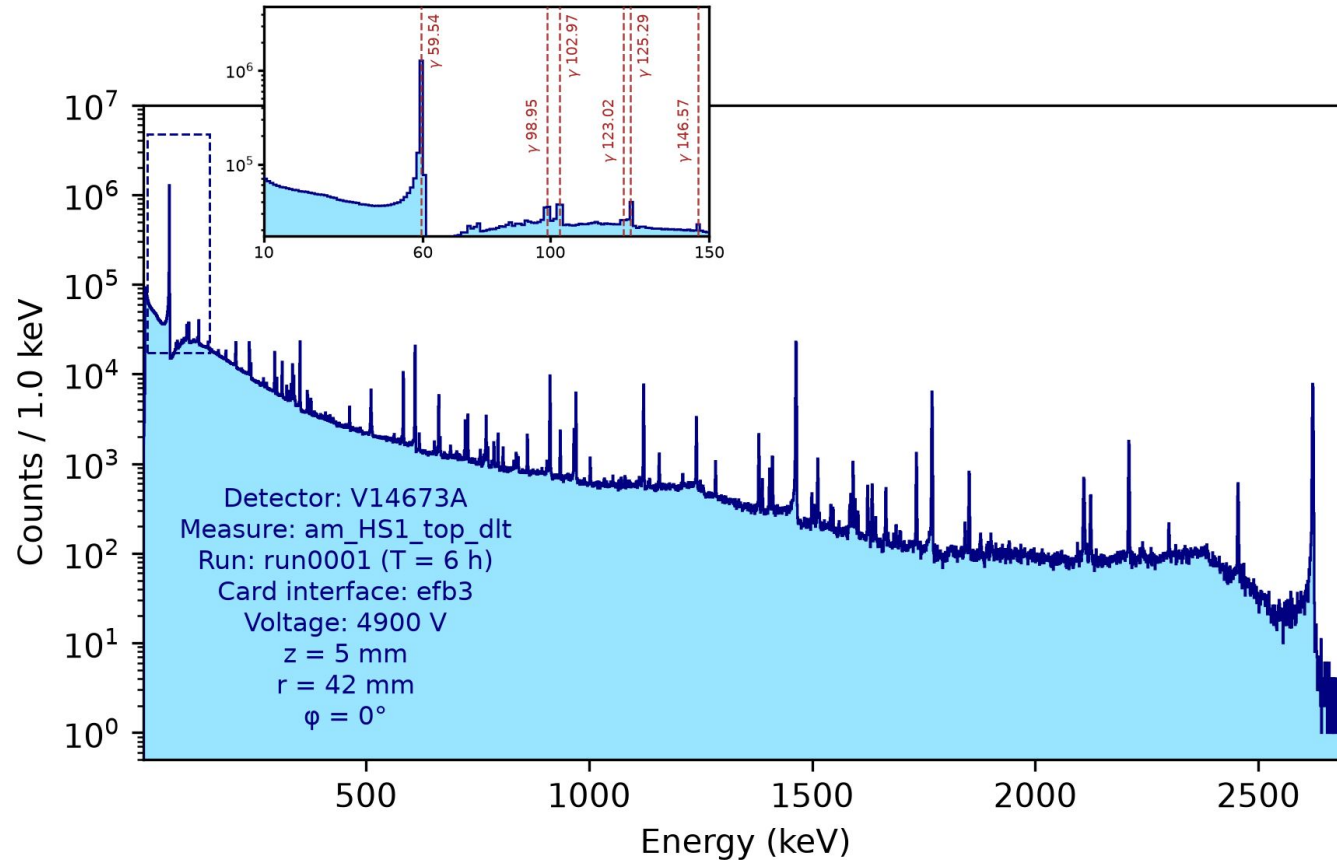


- charge
- × Li center

CCE simulation parameters

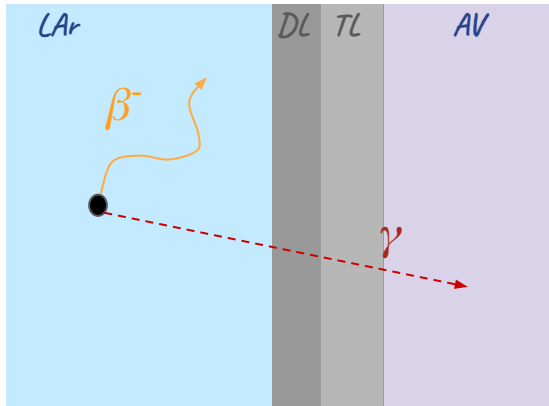
Parameter	Description	Value
FCCD [μm]	Depth where CCE = 1	1 mm
α	How much lithium becomes a precipitates	10^{-11}
N_{sat} [cm^{-3}]	Concentration of saturation of lithium in germanium	10^{14}
T_{ann} [K]	Temperature of annealing (diffusion)	475
t_{ann} [h]	Time of annealing (diffusion)	4
σ [μm]	Standard deviation of radii distribution	20
N_{tot}	Total holes generated	250
N_{sim}	Number of simulation performed	250

Americium low energy gamma lines

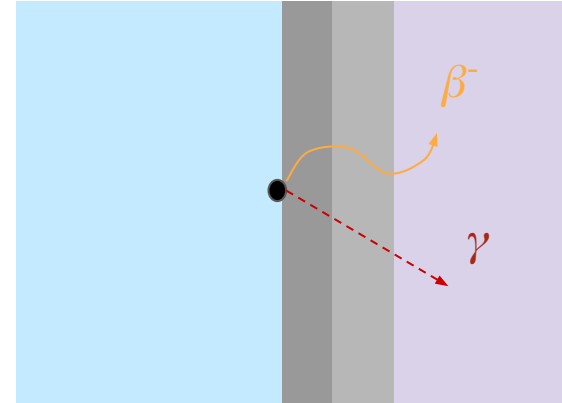


^{42}K events

LAr decay

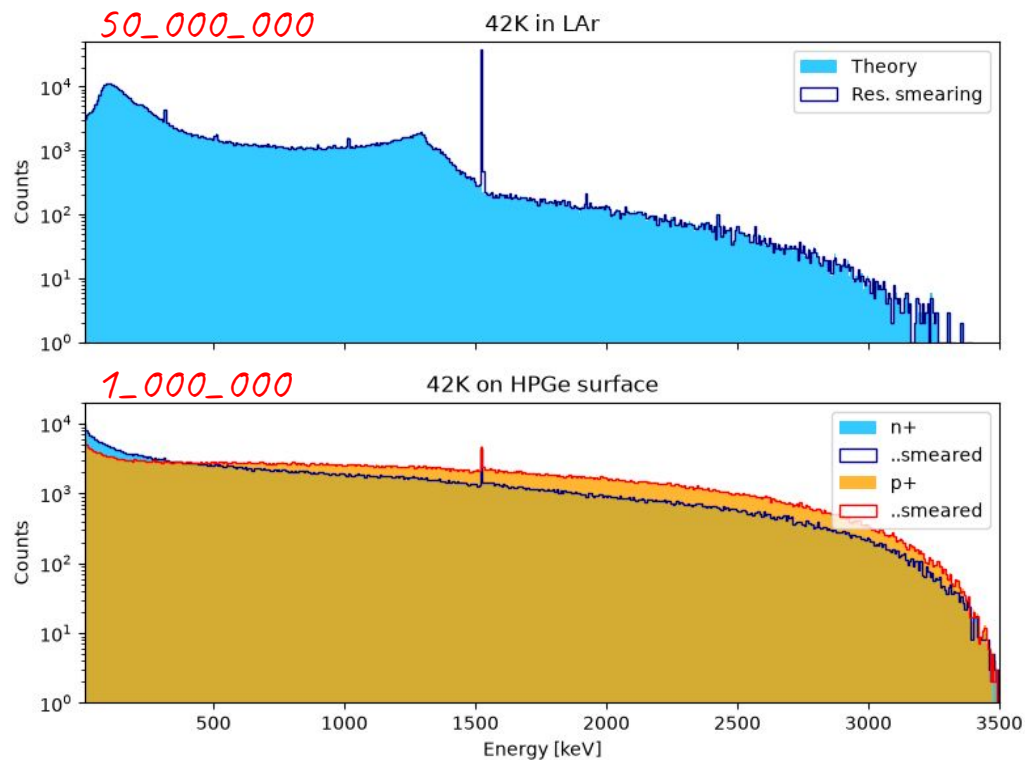


n+ decay



^{42}K events

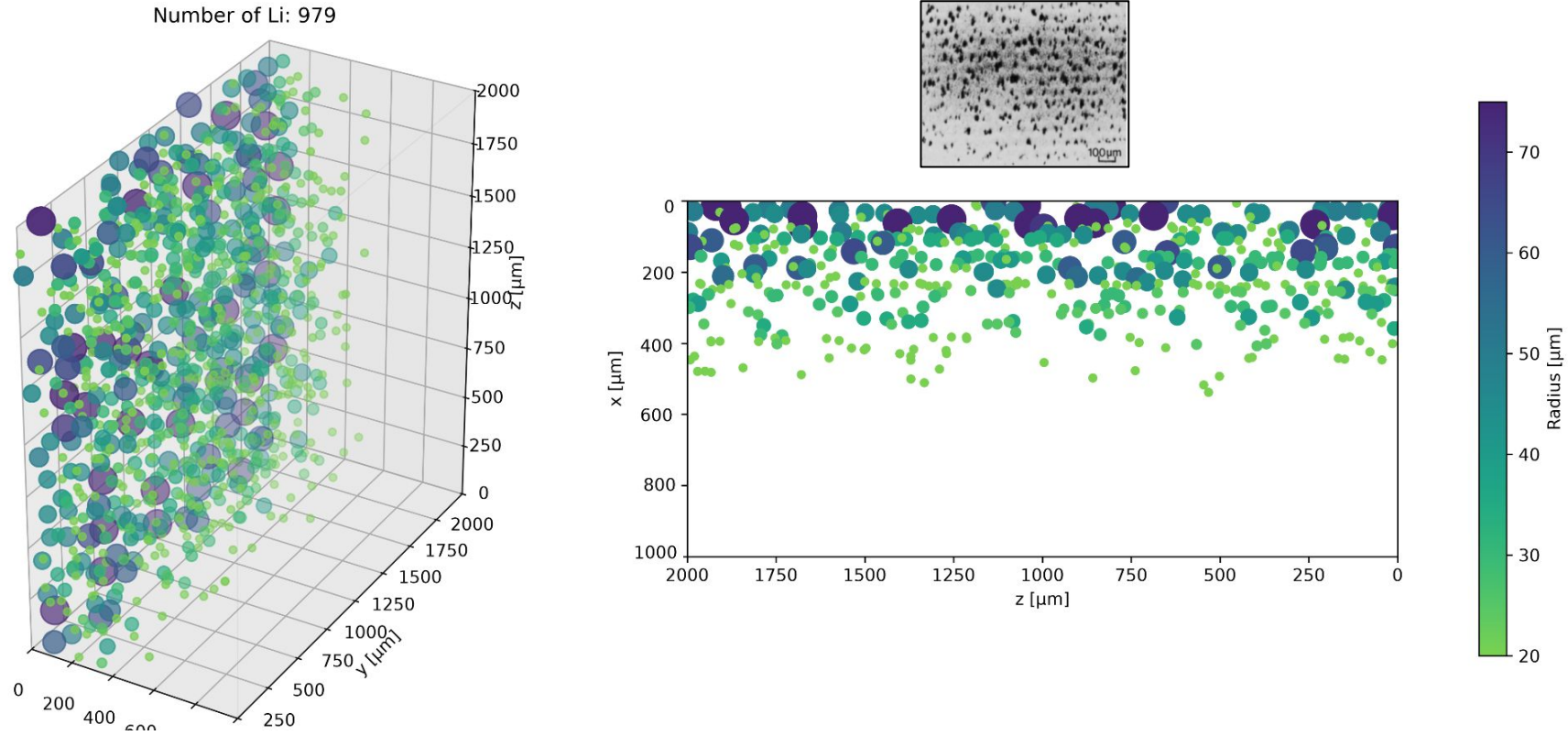
- Allowing ^{42}K to decay in the LAr + ^{42}K on HPGe surface



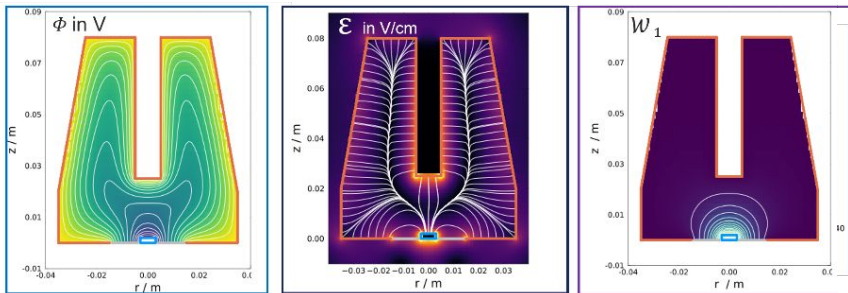
Requiring ^{42}K decay on the surface of HPGe generates:

- $^{42}\text{K}^-$: read by p+
- $^{42}\text{K}^+$: read by n+

The dead layer



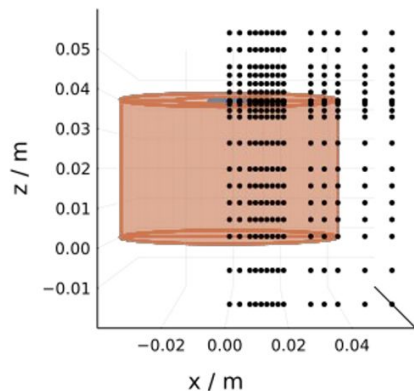
Weighting Potential convergence



Starting from the **4th Maxwell law** in the integral from

$$\iiint \nabla \cdot (\epsilon_r(r) \cdot \nabla \Phi(r)) dV = \iiint \rho(r) / \epsilon_0 dV$$

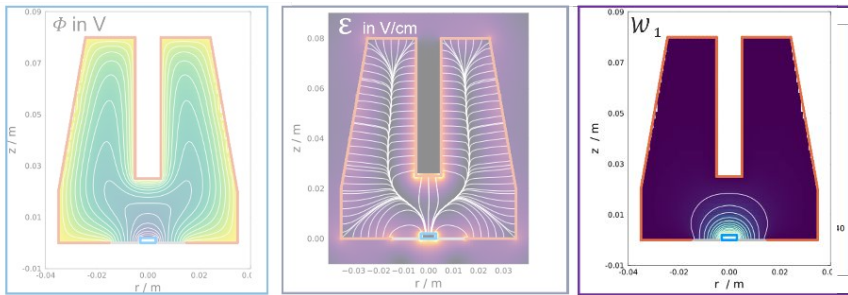
Geometry divided in $\mathbf{N} = \mathbf{N}_r \times \mathbf{N}_\phi \times \mathbf{N}_z$ grid points, obtaining a system of N linear equations. Solved numerically with **Successive Over-Relaxation (SOR)** algorithm.



$$\underbrace{\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{N_p} \end{bmatrix}}_{\vec{\phi} \in \mathbb{R}^{N_p}} = \underbrace{\begin{bmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,N_p} \\ a_{2,1} & a_{2,2} & \dots & a_{2,N_p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{N_p,1} & a_{N_p,2} & \dots & a_{N_p,N_p} \end{bmatrix}}_{A \in \mathbb{R}^{N_p \times N_p}} \cdot \underbrace{\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{N_p} \end{bmatrix}}_{\vec{\phi} \in \mathbb{R}^{N_p}} + \underbrace{\begin{bmatrix} a_1^0 Q_1^{\text{eff}} \\ a_2^0 Q_2^{\text{eff}} \\ \vdots \\ a_{N_p}^0 Q_{N_p}^{\text{eff}} \end{bmatrix}}_{\vec{b} \in \mathbb{R}^{N_p}}$$

$$\Phi^{(k+1)} = A \times \Phi^k + Q$$

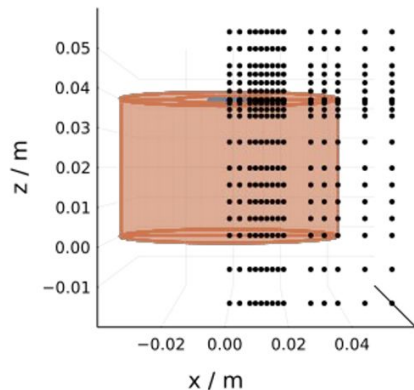
Weighting Potential convergence



Starting from the **4th Maxwell law** in the integral form

$$\iiint \nabla \cdot (\epsilon_r(r) \cdot \nabla \Phi(r)) \, dV = \mathbf{0}$$

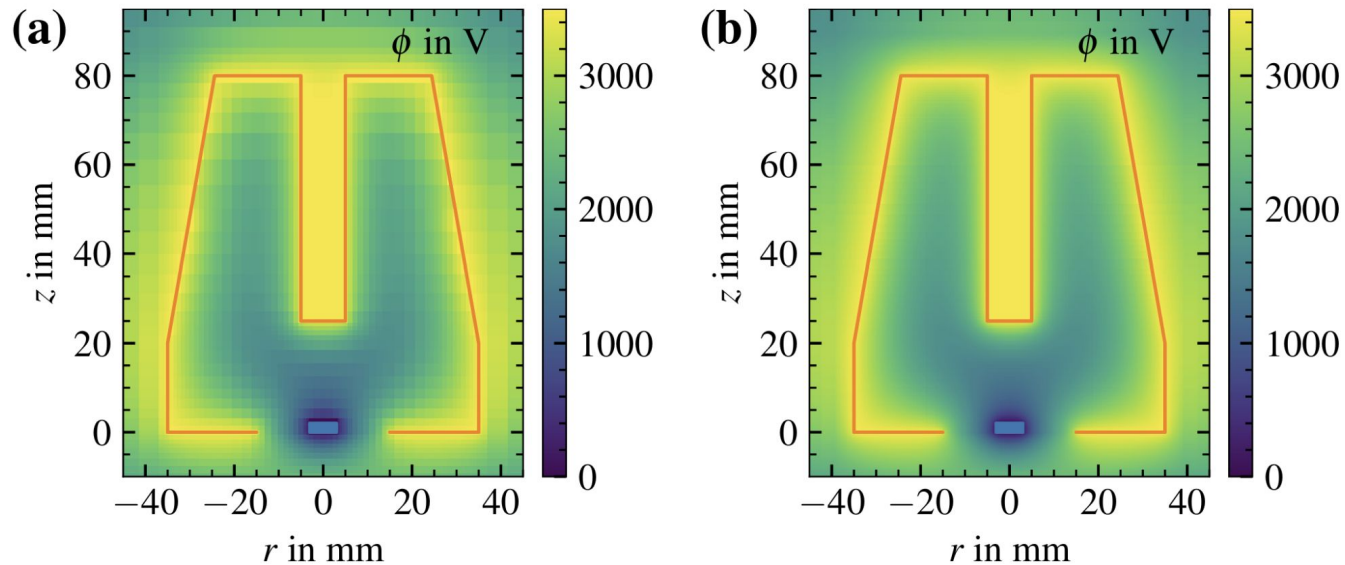
Geometry divided in $\mathbf{N} = \mathbf{N}_r \times \mathbf{N}_\phi \times \mathbf{N}_z$ grid points, obtaining a system of N linear equations. Solved numerically with **Successive Over-Relaxation (SOR)** algorithm.



$$\underbrace{\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{N_p} \end{bmatrix}}_{\vec{\phi} \in \mathbb{R}^{N_p}} = \underbrace{\begin{bmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,N_p} \\ a_{2,1} & a_{2,2} & \dots & a_{2,N_p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{N_p,1} & a_{N_p,2} & \dots & a_{N_p,N_p} \end{bmatrix}}_{A \in \mathbb{R}^{N_p \times N_p}} \cdot \underbrace{\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{N_p} \end{bmatrix}}_{\vec{\phi} \in \mathbb{R}^{N_p}} + \underbrace{\begin{bmatrix} a_{1,1}^0 Q_1^{\text{eff}} \\ a_{2,1}^0 Q_2^{\text{eff}} \\ \vdots \\ a_{N_p,1}^0 Q_{N_p}^{\text{eff}} \end{bmatrix}}_{\vec{b} \in \mathbb{R}^{N_p}}$$

$$\Phi^{(k+1)} = A \times \Phi^k + \mathbf{0}$$

Weighting Potential convergence



Weighting Potential convergence



- user/default convergence limit **CL** (10^{-7})

- Define “ initial error ”

$$c = 10 \times (CL + 1)$$

- Array cs = [c, c, c, c]

- Enters in the main loop

- **While** $c > CL$:

- After **N** steps, update the potential using SOR algorithm
- Saves the **last potential** , perform **one extra SOR** update and computes

$$c_{new} = \max | \phi_{\omega}^n - \phi_{\omega}^{n+1} |$$

- Update the errors array

$$[c, c, c, c_{new}]$$

- Compute the **means** and the **std**

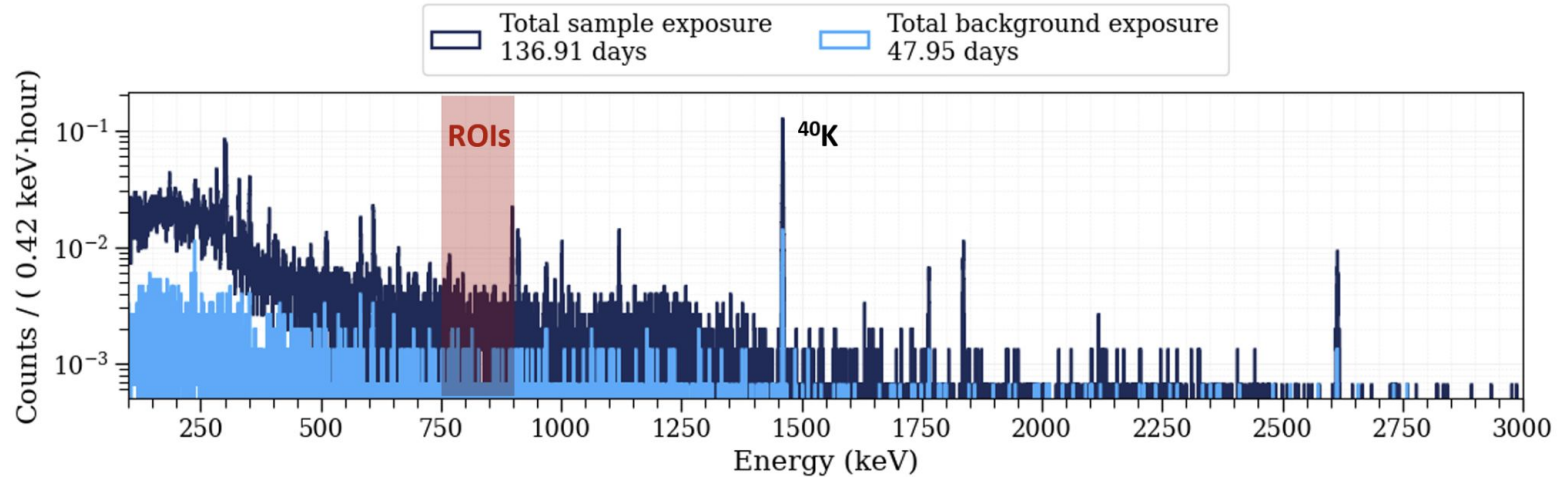
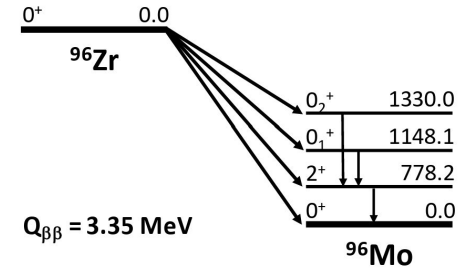
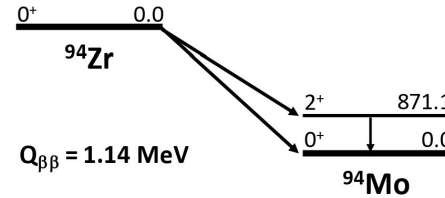
- Algorithm stops if:

1. **Sigma** < CL
2. **Mean** < CL
3. $N_{iteration} > N$

Side project : New limit on $^{94,96}\text{Zr}$ $0\nu\beta\beta$ decay



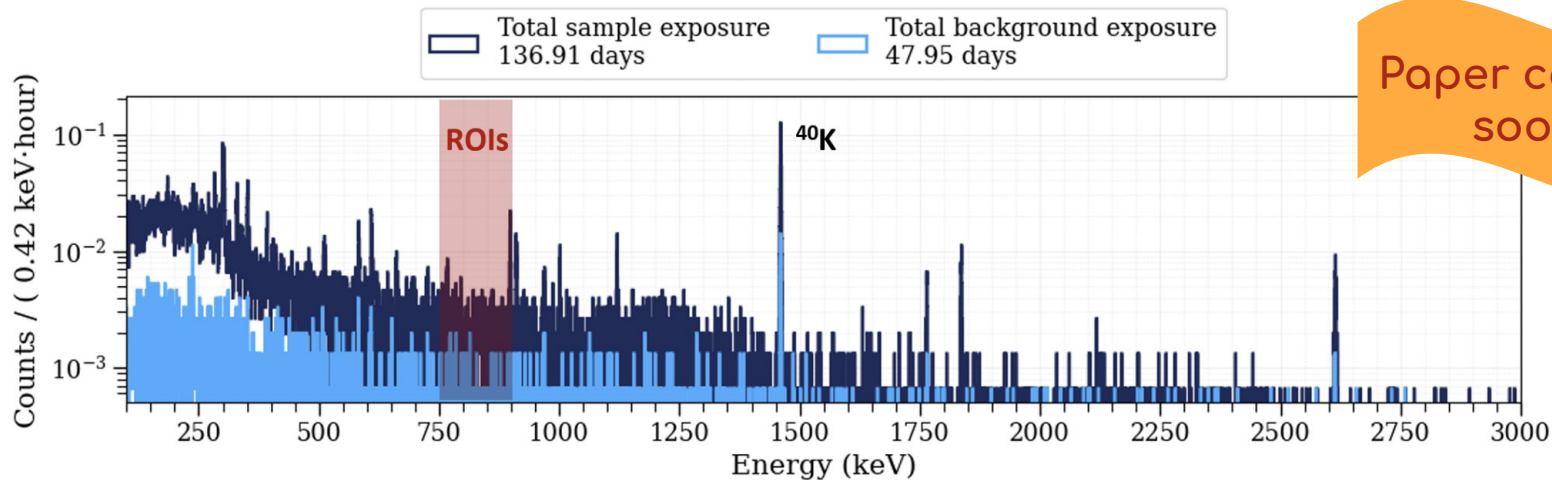
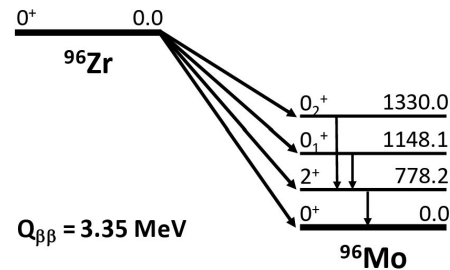
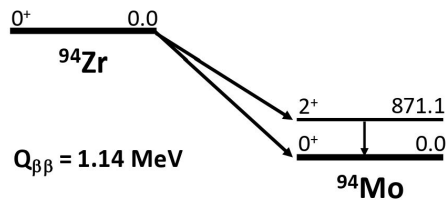
551.3 g of Zirconium
Oxide (ZrO_2) powder



Side project : New limit on $^{94,96}\text{Zr}$ $0\nu\beta\beta$ decay



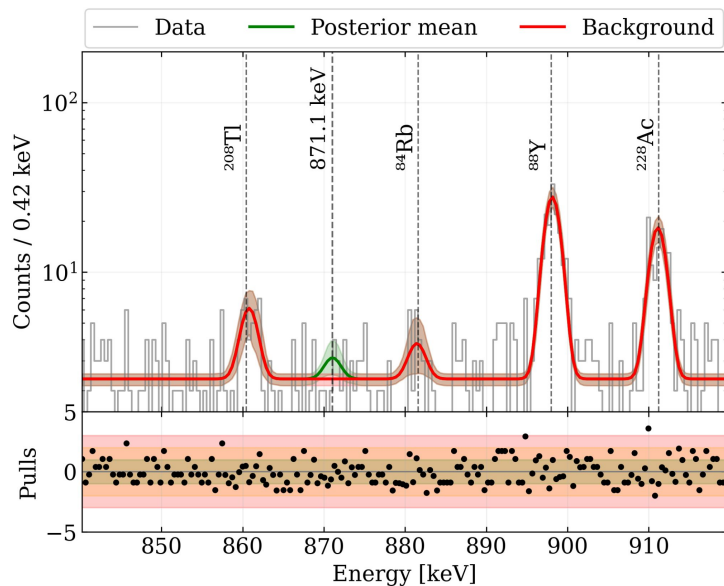
551.3 g of Zirconium
Oxide (ZrO_2) powder



Paper coming
soon!

Side project : New limit on $^{94,96}\text{Zr}$ $0\nu\beta\beta$ decay

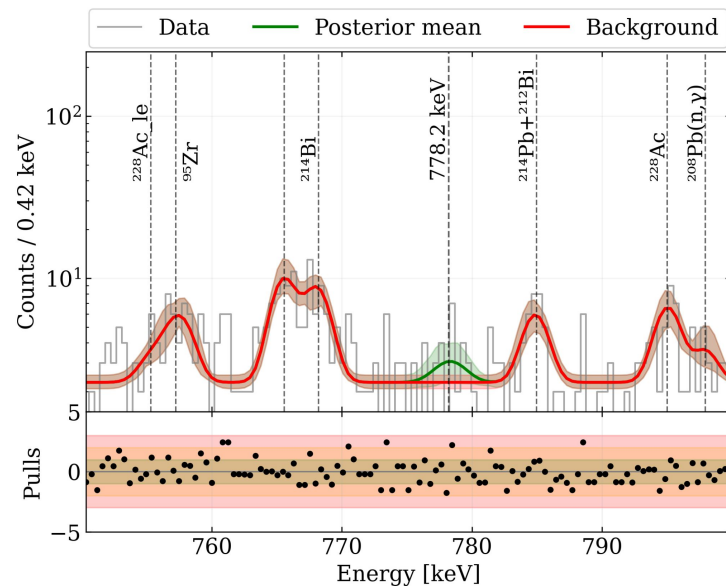
^{94}Zr



$$\varepsilon_{^{94}\text{Zr}} = 2.9 \%$$
$$f_{^{94}\text{Zr}} = 1.7 \%$$

$$T_{1/2} > 3.0 \cdot 10^{20} \text{ years}$$

^{96}Zr

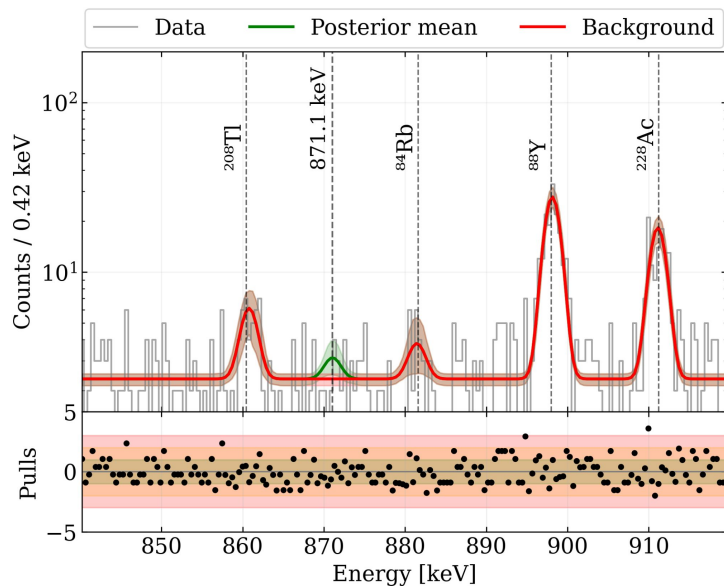


$$\varepsilon_{^{96}\text{Zr}} = 2.4 \%$$
$$f_{^{96}\text{Zr}} = 2.8 \%$$

$$T_{1/2} > 3.4 \cdot 10^{19} \text{ years}$$

Side project : New limit on $^{94,96}\text{Zr}$ $0\nu\beta\beta$ decay

^{94}Zr

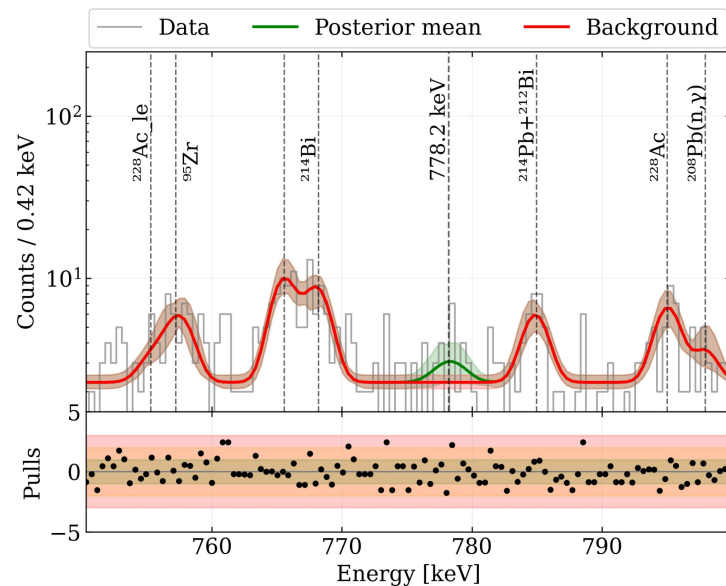


$$\varepsilon_{^{94}\text{Zr}} = 2.9 \%$$
$$f_{^{94}\text{Zr}} = 1.7 \%$$

$$T_{1/2} > 3.0 \cdot 10^{20} \text{ years}$$

(ALMOST 50% BETTER THAN THE BEST PREVIOUS RESULT)

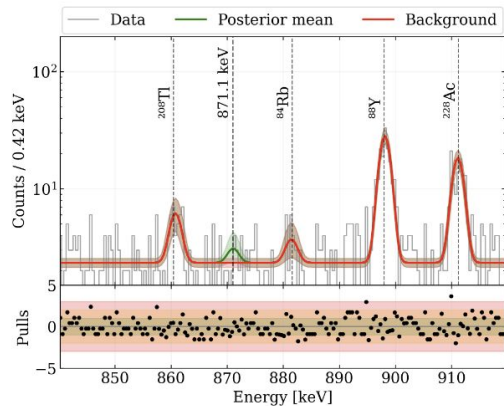
^{96}Zr



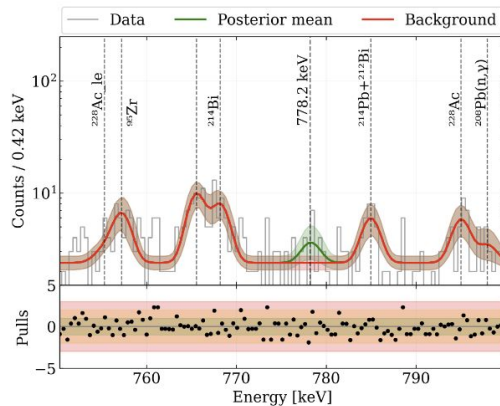
$$\varepsilon_{^{96}\text{Zr}} = 2.4 \%$$
$$f_{^{96}\text{Zr}} = 2.8 \%$$

$$T_{1/2} > 3.4 \cdot 10^{19} \text{ years}$$

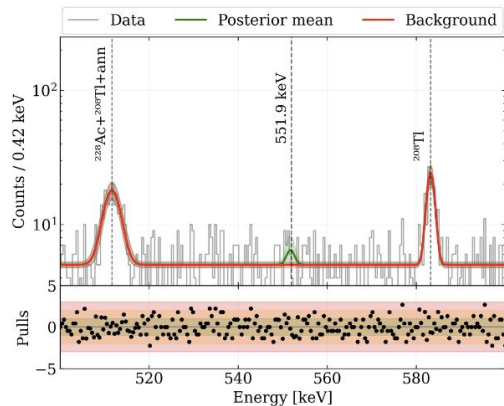
Side project : New limit on $^{94,96}\text{Zr}$ $0\nu\beta\beta$ decay



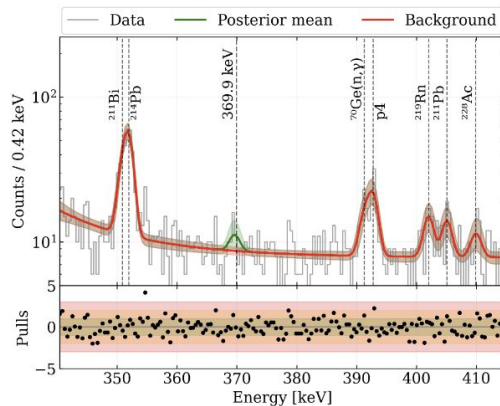
(a) ^{94}Mo de-excitation gamma line $2^+ \rightarrow 0^+$.



(b) ^{96}Mo de-excitation gamma line $2^+ \rightarrow 0^+$.



(c) ^{96}Mo de-excitation gamma line $0^+ \rightarrow 2^+$.



(d) ^{96}Mo de-excitation gamma line $0^+ \rightarrow 2^+$.

Transition	Energy [keV]	ROI [keV]	Efficiency [%]
^{96}Zr			
a) $0^+ \rightarrow 2^+$	369.9	345 - 415	3.33 ± 0.22
b) $0^+ \rightarrow 2^+$	551.8	500 - 600	2.88 ± 0.16
c) $2^+ \rightarrow 0^+$	778.2	750 - 800	2.41 ± 0.29
^{94}Zr			
d) $2^+ \rightarrow 0^+$	871.1	840 - 920	2.29 ± 0.29

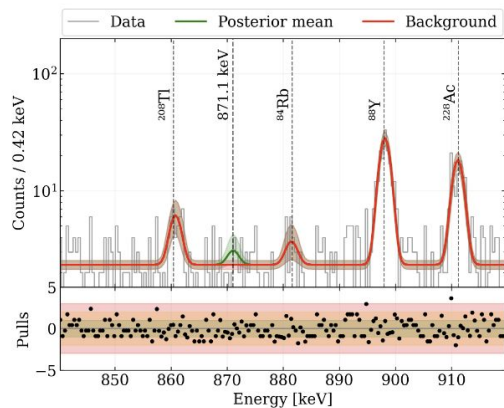
$$T_{1/2}^{0\nu\beta\beta}({}^{96}\text{Zr}, E = 778.2 \text{ keV}) > 3.46 \times 10^{19} \text{ years}$$

$$T_{1/2}^{0\nu\beta\beta}({}^{96}\text{Zr}, E = 551.8 \text{ keV}) > 4.27 \times 10^{19} \text{ years}$$

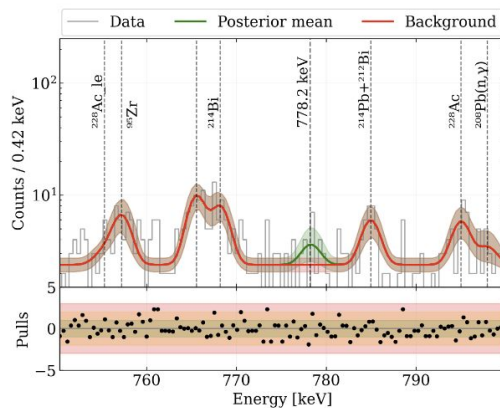
$$T_{1/2}^{0\nu\beta\beta}({}^{96}\text{Zr}, E = 369.9 \text{ keV}) > 2.84 \times 10^{19} \text{ years}$$

$$T_{1/2}^{0\nu\beta\beta}({}^{94}\text{Zr}, E = 871.1 \text{ keV}) > 3.00 \times 10^{20} \text{ years}$$

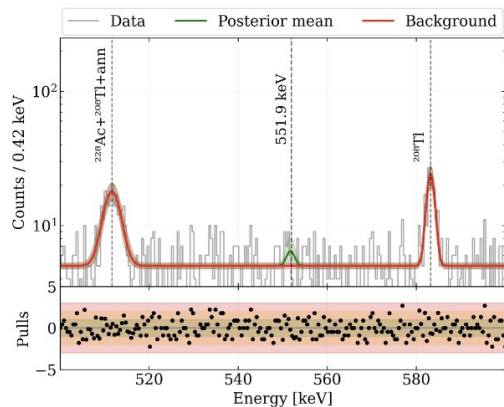
Side project : New limit on $^{94,96}\text{Zr}$ $0\nu\beta\beta$ decay



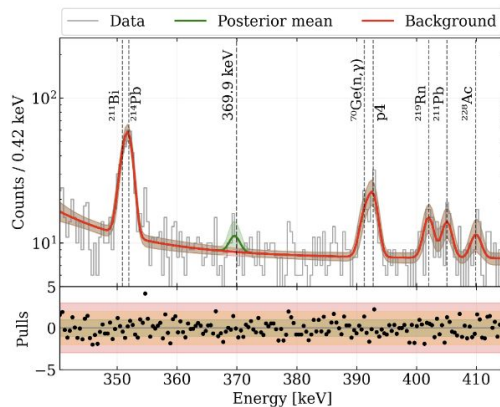
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(d) ^{96}Mo de-excitation gamma line $0^+ \rightarrow 2^+$.

Transition	Energy [keV]	ROI [keV]	Efficiency [%]
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b) $0_2^+ \rightarrow 2^+$	551.8	500 - 600	2.88 ± 0.16
c) $2^+ \rightarrow 0^+$	778.2	750 - 800	2.41 ± 0.29
^{94}Zr			
d) $2^+ \rightarrow 0^+$	871.1	840 - 920	2.29 ± 0.29

$$T_{1/2}^{0\nu\beta\beta} (^{96}\text{Zr}, E = 778.2 \text{ keV}) > 3.46 \times 10^{19} \text{ years}$$

$$T_{1/2}^{0\nu\beta\beta} (^{96}\text{Zr}, E = 551.8 \text{ keV}) > 4.27 \times 10^{19} \text{ years}$$

$$T_{1/2}^{0\nu\beta\beta} (^{96}\text{Zr}, E = 369.9 \text{ keV}) > 2.84 \times 10^{19} \text{ years}$$

$$T_{1/2}^{0\nu\beta\beta} (^{94}\text{Zr}, E = 871.1 \text{ keV}) > 3.00 \times 10^{20} \text{ years}$$

(almost 50% better than the best previous result)

Celi, E., et al. "New limit on ^{94}Zr double beta decay to the 1st excited state of ^{94}Mo ." *The European Physical Journal C* 83.5 (2023): 396.