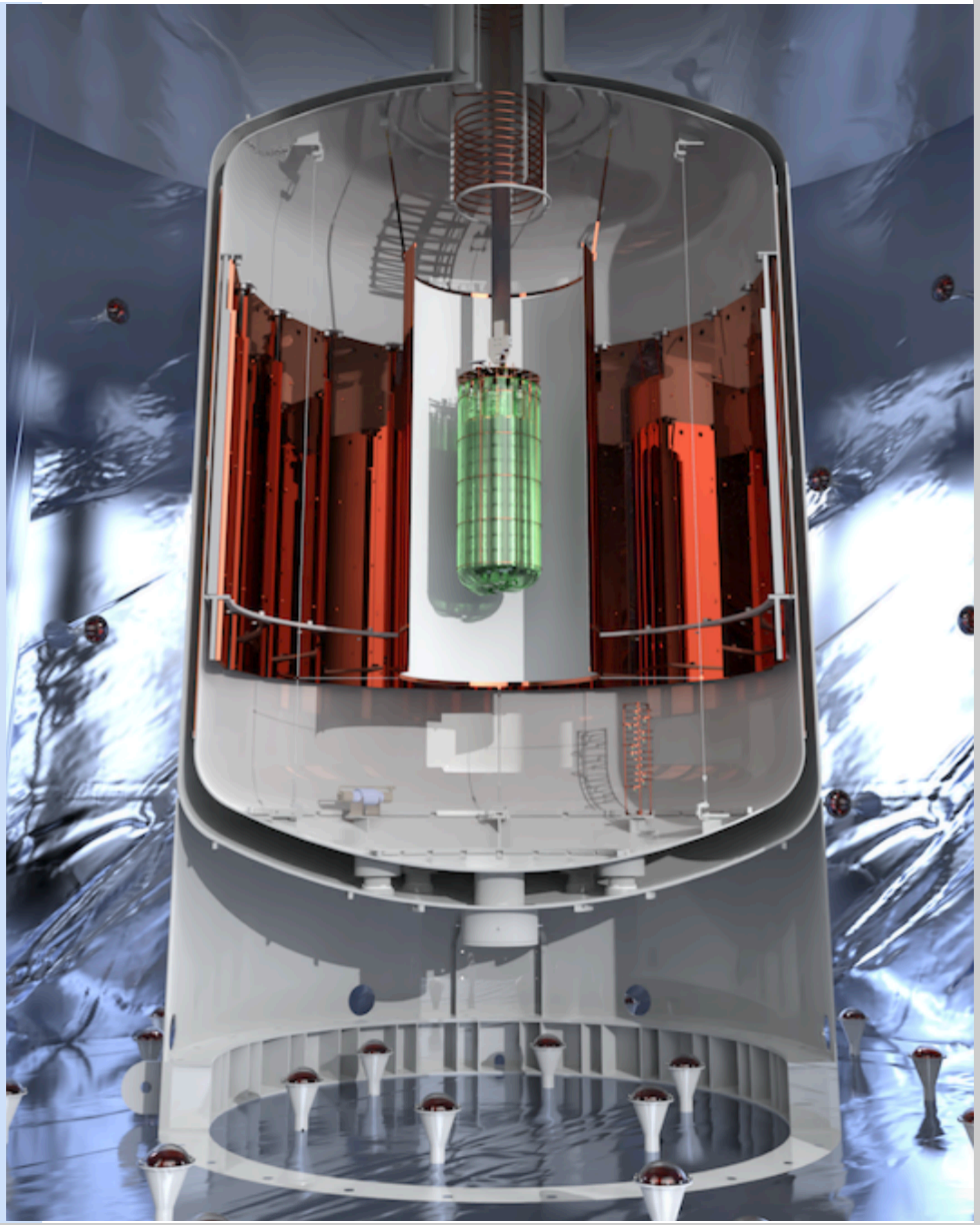
Bayesian Uncertainty Quantification for Neutrinoless Double-Beta Decay

LEGEND

Large Enriched
Germanium Experiment
for Neutrinoless $\beta\beta$ Decay



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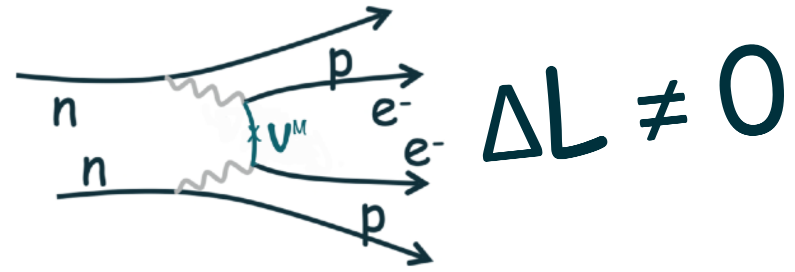


Mass constraints

effective neutrino mass

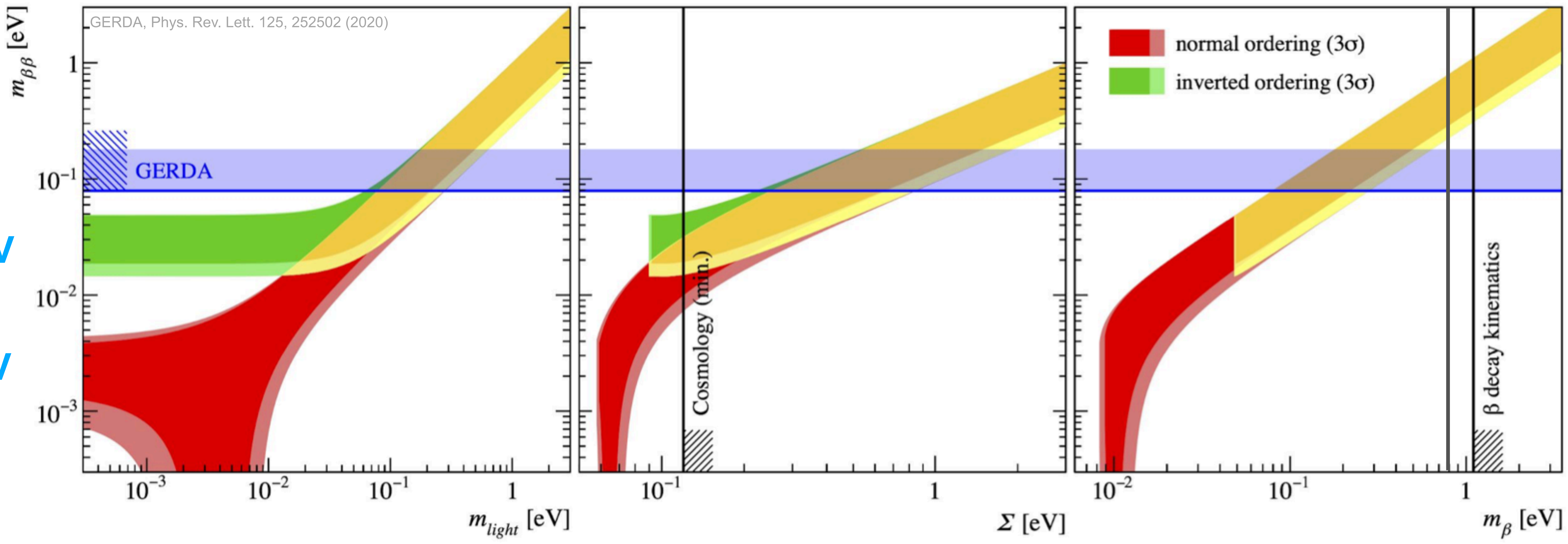
$$1/T^{0\nu}_{1/2} = G \cdot NME^2 \cdot m^2_{\beta\beta}$$

phase space nuclear matrix element

Most obvious decay mechanism: exchange of **light Majorana neutrinos**

LEGEND-200: $m_{\beta\beta}$ < [0.33,0.78] eV

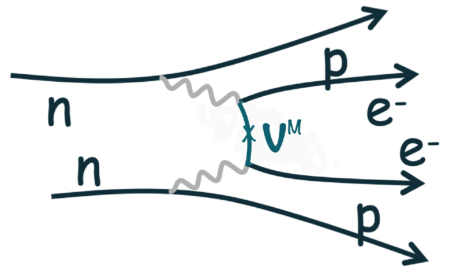
LEGEND-1000: $m_{\beta\beta}$ < [0.09,0.21] eV



Planck+BAO: Σ < 0.12 eV
[Aghanim et al., arXiv:1807.06209]

KATRIN: m_β < 0.8 eV
[*Nat. Phys.* **18**, 160–166 (2022)]

interplay with cosmology / direct mass measurements

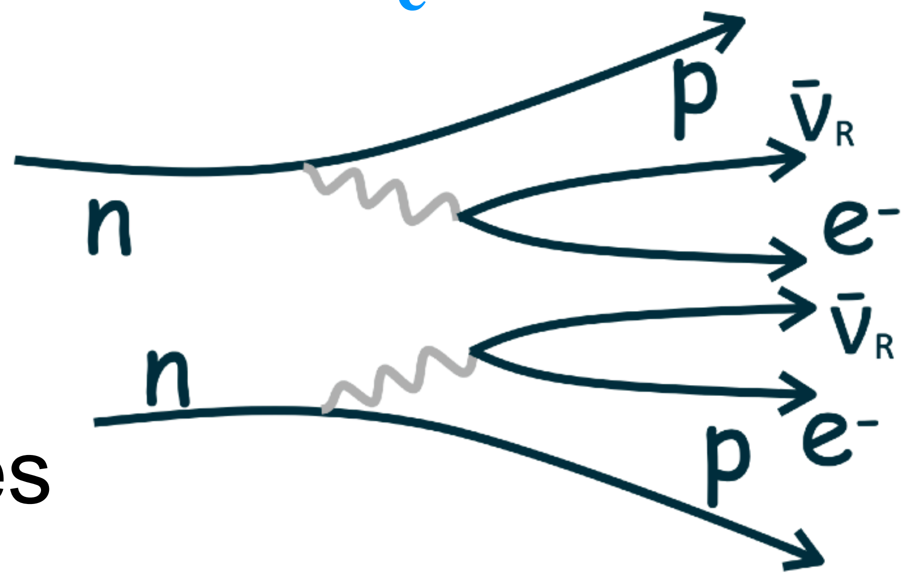


$\Delta L \neq 0$

Double-beta decay and lepton number violation

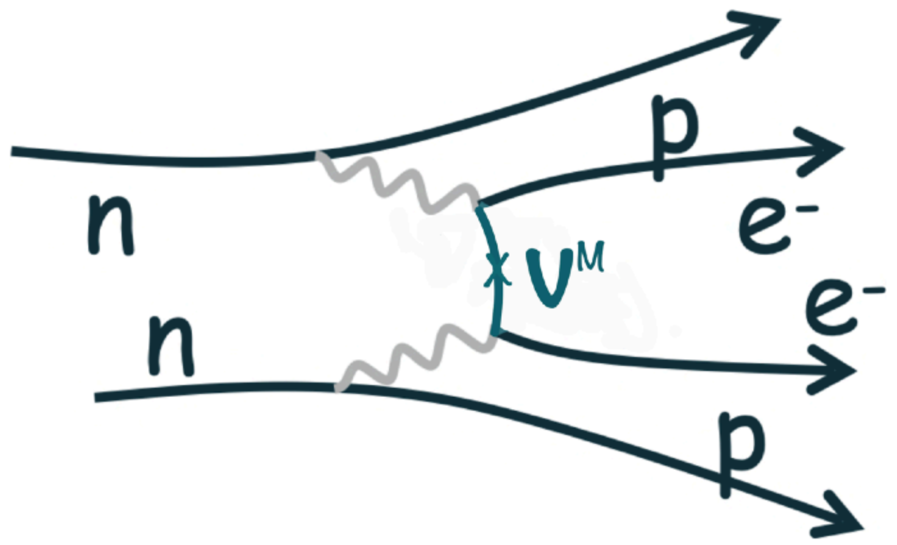
$$2\nu\beta\beta : (A, Z) \rightarrow (A, Z+2) + 2e^- + 2\bar{\nu}_e$$

- ΔL=0
- SM allowed
- observed in many isotopes
- $T_{1/2}$ ~ (10^{18} - 10^{24}) yr

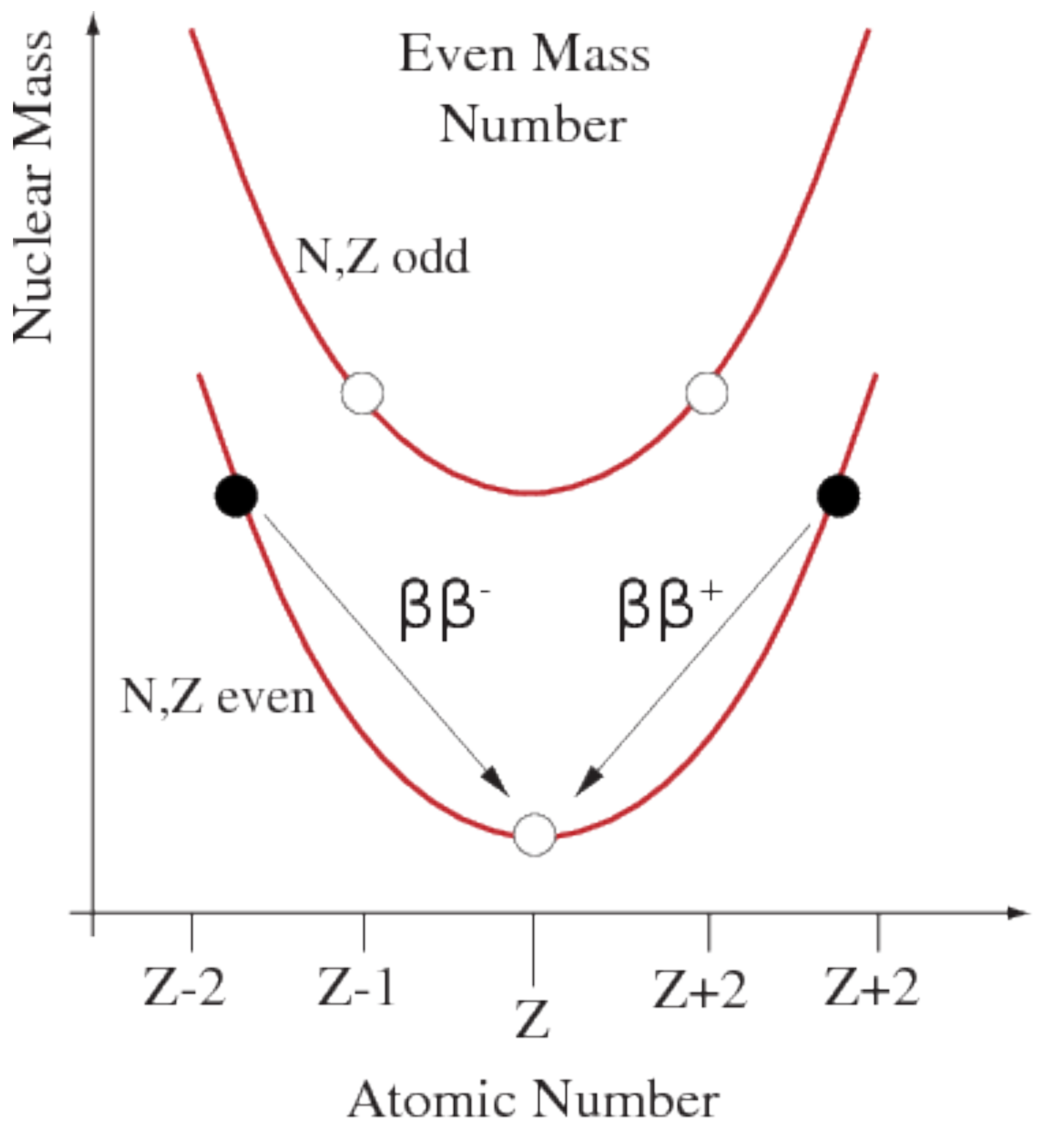


$$0\nu\beta\beta : (A, Z) \rightarrow (A, Z+2) + 2e^-$$

- ΔL=2
- beyond SM
- Majorana mass component
- via light Majorana ν exchange or other L-violating processes



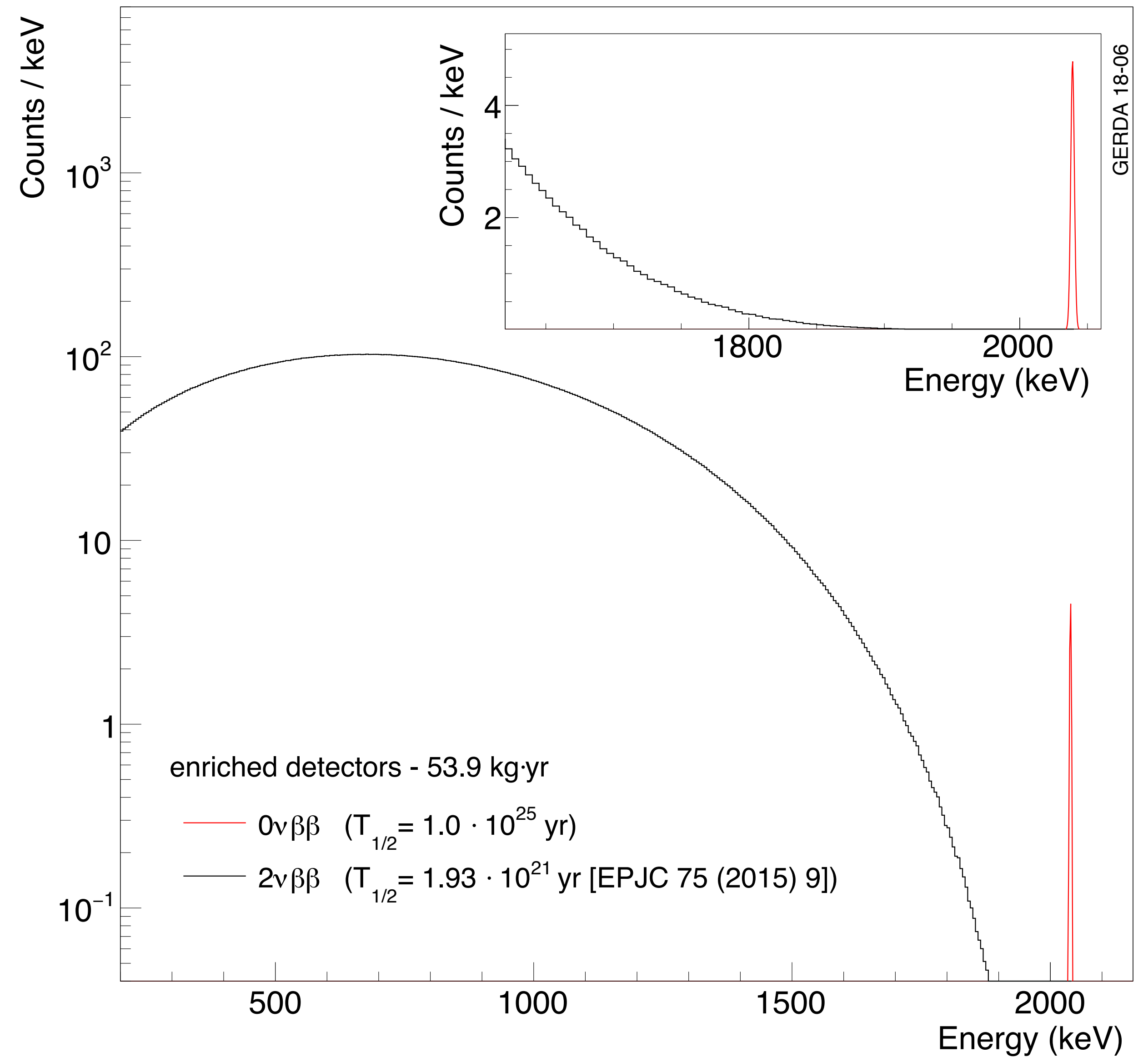
double-beta decay is possible when energetically favored

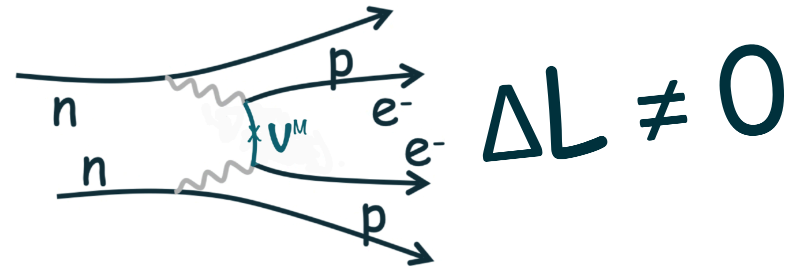


measure sum energy spectrum of electrons

- 2νββ ➞ continuum
- 0νββ ➞ mono-energetic peak @ $Q_{\beta\beta}$

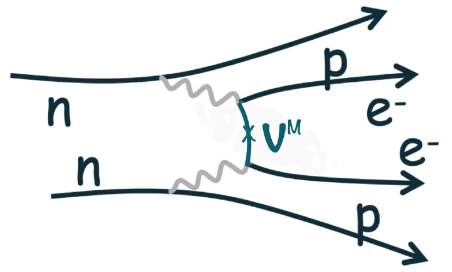
$$Q_{\beta\beta} = E_{e1} + E_{e2} - 2m_e$$





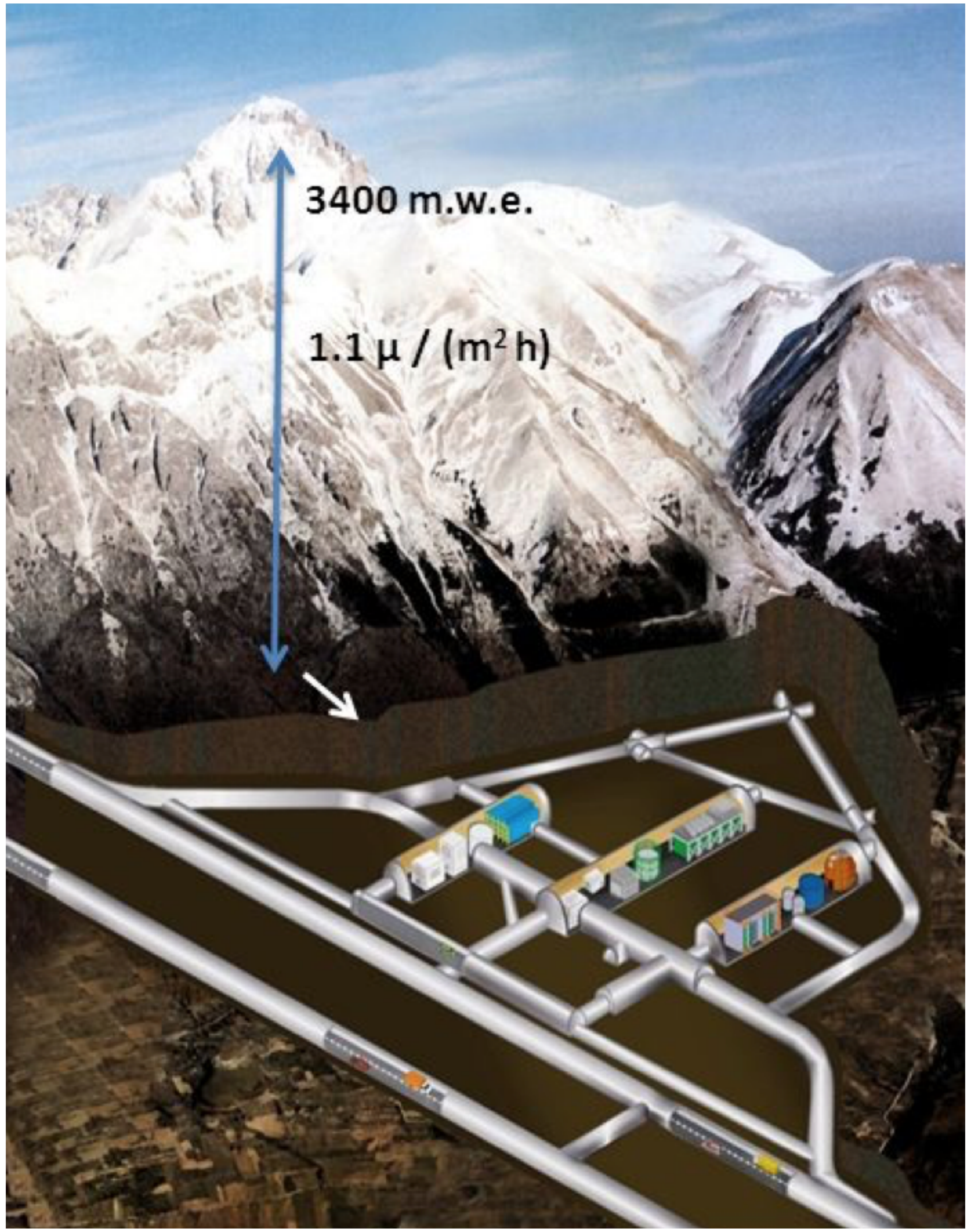
Most measured half-lives for 2vββ are O(10^{21}) years

- Compare to lifetime of the universe: 10^{10} years
- Compare to Avogadro’s number: 6 Å~ 10^{23}
- A mole of the isotope will produce ~1 decay/day
- If it exists, the half-lives of 0vββ would be much longer
- ^{76}Ge 0vββ limit is > 10^{26} years, ^{130}Te 0vββ limit is > 10^{24} years
- A mole of ^{76}Ge produces < 1 neutrinoless decay/year



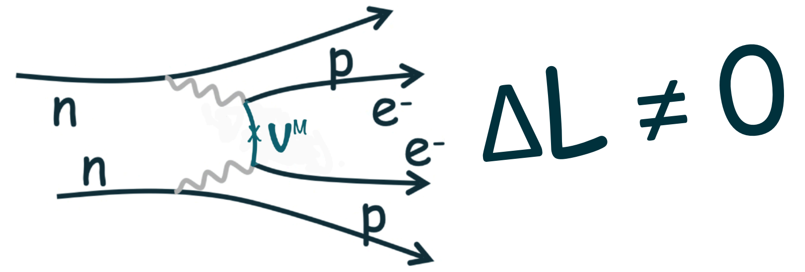
$\Delta L \neq 0$

LEGEND experiment



LEGEND mission: “The collaboration aims to develop a phased, ^{76}Ge based double-beta decay experimental program with discovery potential at a half-life beyond 10^{28} years, using existing resources as appropriate to expedite physics results.“

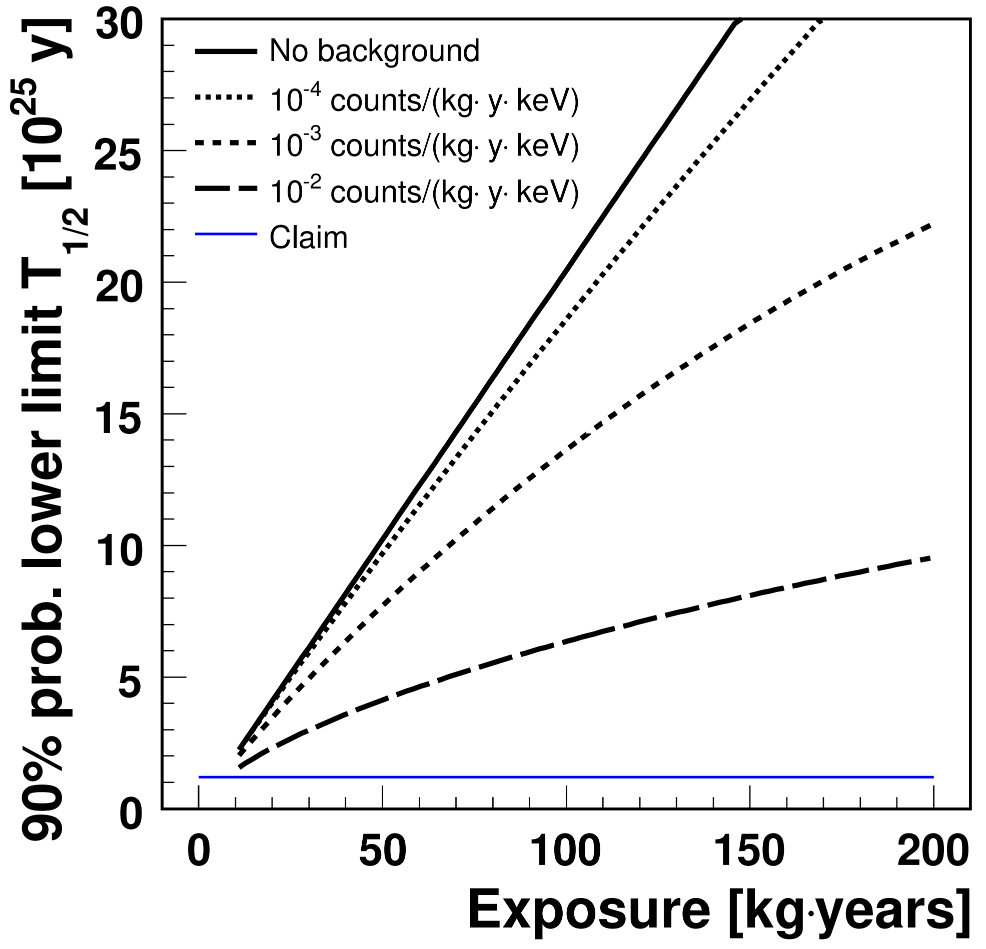
~270 scientists spread over 12 countries and 55 institutes



Experimental sensitivity

background (BI) < 1 $T^{0\nu}_{1/2} \propto \varepsilon \cdot a \cdot M \cdot t$

background (BI) > 1 $T^{0\nu}_{1/2} \propto \varepsilon \cdot a \cdot \sqrt{\frac{M \cdot t}{BI \cdot \Delta E}}$



0vββ search in ^{76}Ge: ^{76}Ge → ^{76}Se + 2e$^-$

✓ source = detector
⇒ **high ε**

✓ high purity Ge (HPGe) detectors
⇒ **low intr. BI**

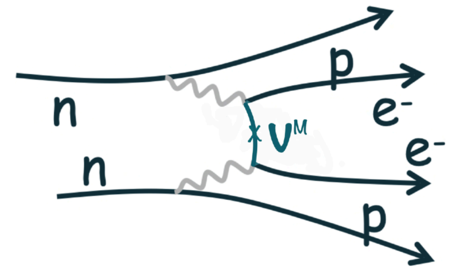
✓ ΔE @ $Q_{\beta\beta}$ ~ 0.2 %
⇒ **excellent ΔE**

✓ high density
⇒ **0vββ peak-like events**

- low $Q_{\beta\beta}$ value ($Q_{\beta\beta}$ = 2039 keV)
⇒ **possible external BI (e.g. ^{208}Tl)**

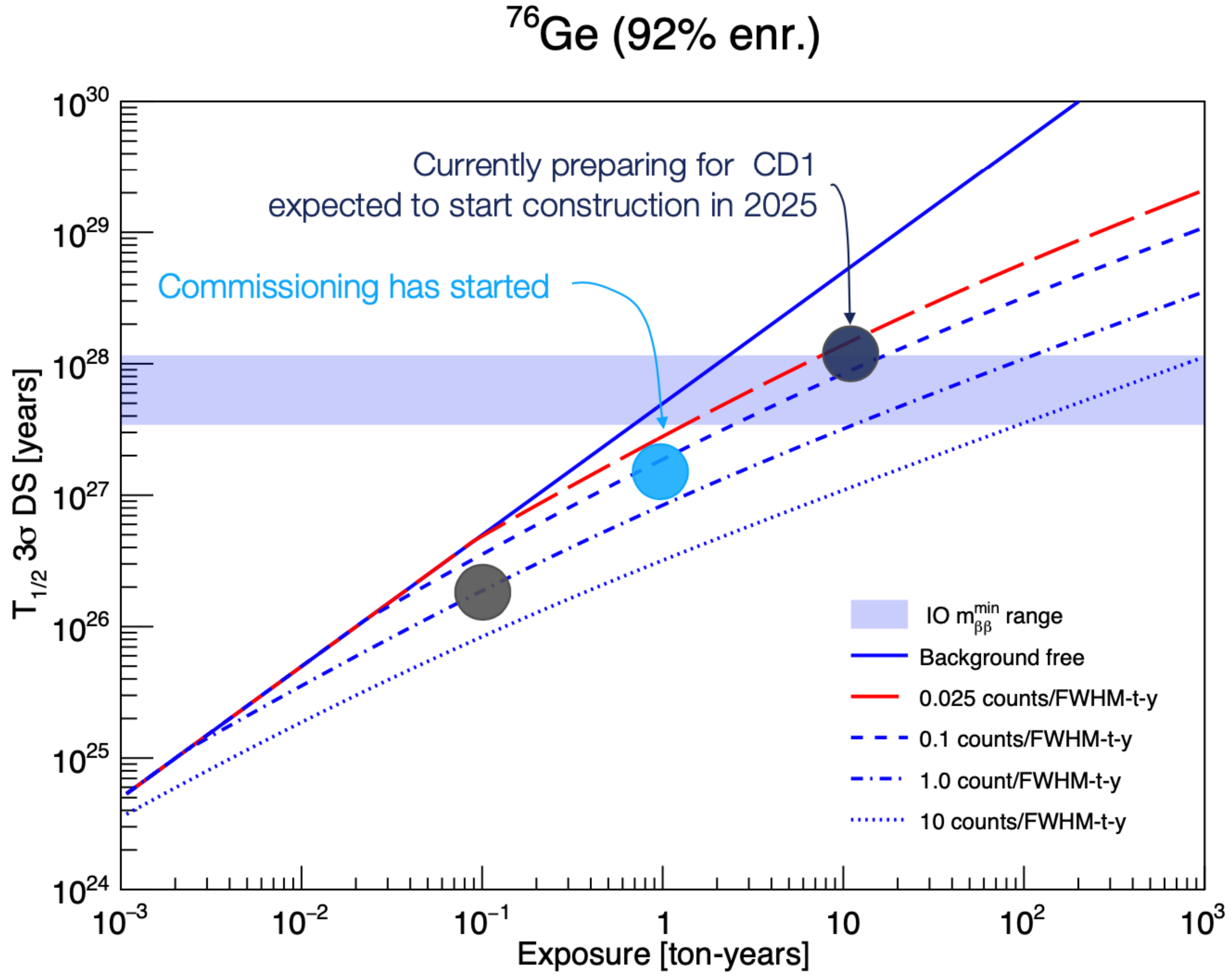
- a=7.8% for ^{76}Ge
⇒ **enrichment necessary**

→ increase sensitivity by background reduction (BI) at $Q_{\beta\beta}$ and simultaneous increase of mass (M) and improvement of the energy resolution (ΔE)



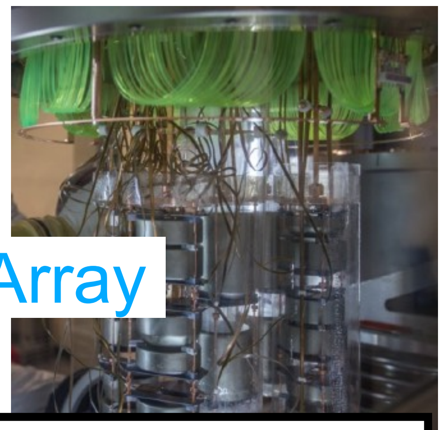
$\Delta L \neq 0$

Building on past strengths



LEGEND-1000	Detector mass: 1000 kg Exposure: 10 ton-yr	$T^{0\nu}_{1/2} > 10^{28}$ yr
LEGEND-200	Detector mass: 200 kg Exposure: 1 ton-yr	$T^{0\nu}_{1/2} > 10^{27}$ yr
GERDA / MAJORANA DEMONSTRATOR	Detector mass: 44/ 44 kg Exposure: 127/ 65 kg-yr	$T^{0\nu}_{1/2} > 10^{26}$ yr / 10^{25} yr

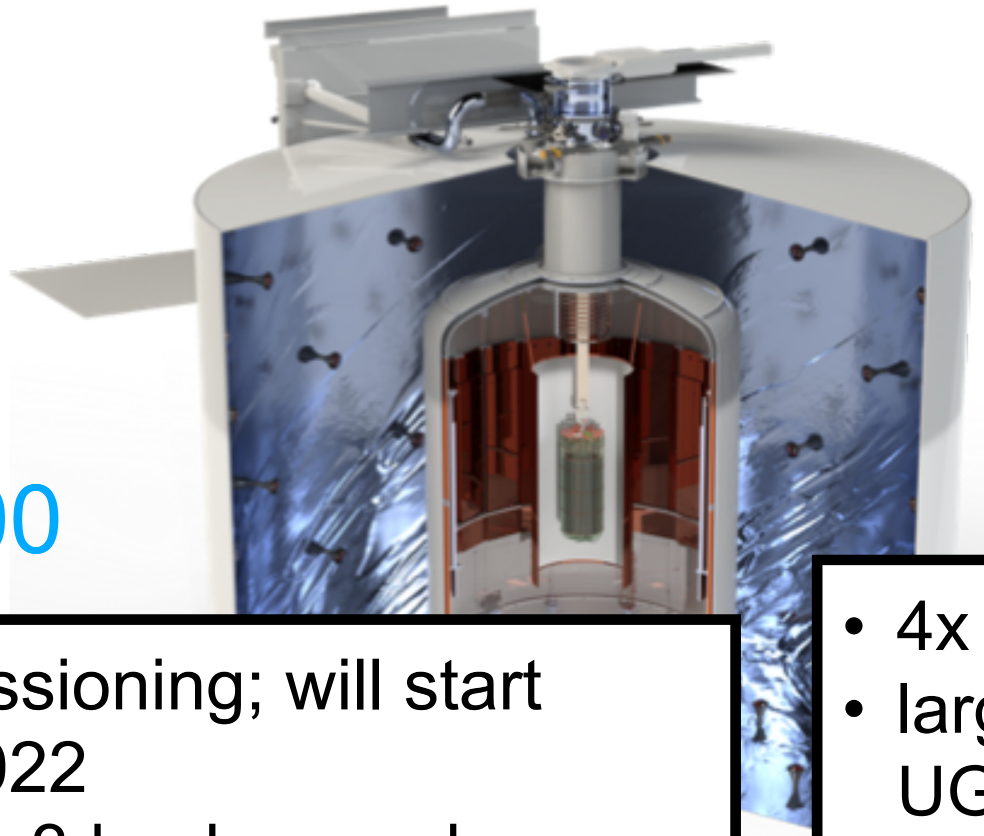
GERDA - Germanium Detector Array



- operation of bare Ge crystals immersed in LAr, LAr scintillation for active veto
- LNGS (Italy) until Nov 2019
- ΔE: 2.6 keV (BEGe FWHM at $Q_{\beta\beta}$)
- **BI: 5.2 x 10^{-4} cts / (kg·keV·yr)**

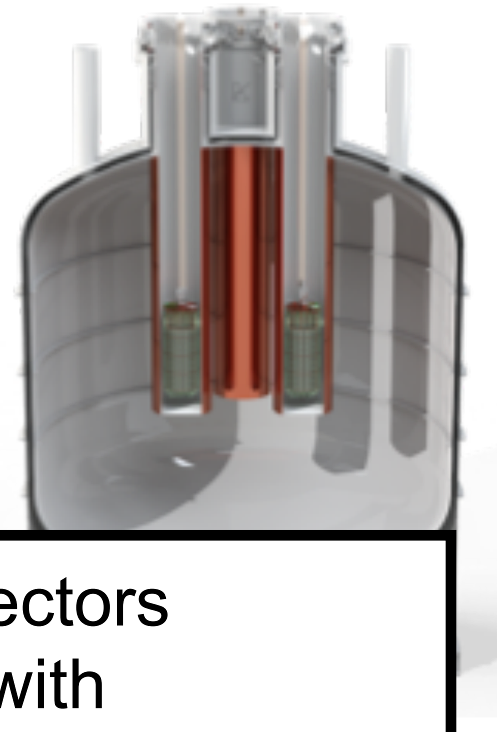
MJD - MAJORANA DEMONSTRATOR

- operation of Ge crystals in vacuum cryostat, ultra-clean underground electro-formed copper
- SURF (South Dakota) until 2020
- **ΔE: 2.53 keV (FWHM at $Q_{\beta\beta}$)**
- BI: 4.7 x 10^{-3} cts / (kg·keV·yr)



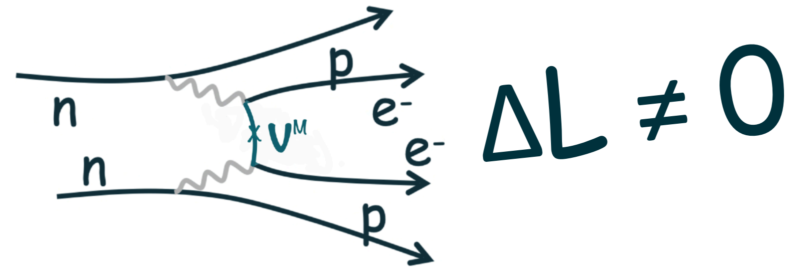
LEGEND-200

- currently commissioning; will start data-taking in 2022
- requires only ×2–3 background improvement w.r.t. GERDA
- goal (5 yr runtime):
- discovery sensitivity $T_{1/2} > 10^{27}$ yr (90% C.L.) → $m_{\beta\beta}$ < 33–71 meV



LEGEND-1000

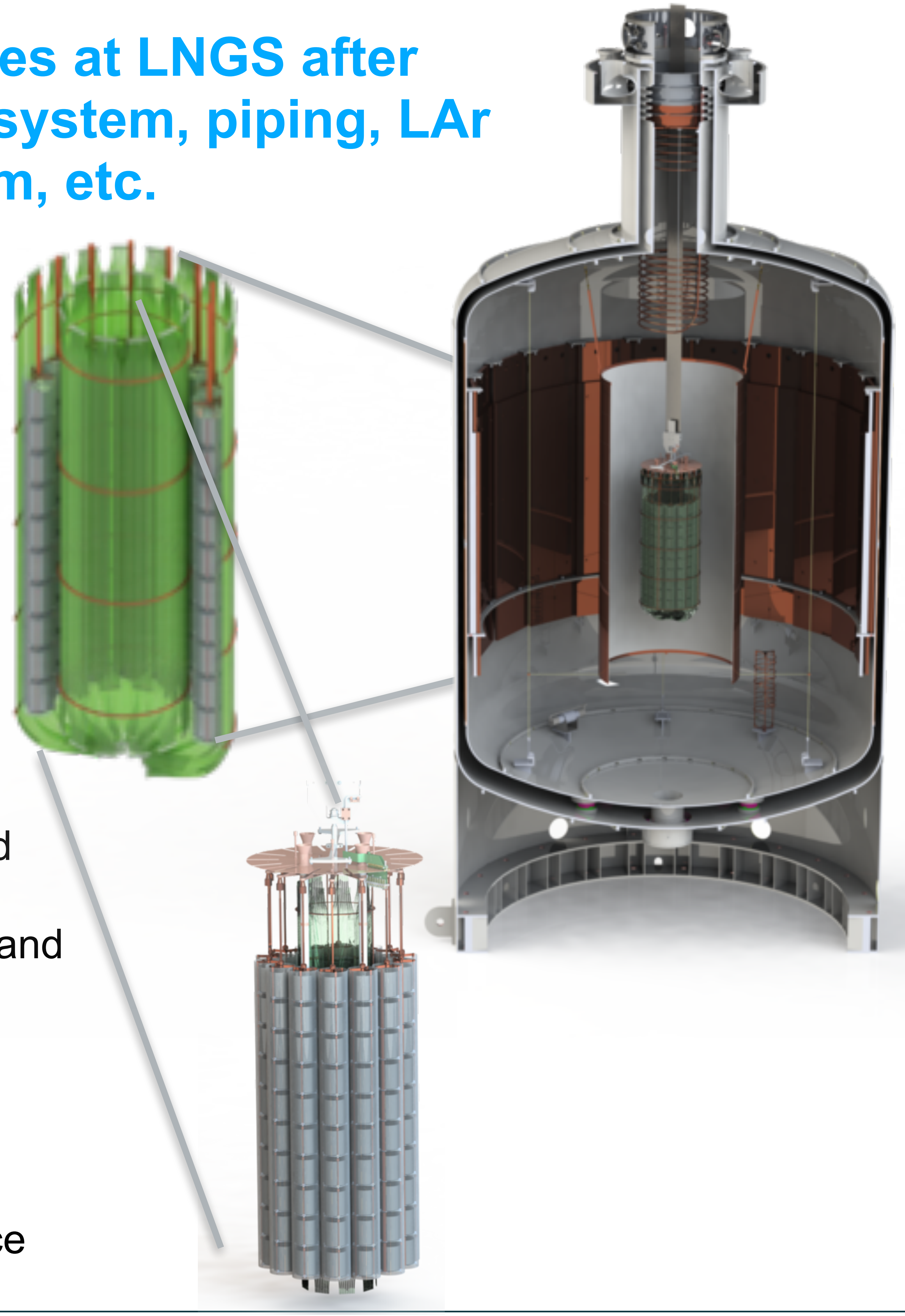
- 4x L-200 design ~400 detectors
- large reentrant tube filled with UGLAr/ all LAr vol. with veto system
- baseline site is SNOLAB but LNGS possible → rich R&D program
- goal (10 yr runtime):
- discovery sensitivity $T_{1/2} > 10^{28}$ yr (90% C.L.) → $m_{\beta\beta}$ < 9-19 meV



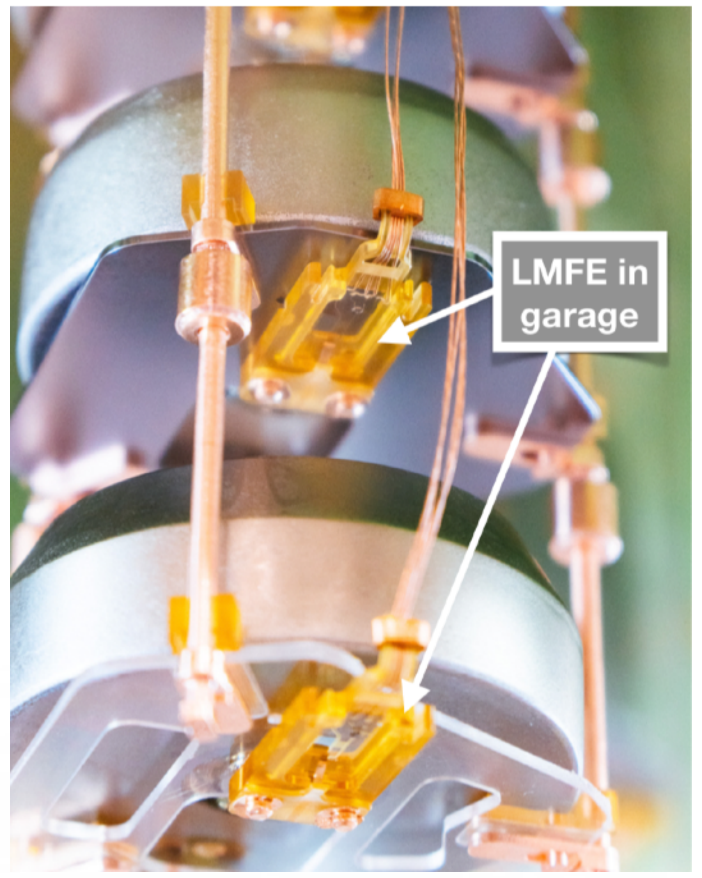
First stage: LEGEND-200

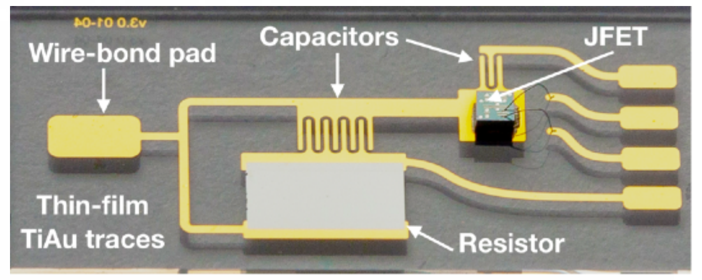
Reuse of GERDA facilities at LNGS after upgrades on e.g. lock system, piping, LAr veto, calibration system, etc.

- detect LAr scintillation light
- fiber shroud: fibers were coated with tetraphenyl butadiene (TPB) for wavelength shifting from VUV to blue regime



- ~ 200 kg of detectors distributed over 12 strings
- reuse of detectors from GERDA and MJD + 140 kg of additional inverted-coaxial point-contact (ICPC) detectors
- ICPC detectors:
  - Active mass > 3 kg
  - Excellent PSD performance





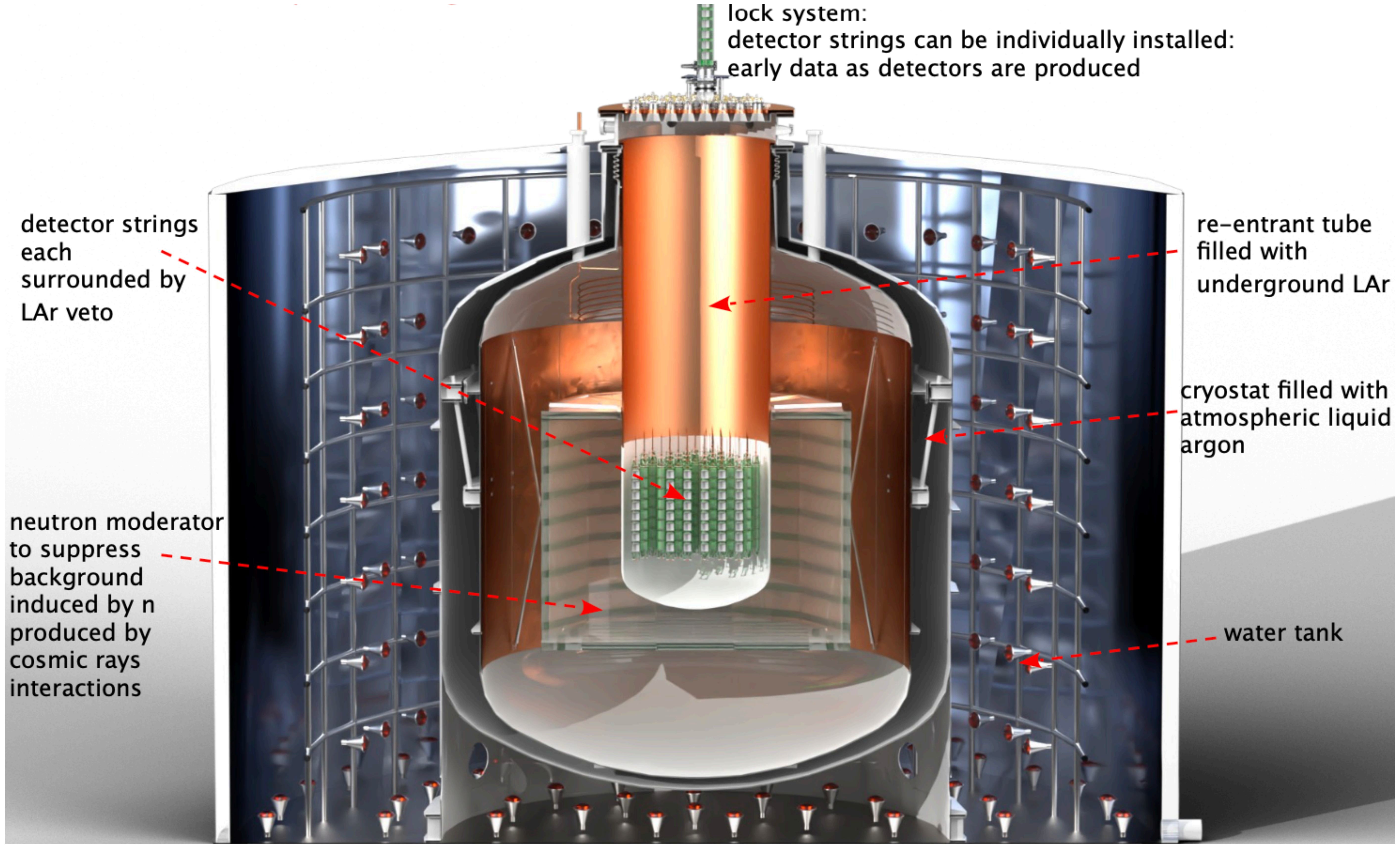
Read-out: *New in LEGEND-200*
- Low-mass front end (LMFE) close to detector (MJD-style)
- differential signal output (reducing noise)
- new digitizer: Flashcam
- new custom made head electronics, HV filter boards, slow control

LAr veto: *New in LEGEND-200*
- independent trigger (veto $^{77(m)}$Ge, neutrons)
- in-situ LAr purity monitoring (LLAMA)
- measuring light yield and triplet lifetime
- Scintillating/ transparent detector holders (PEN)
- LAr purification system (fill and continuous)
- cryostat refilled with new LAr Sep.2021

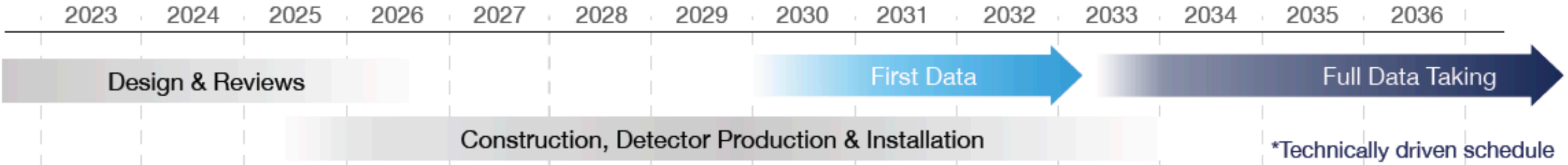
Second stage: LEGEND-1000

Performance parameters

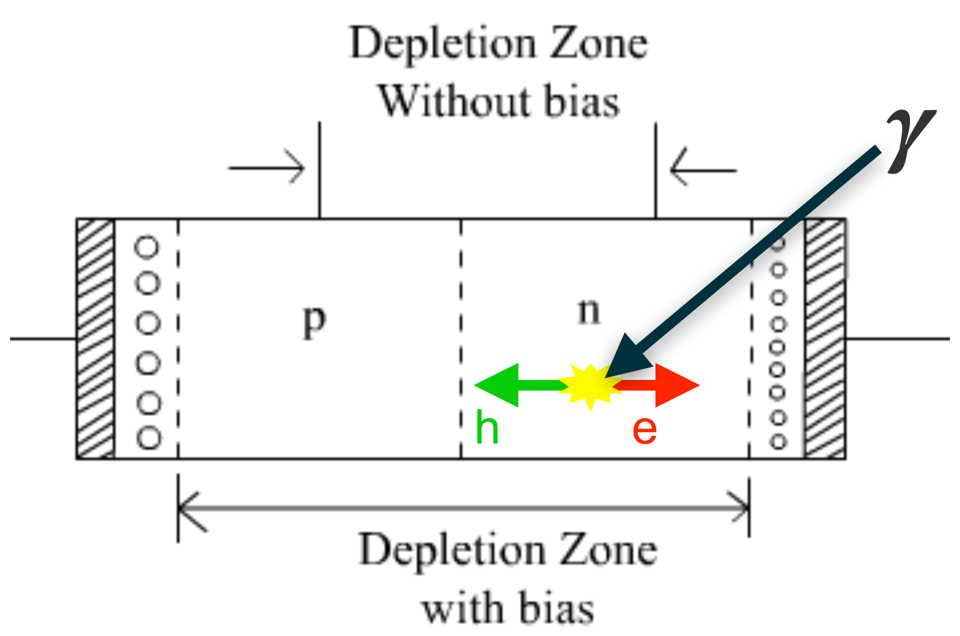
0νββ isotope	^{76}Ge
$Q_{\beta\beta}$	2039 keV
Total masss	1000 kg
ΔE at $Q_{\beta\beta}$	2.5 keV FWHM
Signal acceptance	0.69
Total exposure	10 t·yr
Background goal	< 10^{-5} cts/(keV·kg·yr)
$T^{0\nu}_{1/2}$	$1.3\cdot10^{28}$ yr (90% C.L. discovery) $1.8\cdot10^{28}$ yr (90% C.L. sensitivity)
$m_{\beta\beta}$	9.4-21.4 meV (99.7% C.L. discovery) 8.5-19.4 meV (90% C.L. sensitivity)

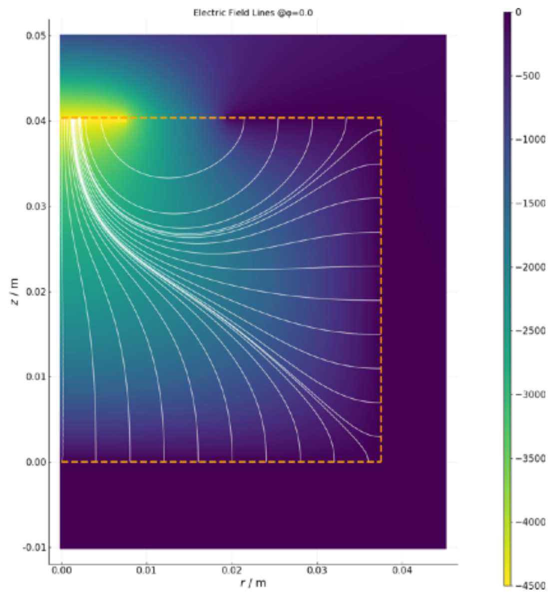


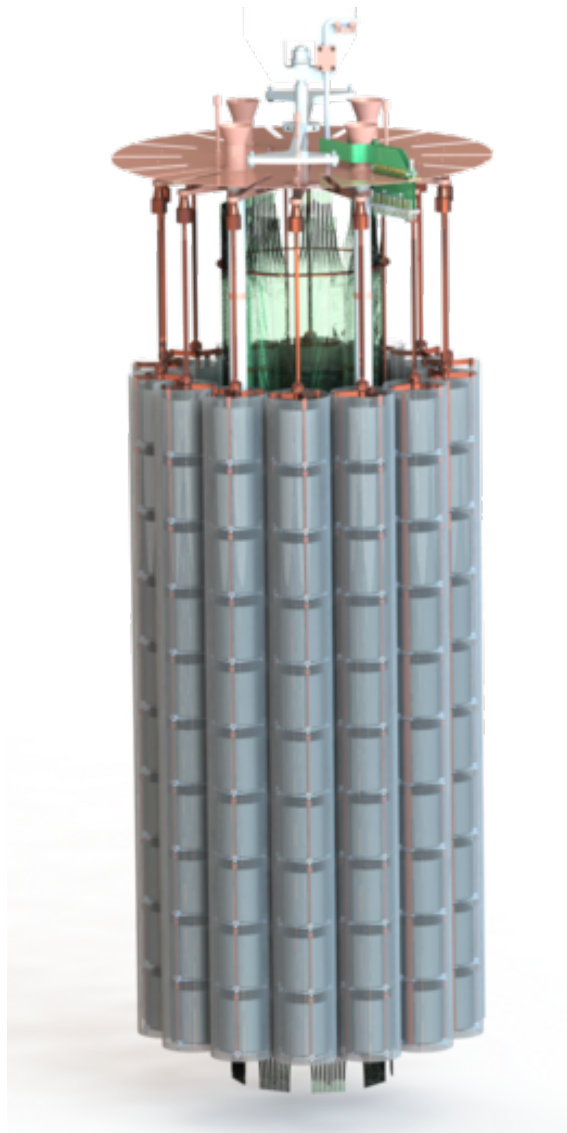
Timeline

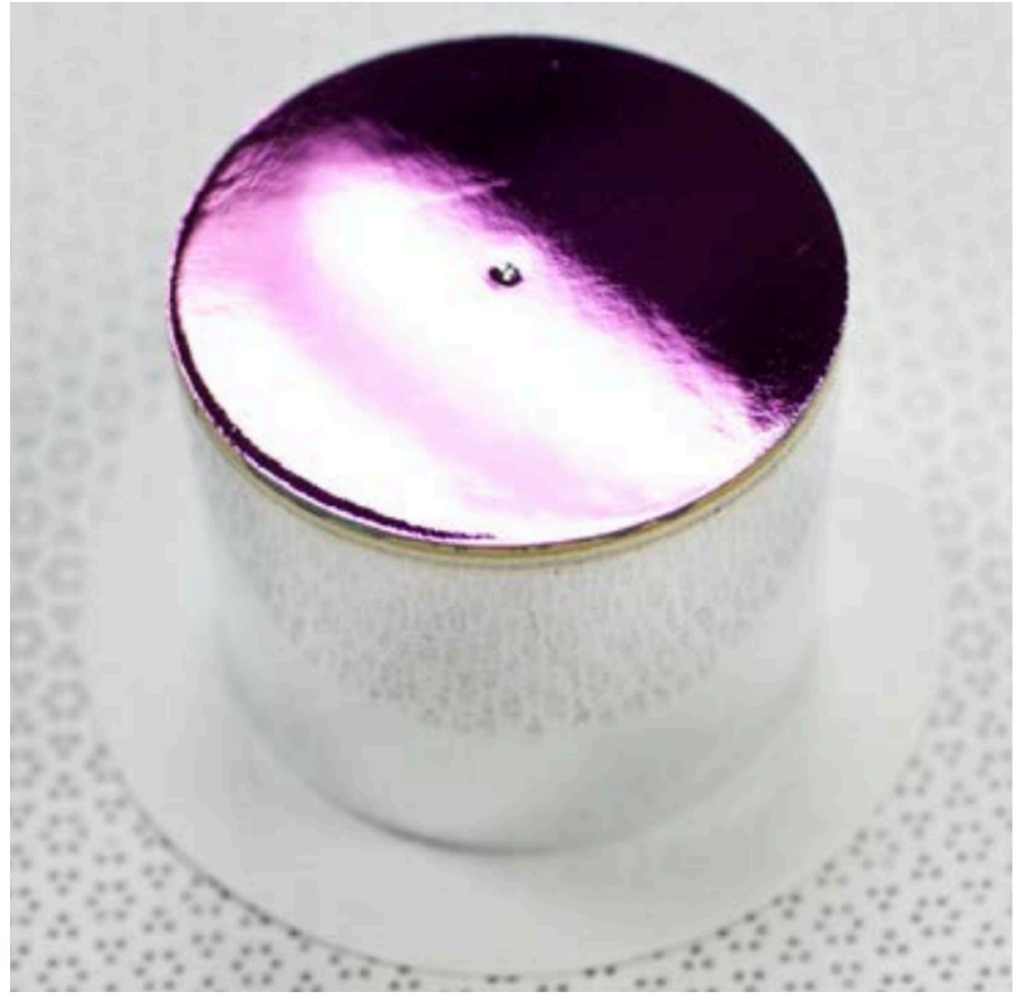


Point contact HPGe detectors





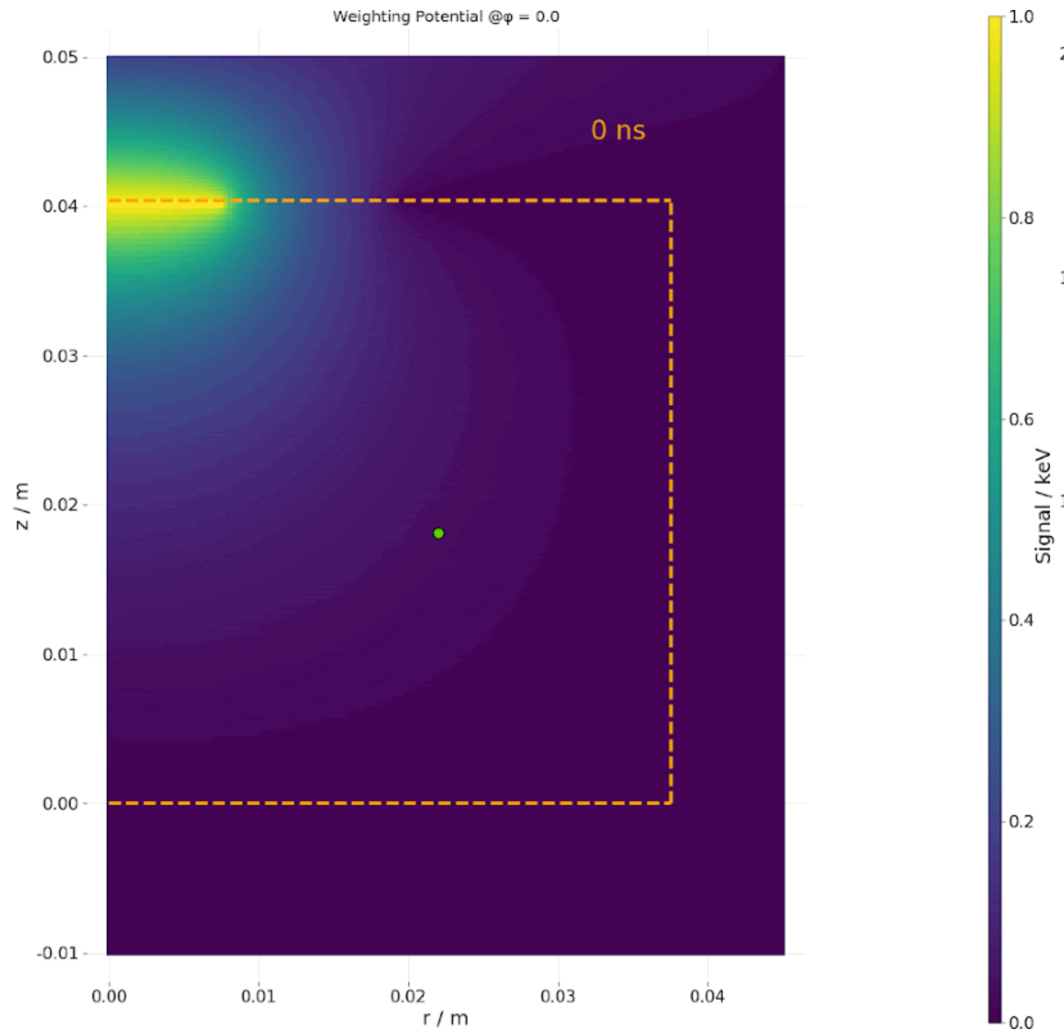


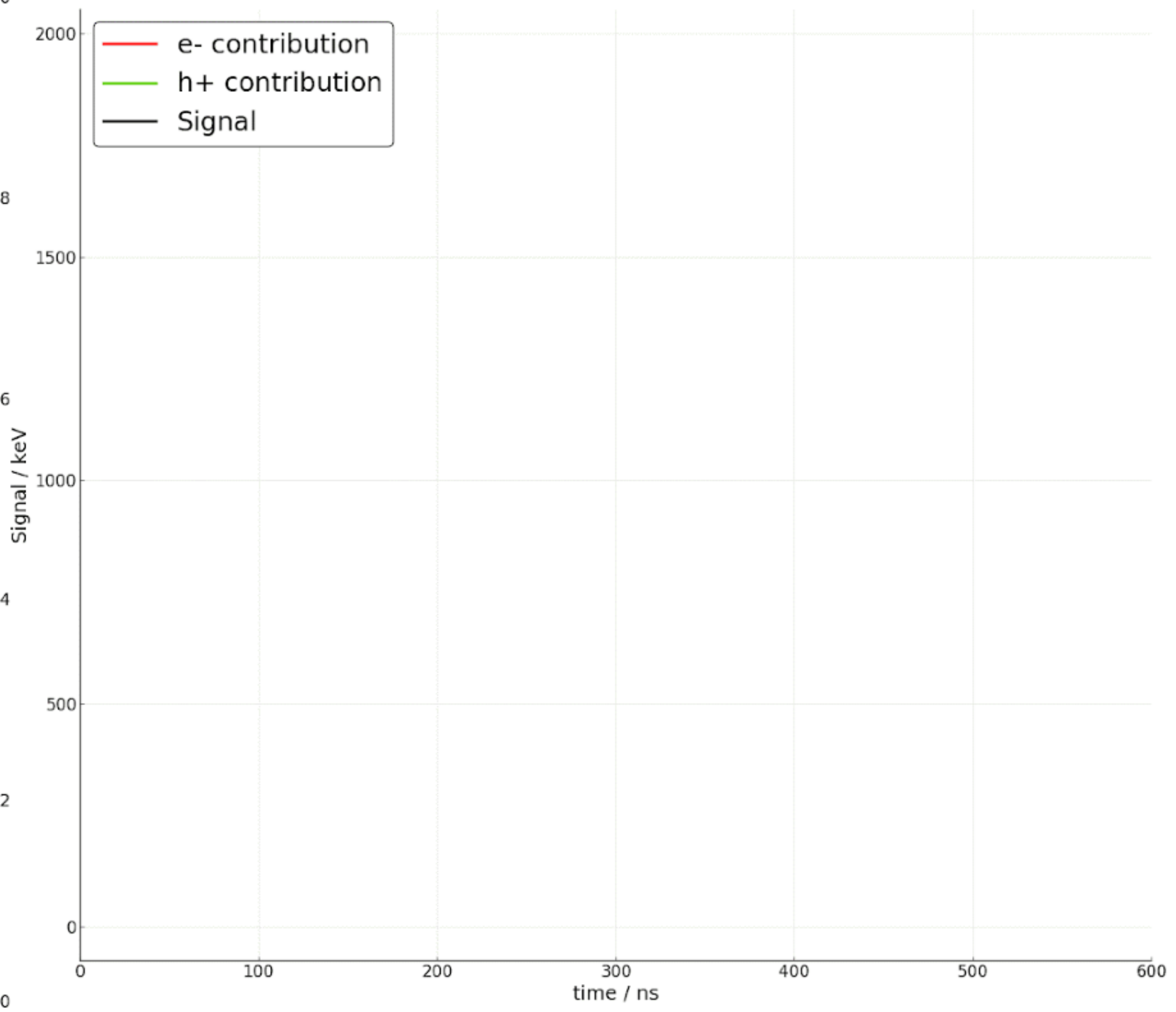


P-type Point Contact Detector

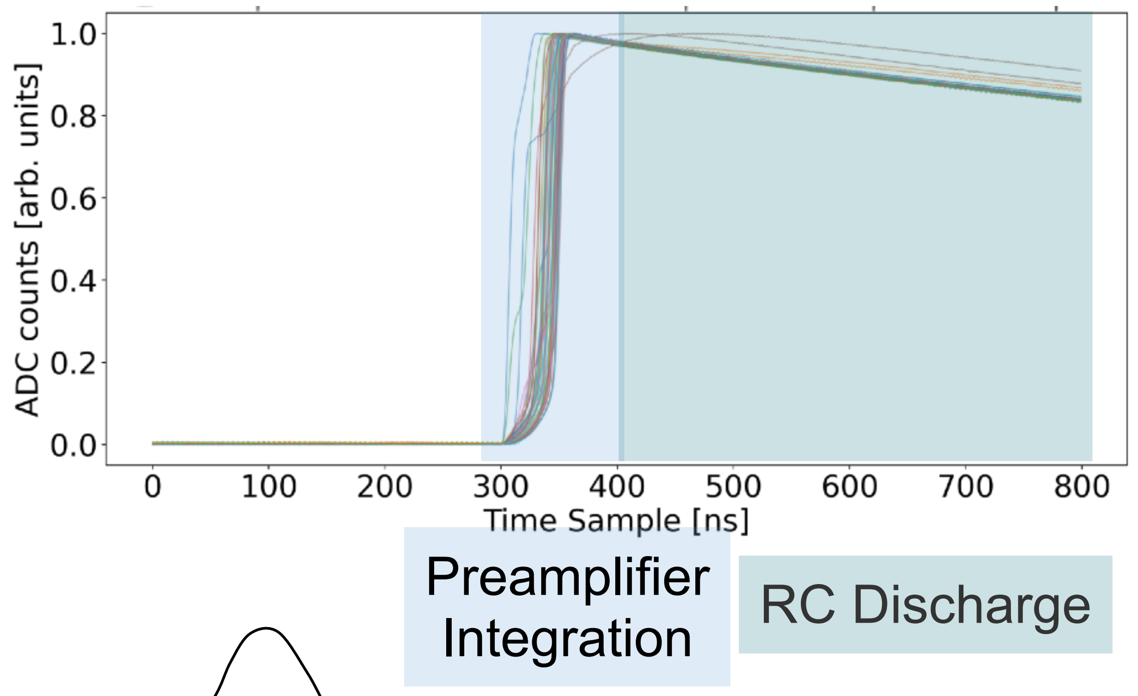
- Signal cable
  ➡Less background
- Small p-contact
  ➡Low capacitance
  ➡Less noise
- Thick dead layer
  ➡Less alpha and beta events
- Lower bias voltage
- Bigger detectors
- Smaller surface to volume ratio

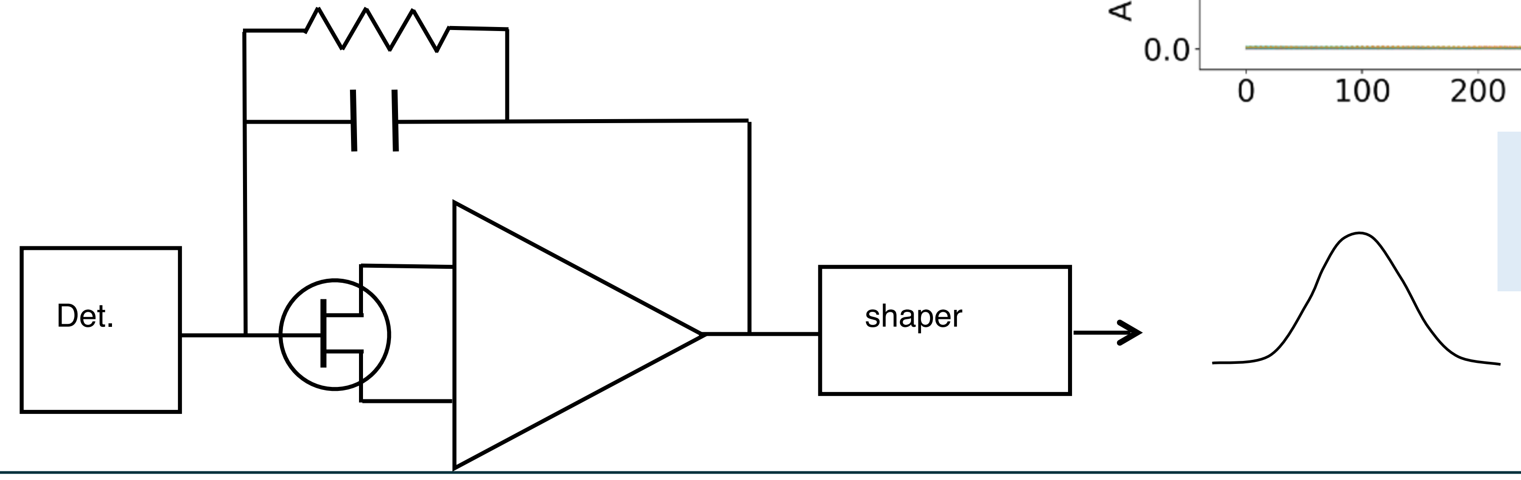
- Incident ionizing radiation creates electron - hole pairs ∝E
- e^- and h created in the depletion region move to the respective electrodes → **detectable current**

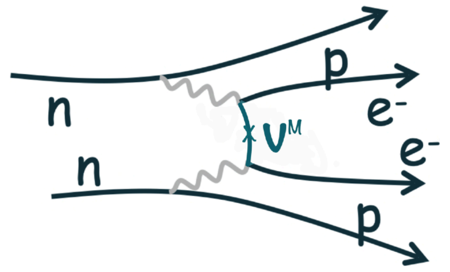




- Charge drift & signal formation by using Shockley-Ramo Theorem: Charge induced on given electrode by motion of charge carriers
- Resulting signal convoluted with the electronic response function (detector-channels-wise)







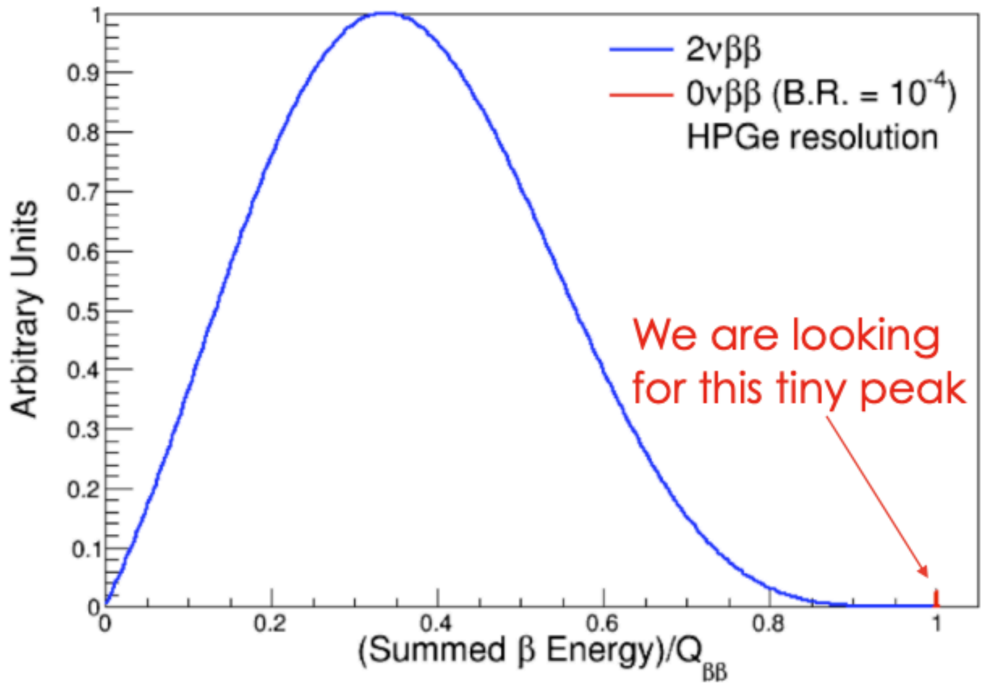
$\Delta L \neq 0$

Bayesian Inference and UQ for 0νββ decay

Experimental goal is to measure mono-energetic peak at Q$_{bb}$

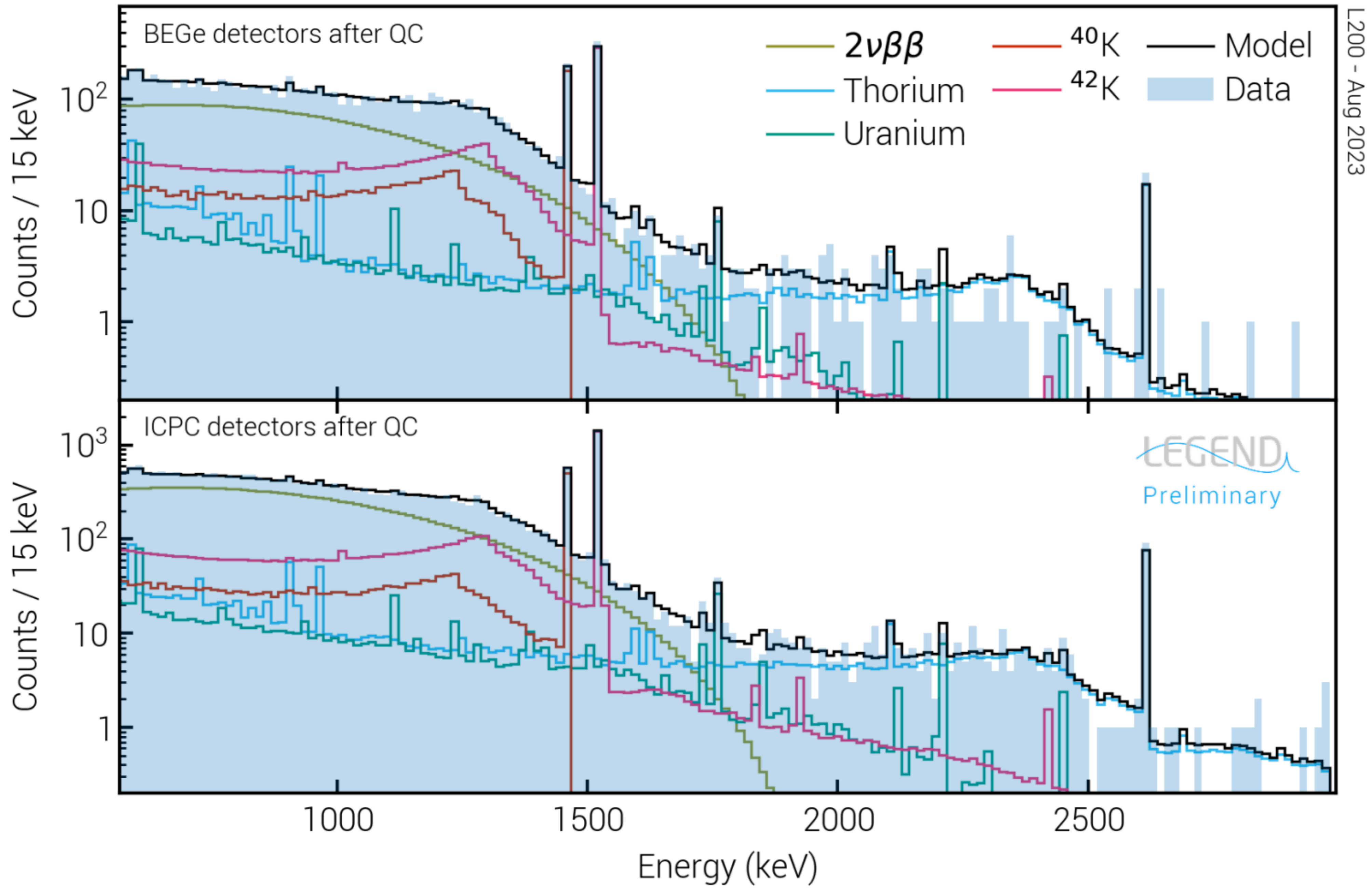
$$0\nu\beta\beta : (\mathbf{A}, \mathbf{Z}) \rightarrow (\mathbf{A}, \mathbf{Z}+\mathbf{2}) + \mathbf{2e^-}$$

Experimental sensitivity: background (BI) > 1 $T^{0\nu}_{1/2} \propto \varepsilon \cdot a \cdot \sqrt{\frac{M \cdot t}{BI \cdot \Delta E}}$

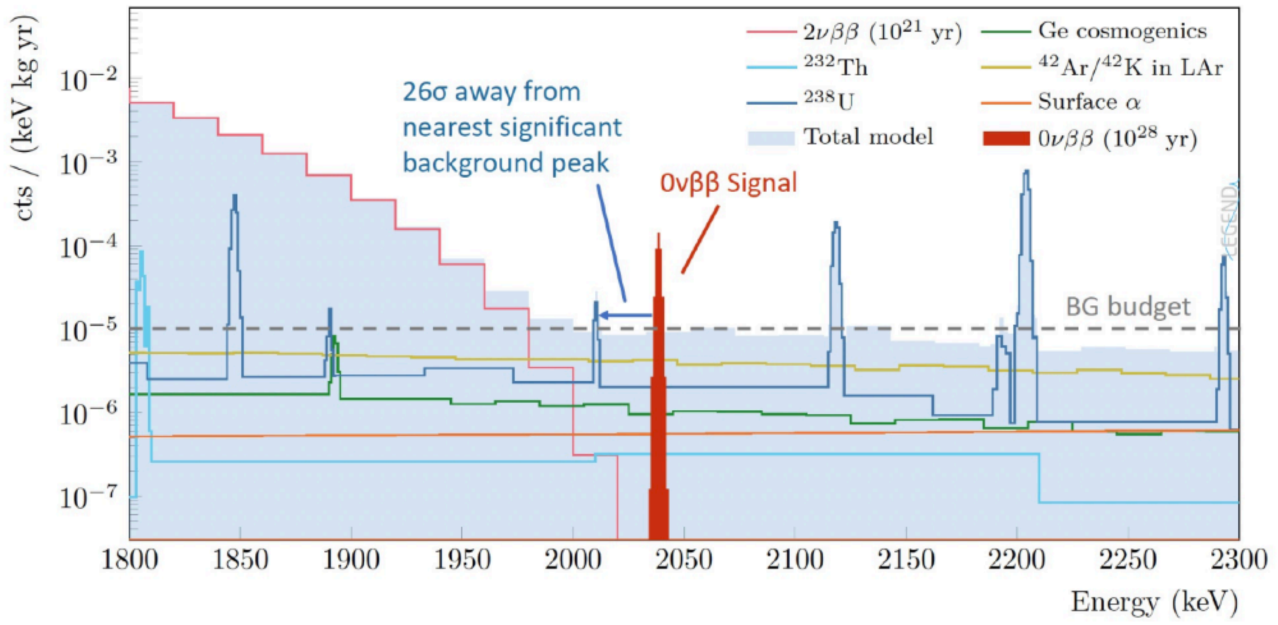


measure sum energy spectrum of electrons

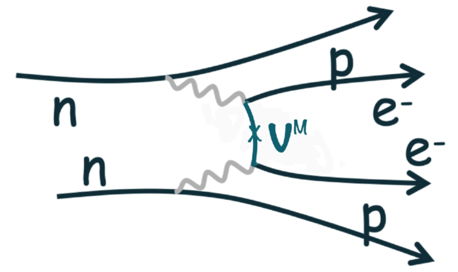
- 2vββ ➞ continuum
- 0vββ ➞ mono-energetic peak @ $Q_{\beta\beta}$



But this signal is buried under other backgrounds…



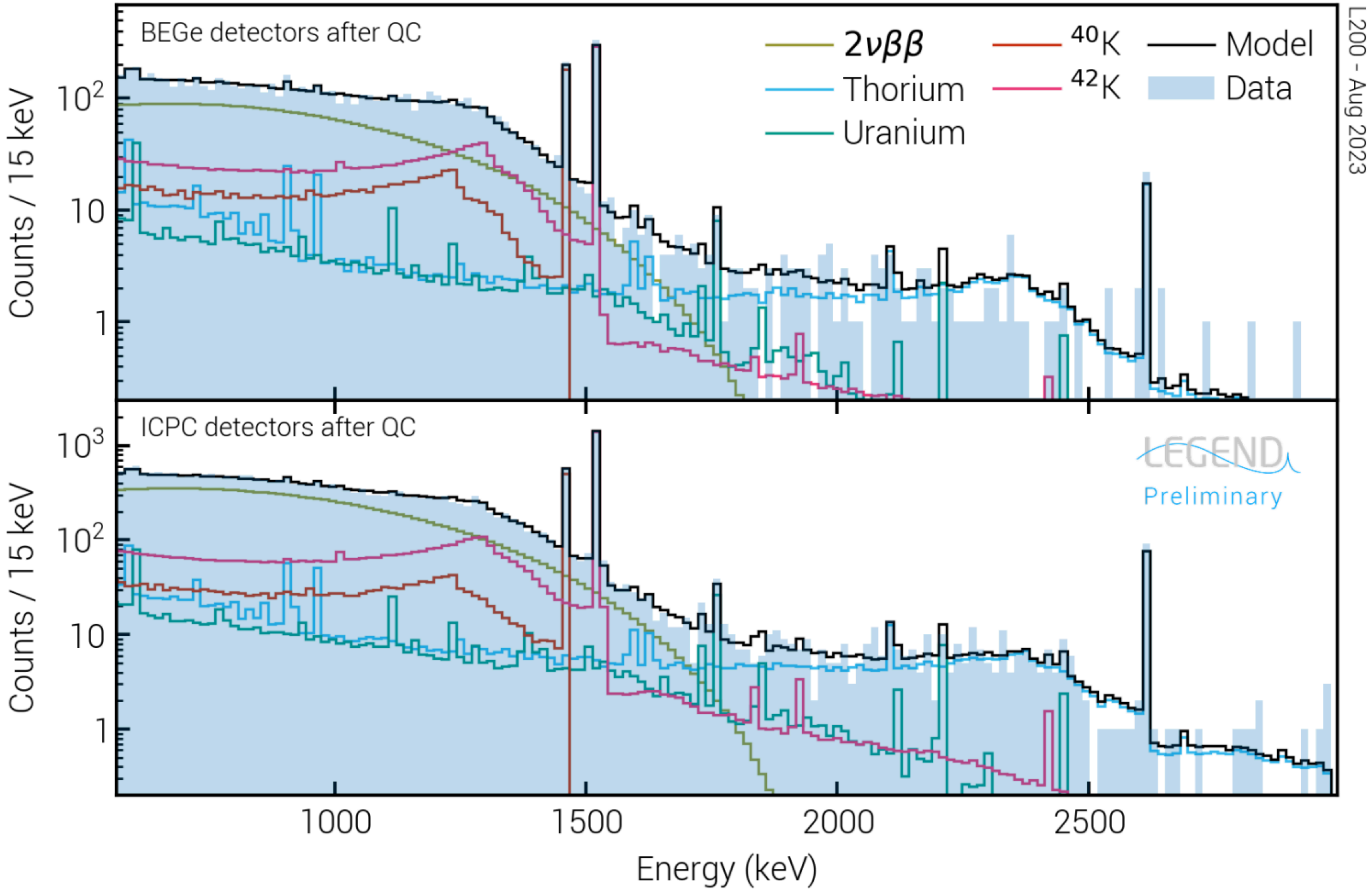
→ increase sensitivity by **background reduction (BI)** at $Q_{\beta\beta}$ and simultaneous increase of mass (M) and improvement of the energy resolution (ΔE)

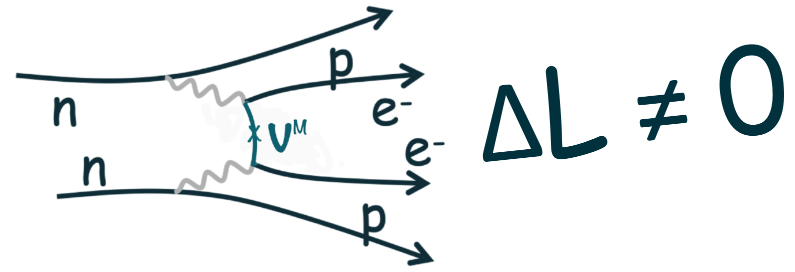


Background Decomposition

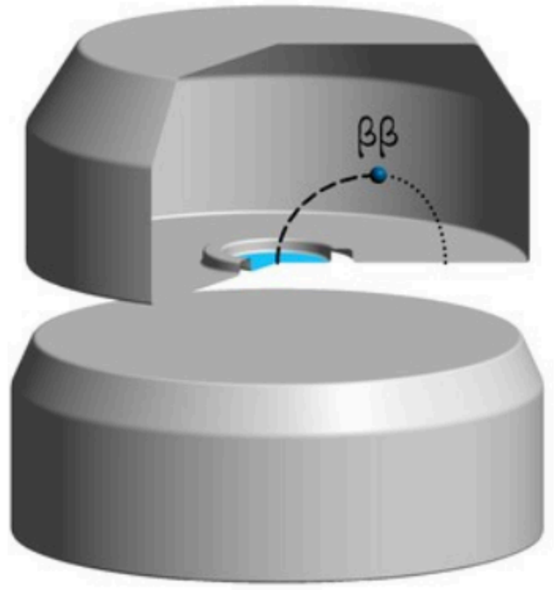
Decomposition before analysis cuts

- Well described by expected contributions with current statistics



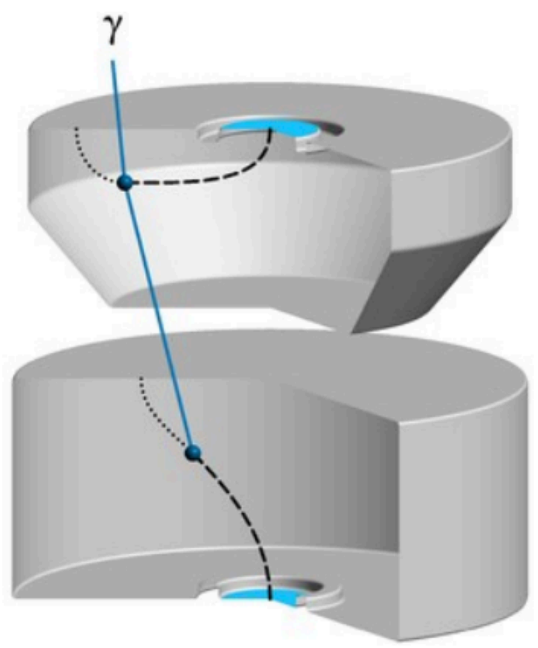


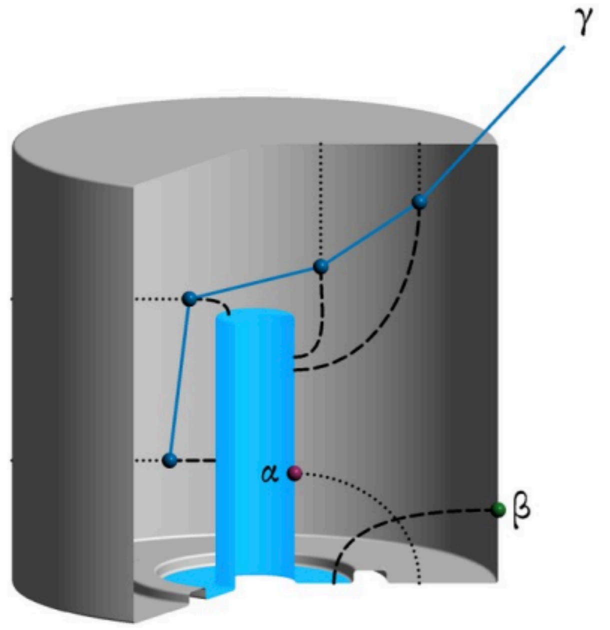
Background reduction



Signal-like events (0νββ/ 2νββ events)
local energy deposit in single detector

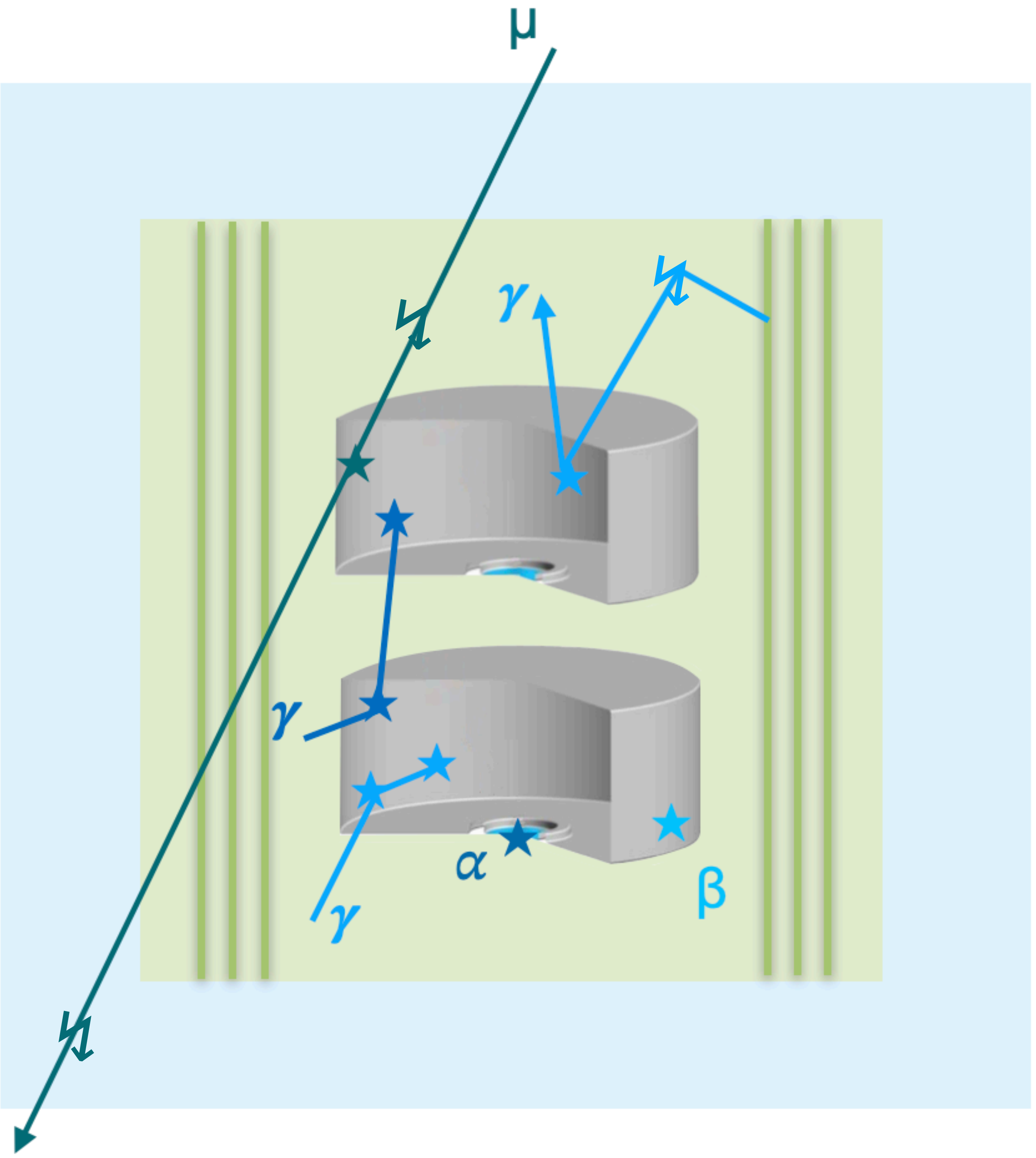
(1) Background events (γ events)
coincident energy deposition in more than one detector
→ detector anti-coincindence



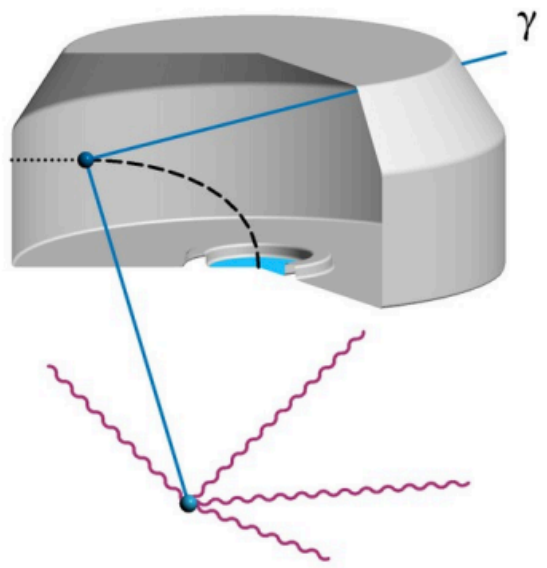


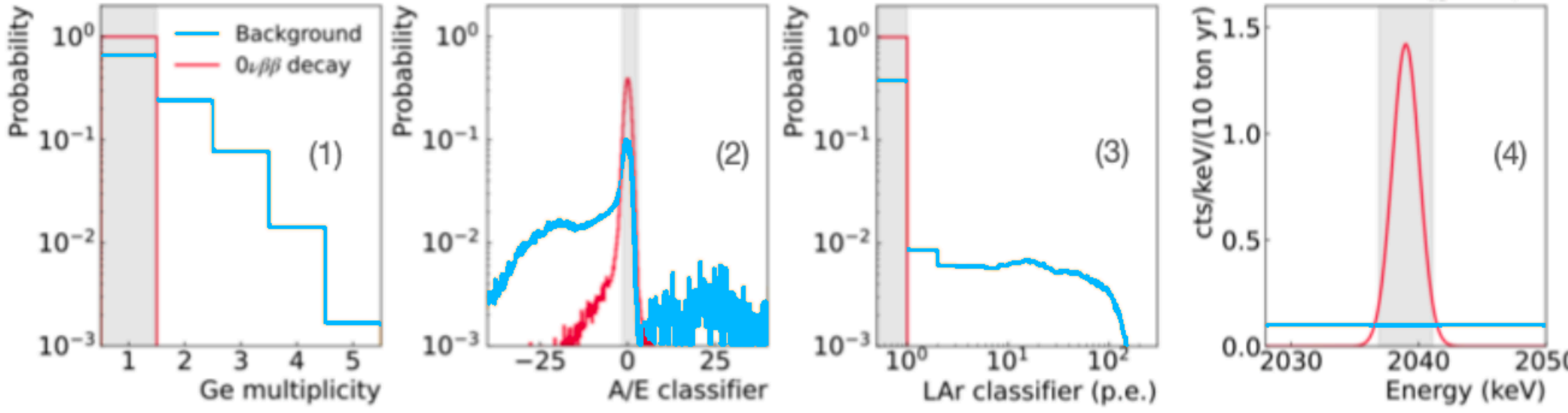
(2) Background events (γ events)
deposition in multiple locations (MSE)
→ PSD (analysis of time profile of current signal)

Surface events (α/β events)
energy deposited on or close by the detector contacts
→ PSD (short (p+) or long (n+) current pulse)



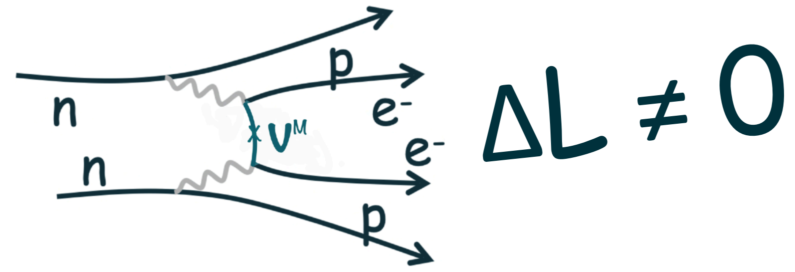
(3) Background events (γ events)
additional energy deposition in LAr
→ LAr veto



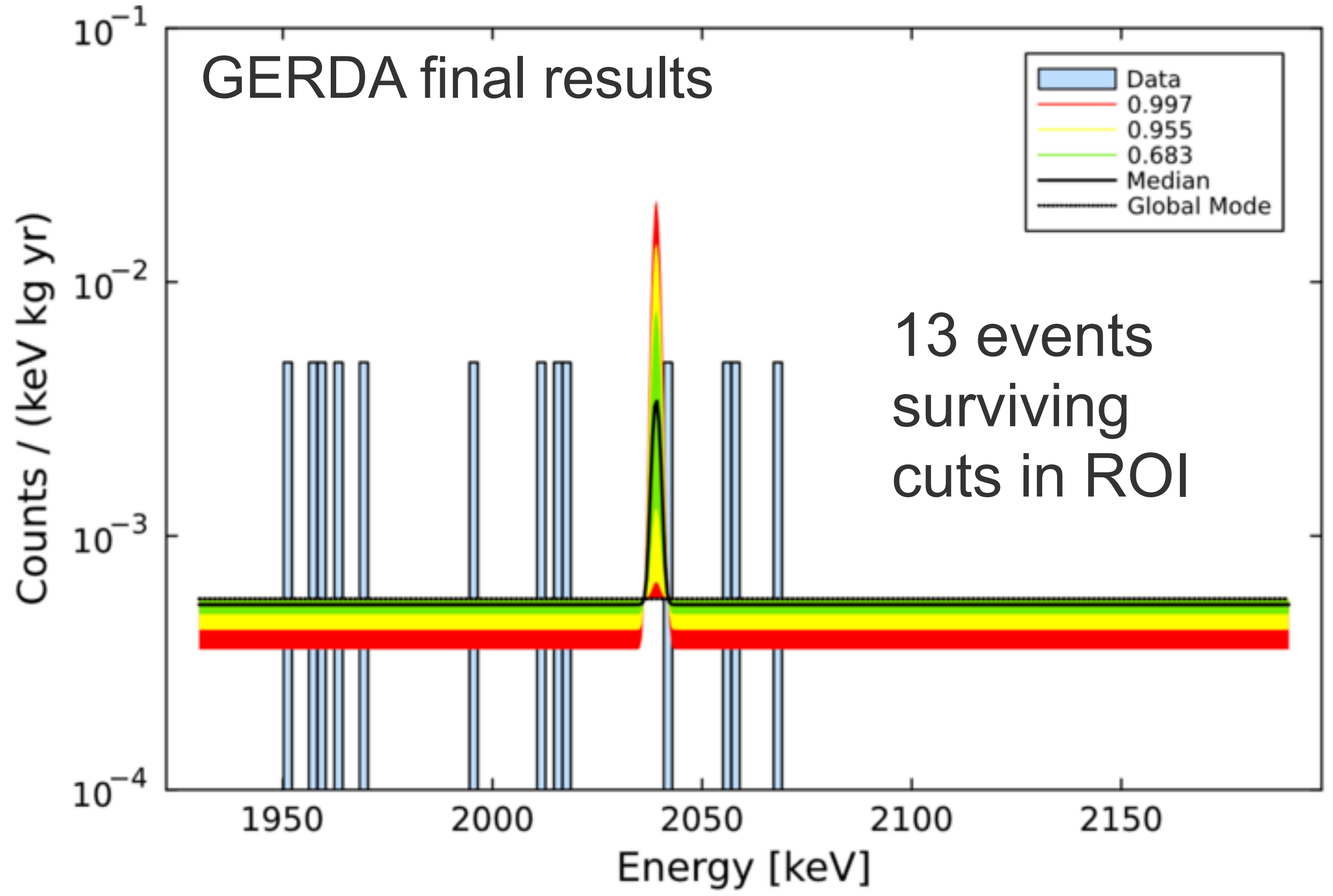


Energy resolution:

all backgrounds with continuous energy



Bayesian Inference and UQ for 0νββ decay



Example GERDA/ L200 commissioning:
< 10 detector datasets (< 20 cts in all datasets)
$Q_{\beta\beta}$, σ_i, μ_i^B, μ_i^S
→ < 50 nuisance parameters

LEGEND-1000: 10x detector channels
~ 100 measurement campaigns
~ 150 detector datasets
$Q_{\beta\beta}$, σ_i, μ_i^B, μ_i^S
→ 10^5-10^6 nuisance parameters

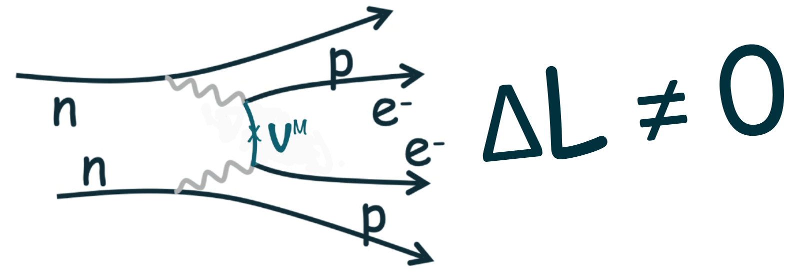
The total likelihood is constructed as the product of all $\mathcal{L}_i$ weighted with the Poisson term:

$$\mathcal{L} = \prod_k \left[\frac{(\mu_{s,k}+\mu_{b,k})^{N_k} e^{-(\mu_{s,k}+\mu_{b,k})}}{N_k!} \times \prod_{i=1}^{N_k} \frac{1}{\mu_{s,k}+\mu_{b,k}} \times \left(\frac{\mu_{b,k}}{\Delta E} + \frac{\mu_{s,k}}{\sqrt{2\pi}\sigma_k} e^{-\frac{(E_i-Q_{\beta\beta})^2}{2\sigma_k^2}} \right) \right]$$

Poisson weight
Flat background
Gaussian signal
Expected counts

where:

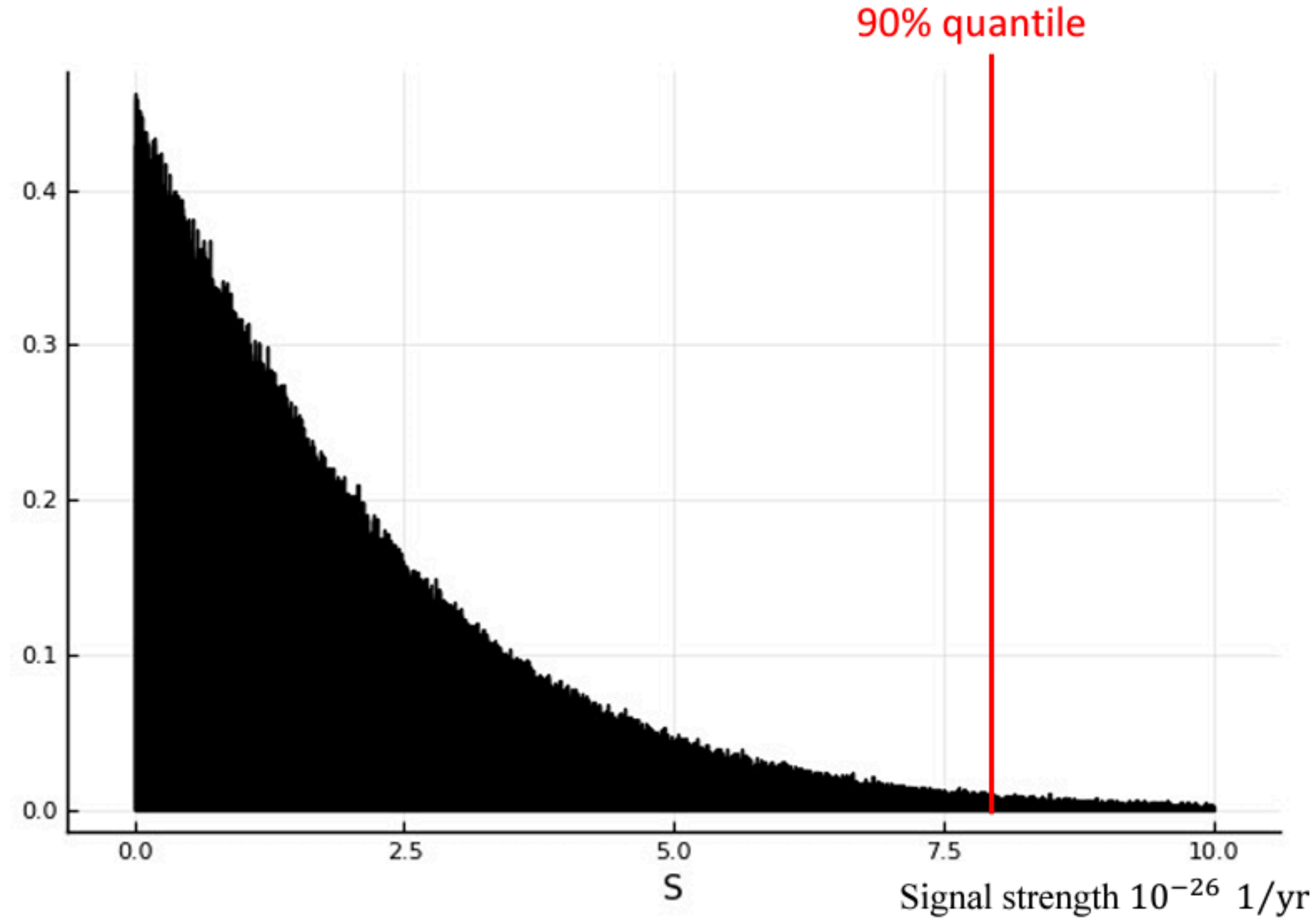
- N_k total number of events observed in the ith partition
- E_i individual event energies in the ith partition
- $\sigma_k = FWHM_i/(2\sqrt{2ln2})$: energy resolution in ROI
  - the average FWHM across partitions is $3.29\ keV$



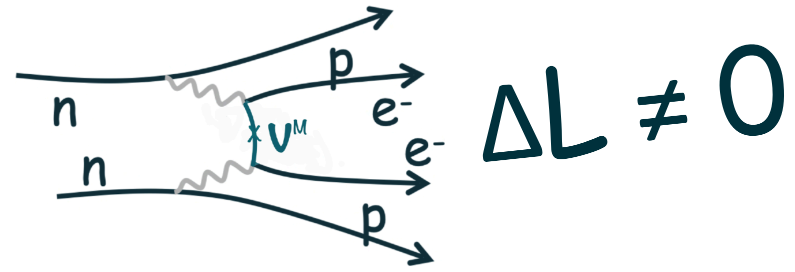
Models for the Signal strength

There are 2 different priors on the signal strength $S = \frac{1}{T_{1/2}^{0\nu}}$ (which ranges from 0 to 10^{-24} $1/\mathrm{yr}$):

- $p(S) \sim Uniform$
  - equiprobable signal strengths
- $p(S) \sim \frac{1}{\sqrt{S}}$
  - equiprobable Majorana neutrino masses $m_{\beta\beta}$
  - $S \propto m_{\beta\beta}^2$



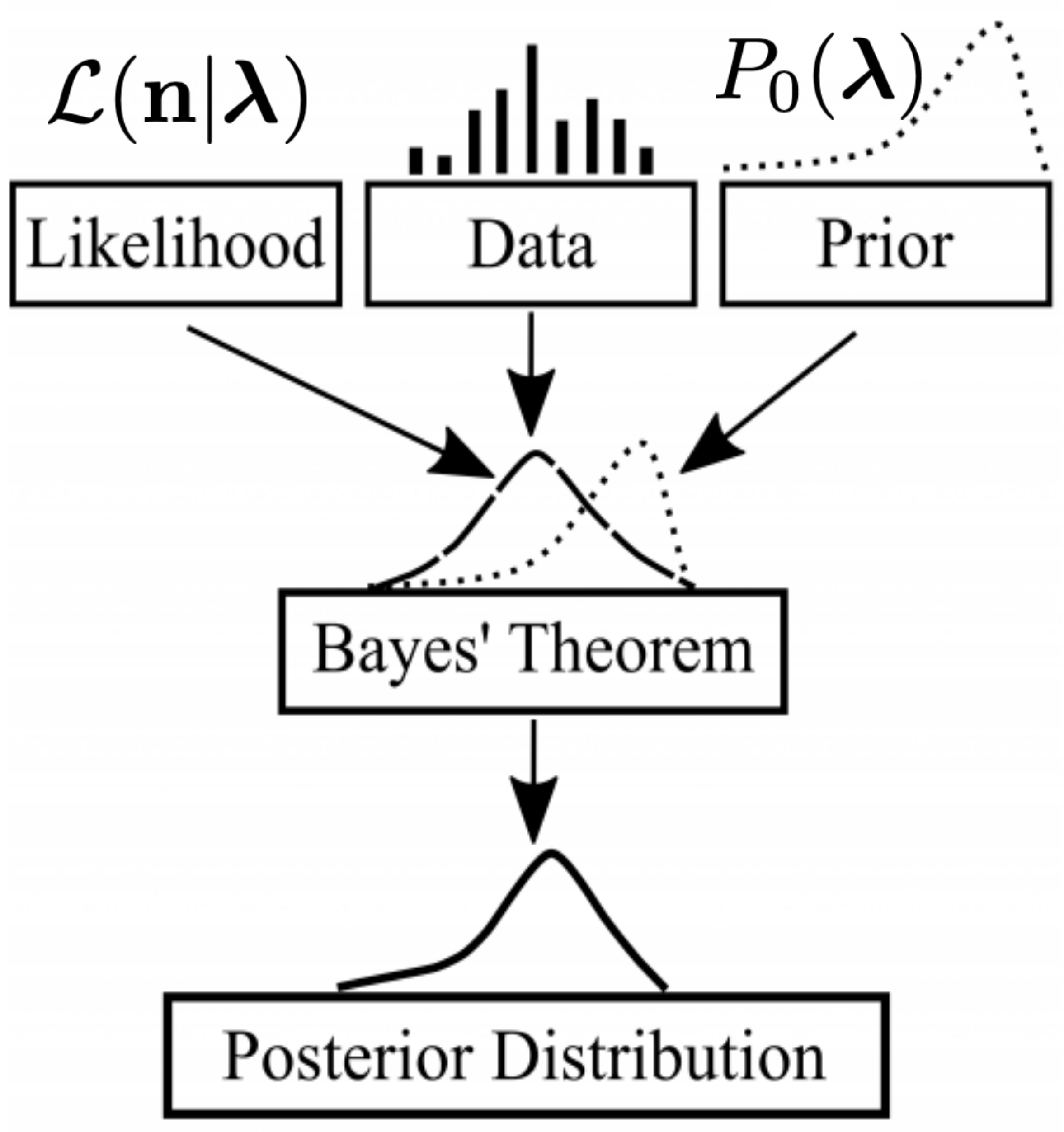
Get limit at 90% C. I. from posterior distribution of S



Limitation MCMC sampling

Limitation: High dimensional parameter space:

- Metropolis-Hastings sampling with random walk → expensive
- gradient-based sampling like Hamiltonian Monte Carlo → slow for high dimensional correlations

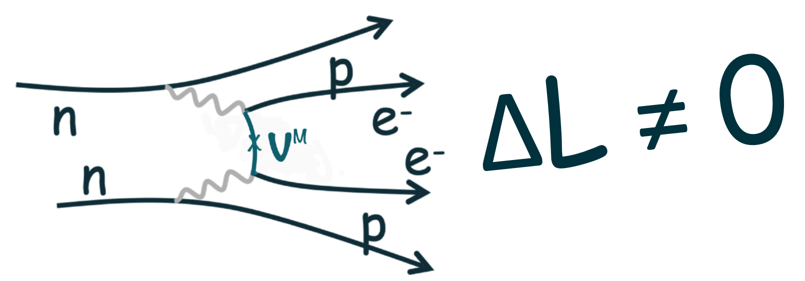


$$P(\boldsymbol{\lambda}|\mathbf{n}) \propto P(\mathbf{n}|\boldsymbol{\lambda})P_0(\boldsymbol{\lambda})$$

How can we address MCMC sampling limitations?

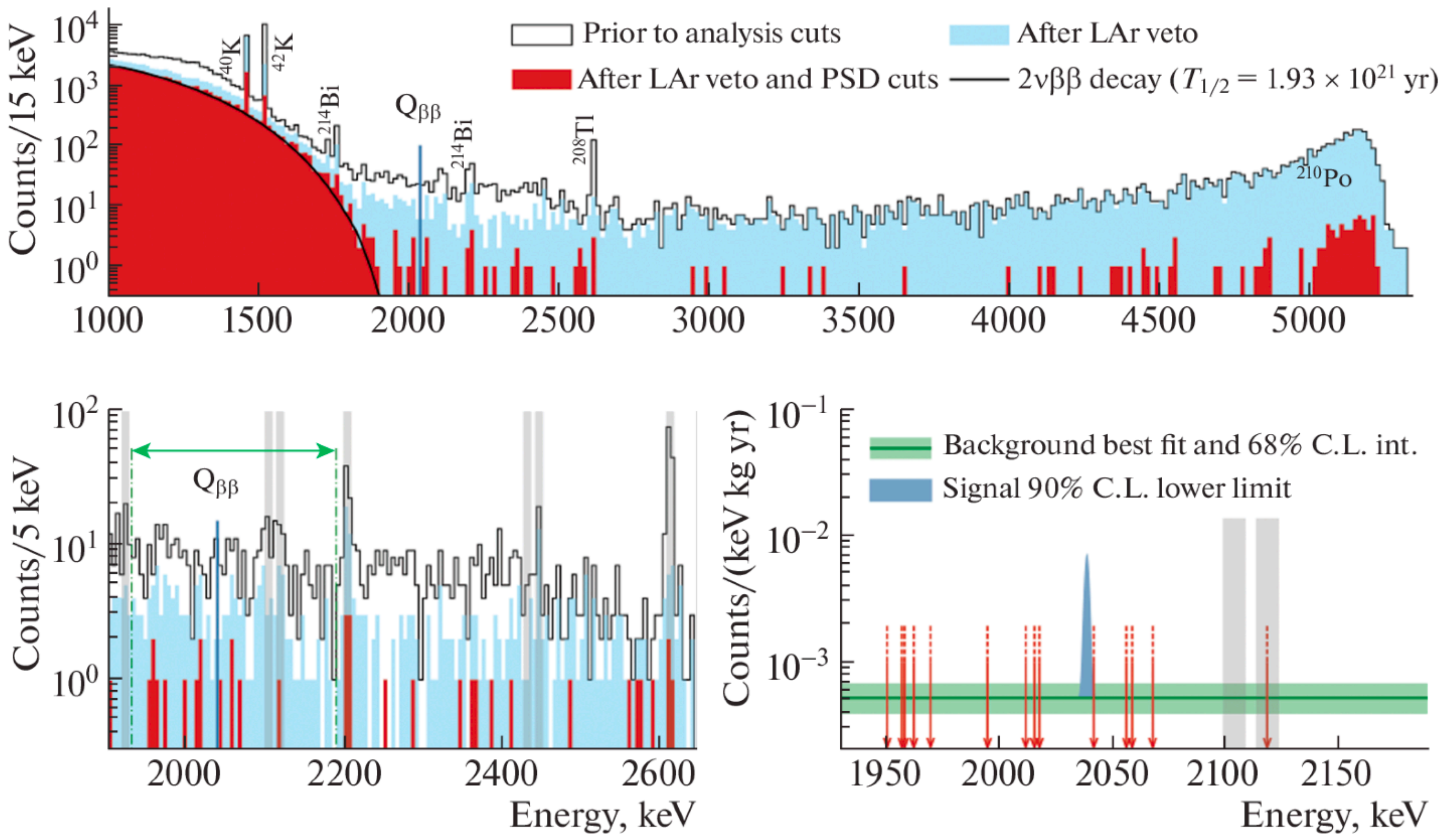
Ideas:

- GP surrogates for Bayesian inference [arXiv:1809.10784] → *physics posteriors densities mostly non-gaussian with tails*
- Variational Bayesian Monte Carlo with Noisy Likelihoods
- Hamiltonian Monte Carlo
- Langevin Monte Carlo with modifications
  - LMC (w/o MH adjusted)
  - Random coordinate descent LMC → *Is the gradient less expensive to calculate?*
  - Deterministic LMC with Normalizing Flow [arXiv:2205.14240] (proposed by Uroš Seljak)
  - LMC underdamped
- NN which learns the conditional probability (posterior) [arXiv:2006.02369] → *potential large uncertainty?*
- Sampling with support points [arXiv:1609.01811]
- Dimension reduction by embedded (sub-)structures/ correlations

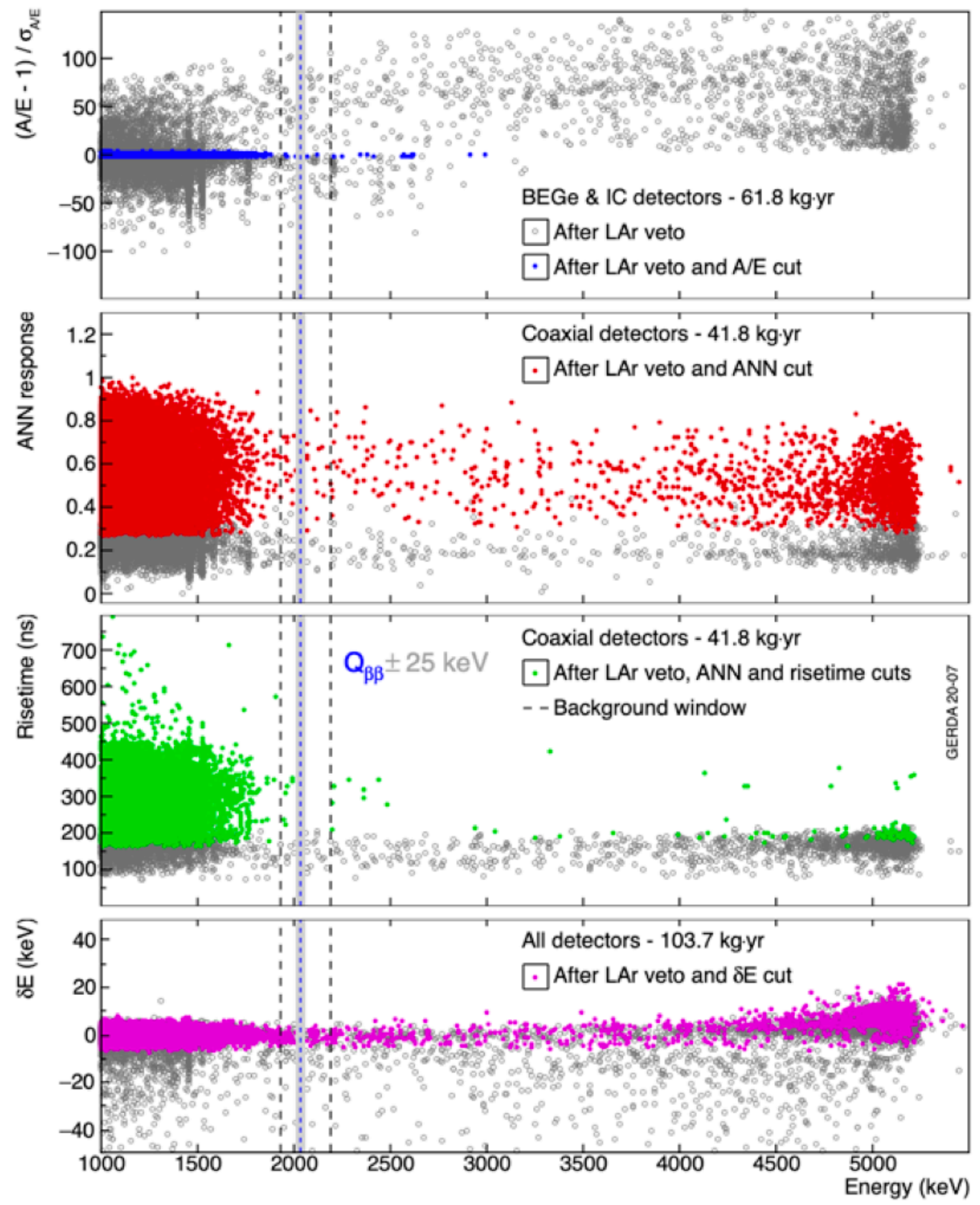


Extended Bayesian Inference and UQ for 0νββ

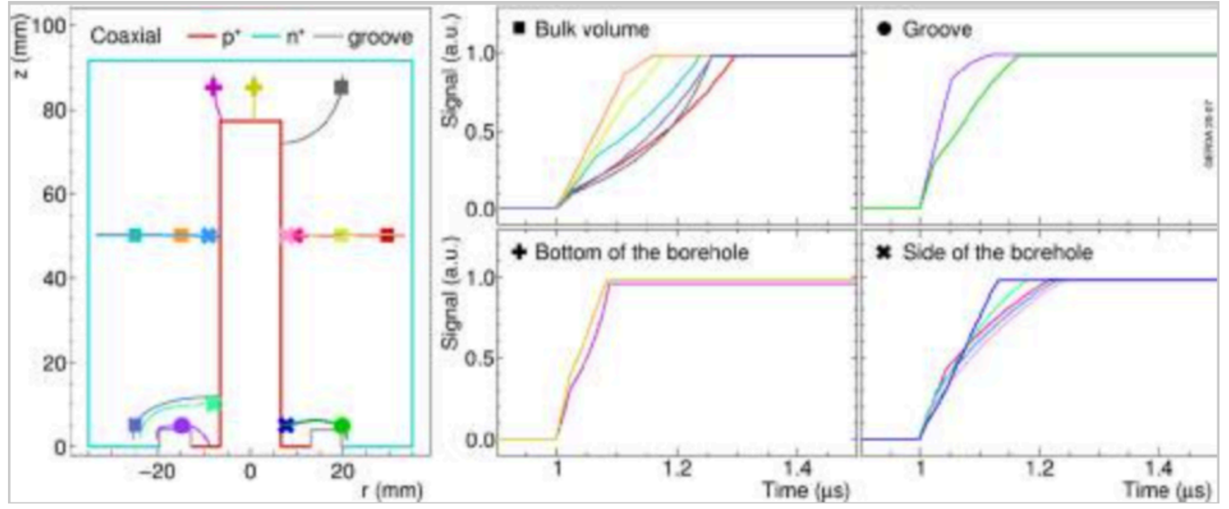
So far, background rejection based on single pulse shape/ veto parameters prior to spectral fit



Correlations are everywhere!

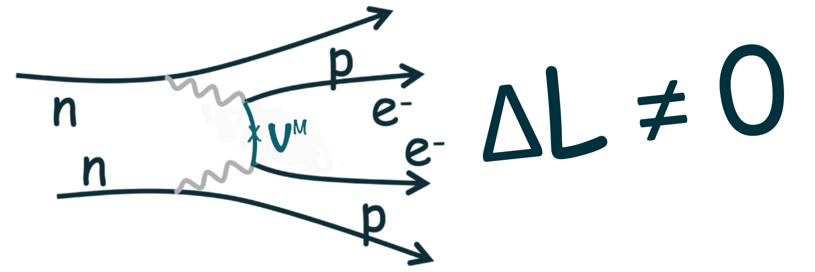


Pulse shape analysis: analysis of the time profile of individual pulses used to reject different backgrounds by a single parameter



Goal: model which incorporates additional informations into the likelihood (e.j. PSD, veto signals,…) indicating the background probability of an event

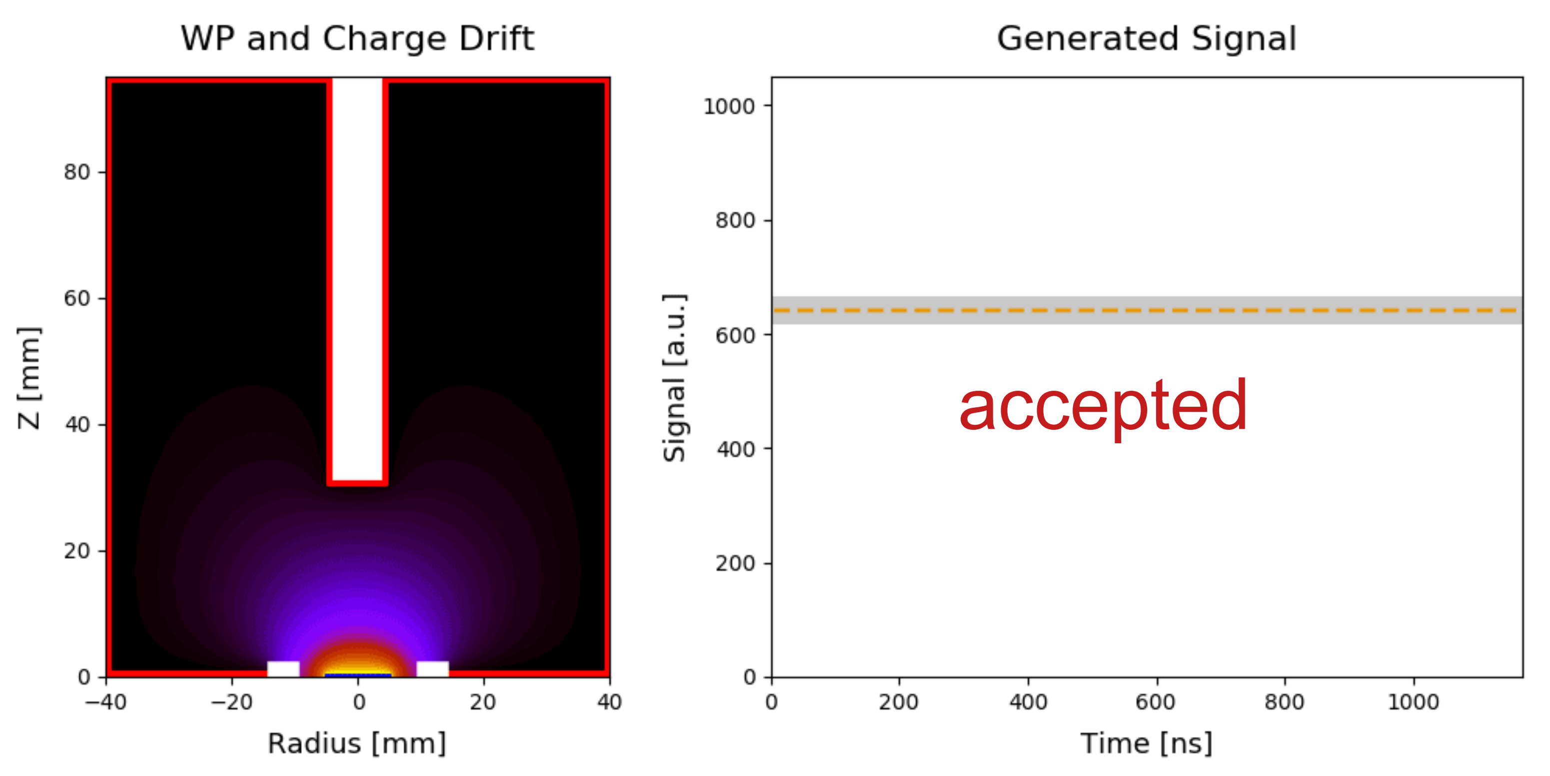
Questions:
- **How to integrate PSD simultaneously for all type of pulse shapes?**
- **How would the mathematical formulation of the fit look like?**



Background rejection in point contact HPGe

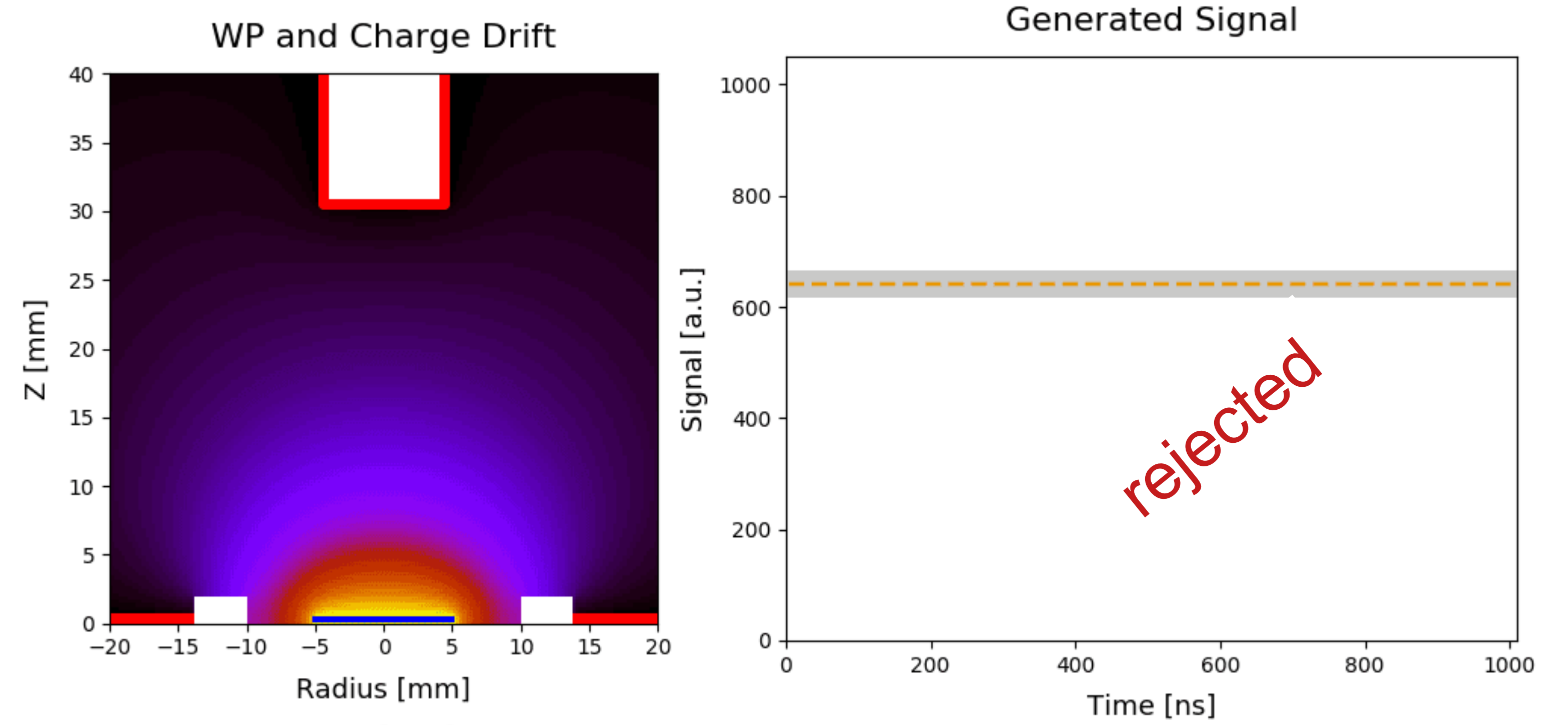
Weighting Potential and Charge Drift

0νββ signal candidate (single-site)

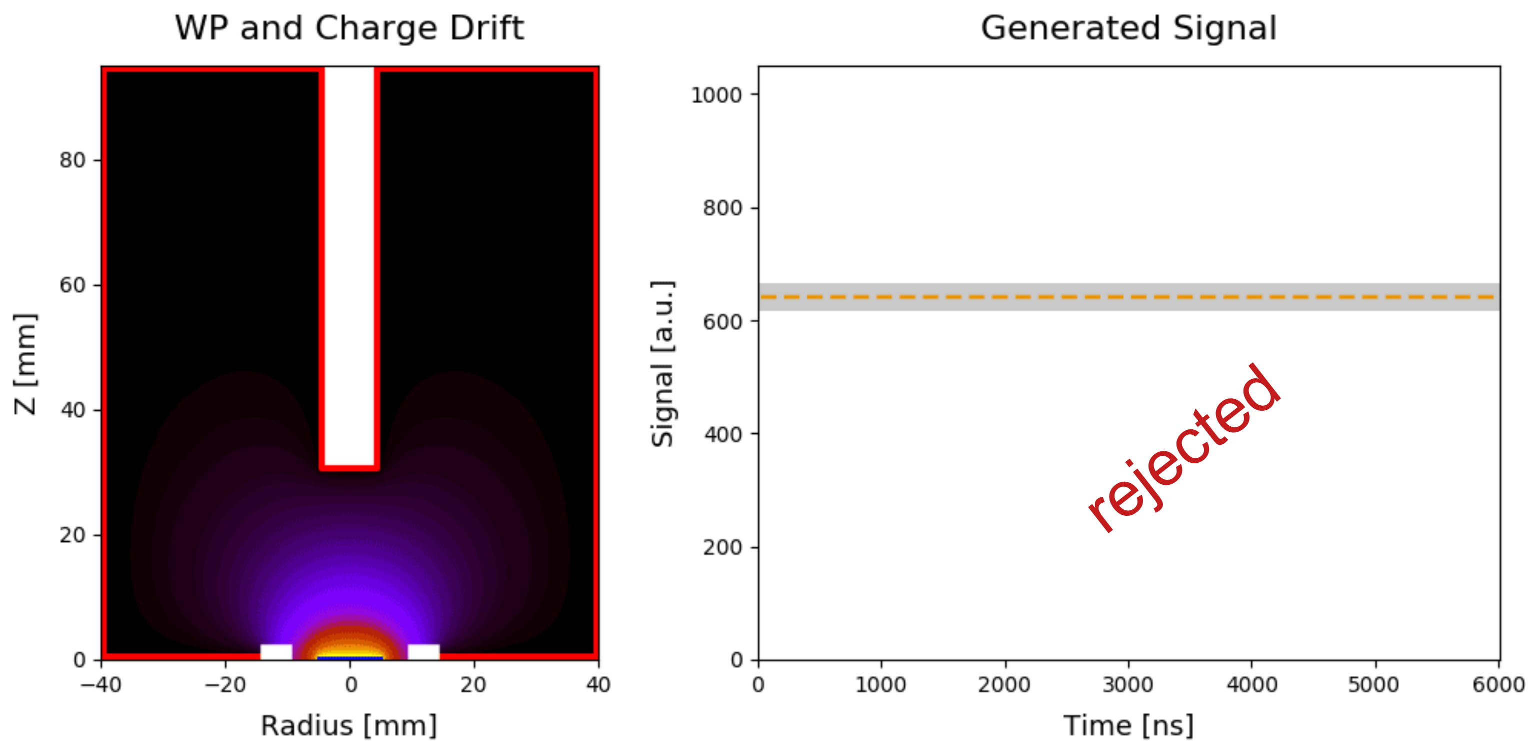


- Charge signal - Current signal

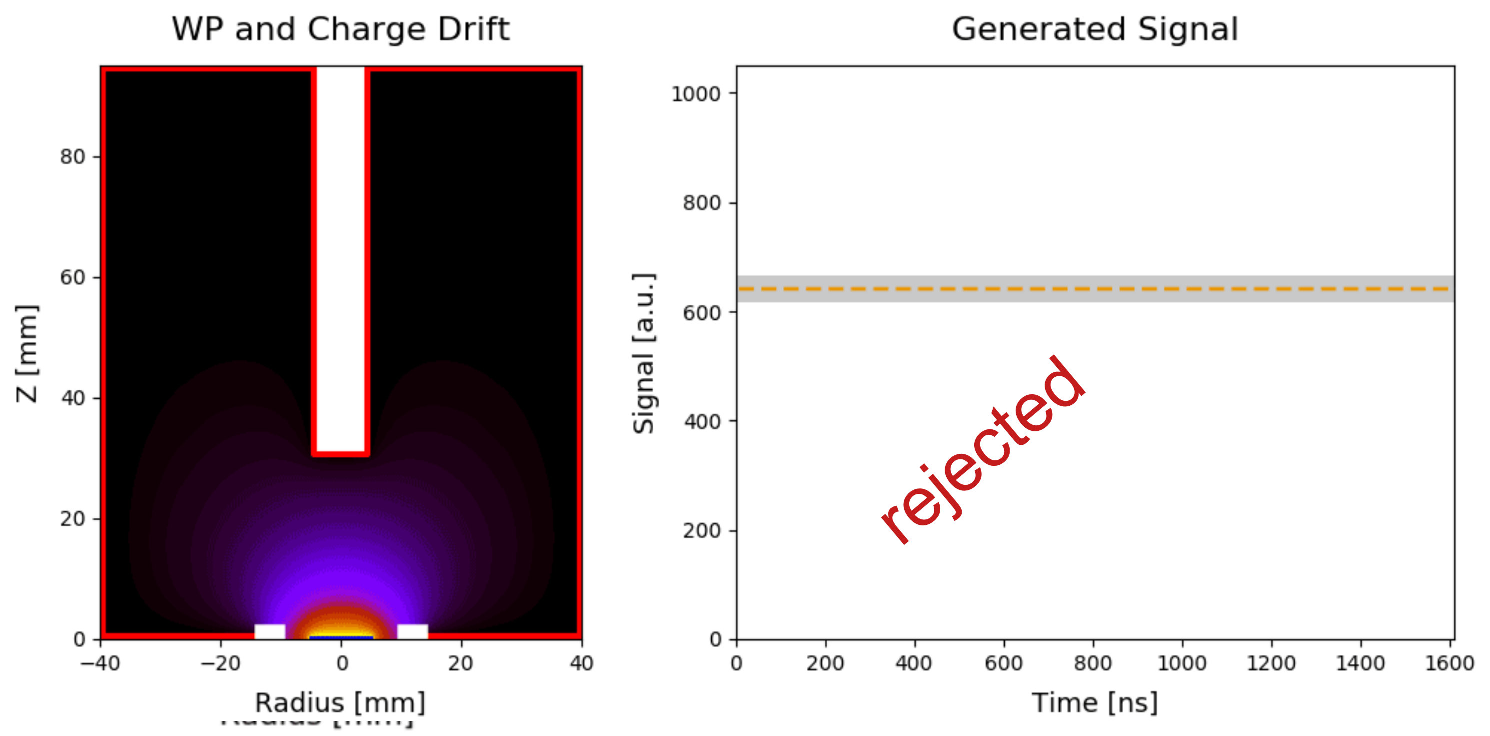
α-background on p+ contact

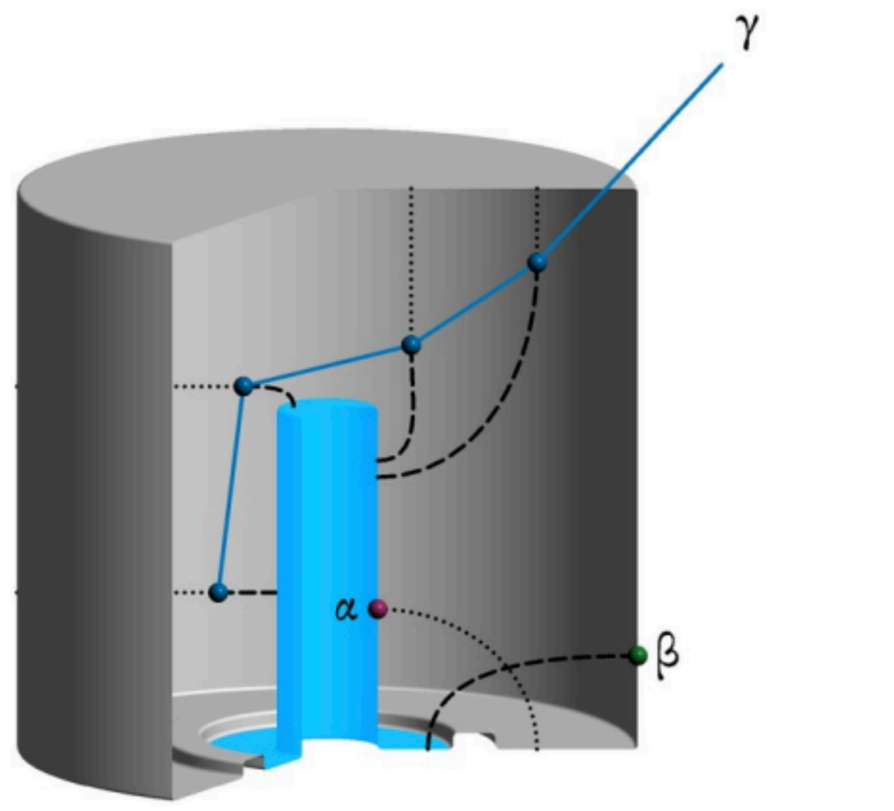


Surface-β-background ^{42}K (^{42}Ar) on n+ contact

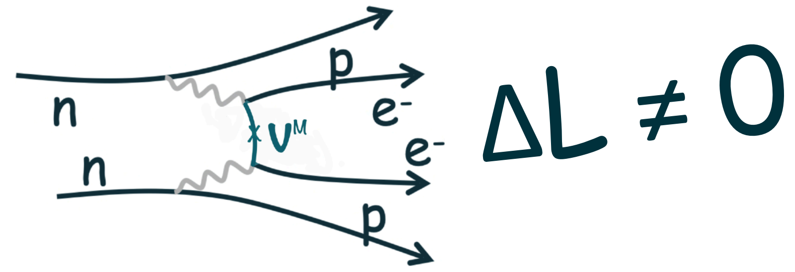


γ-background (multi-site)





- amplitude of current pulse is suppressed for a **multi-site event** compared to a **single-site event** of the same event Energy
- comparing **A against E** effectively rejects multi-site backgrounds
- various powerful PSA event topology tools can be used to reject different backgrounds
- alternative machine learning algorithms are available

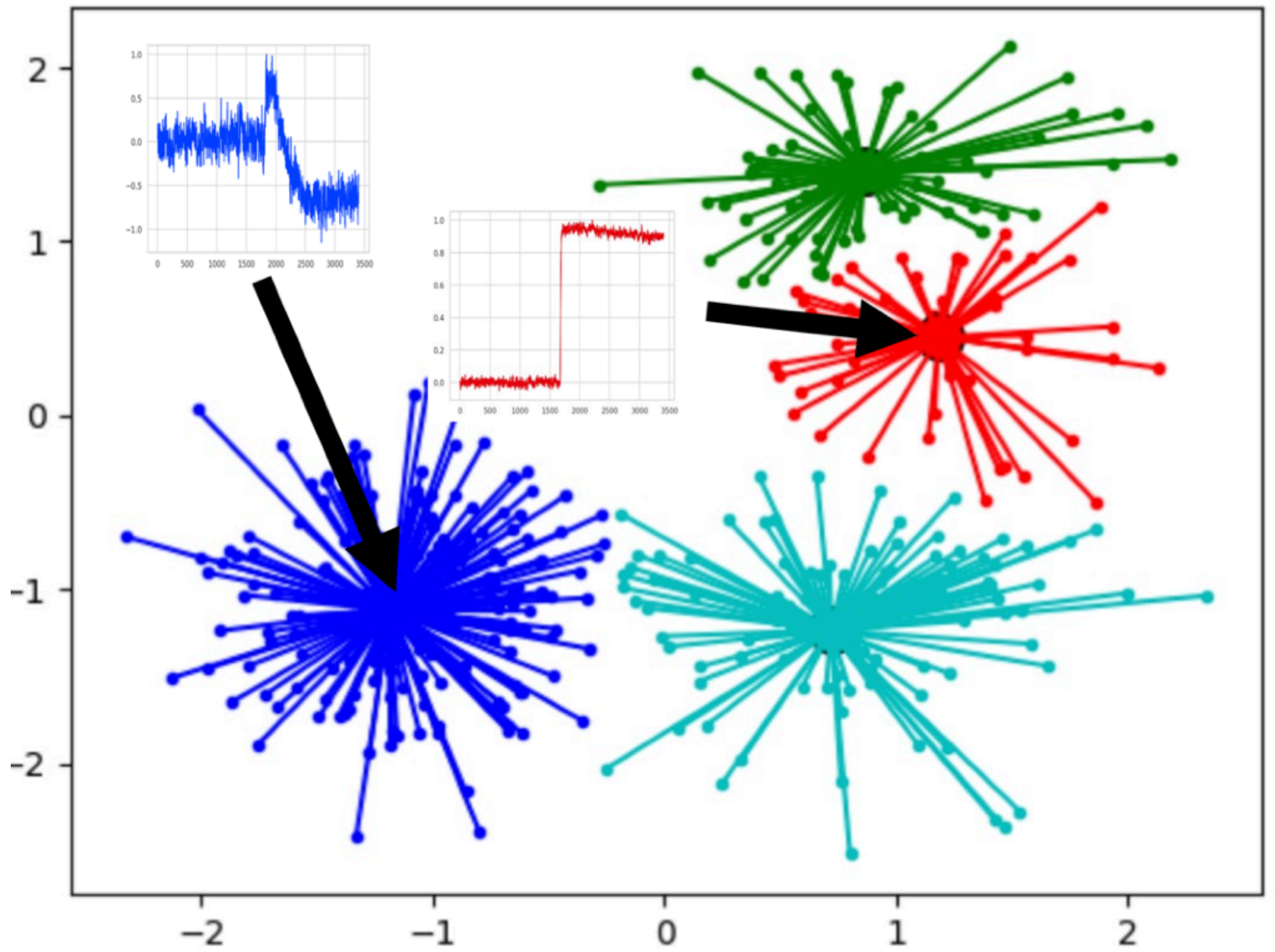


PSD Extended Bayesian Inference0νββ decay

Can we integrate PSD and veto signals?

Find a tool analogue to LEGEND ML Data Cleaning using actual physics waveforms with
→ probability of waveform classification to the categories shown before
+ uncertainty estimation

Extract pulse shape information from waveforms → **Group and label similar waveforms using an unsupervised learning classifier**



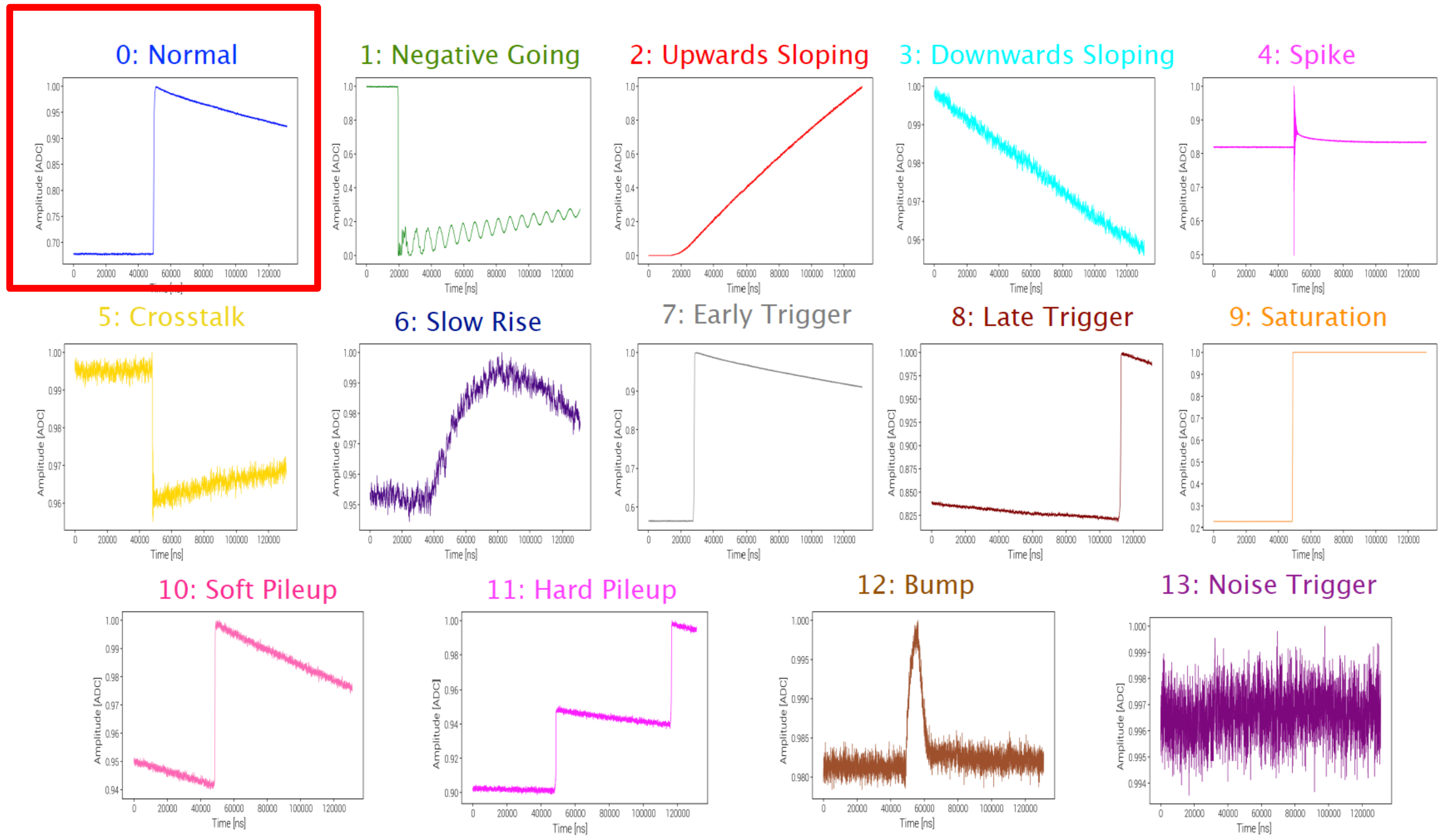
Advantages of ML Data cleaning method over traditional analysis:

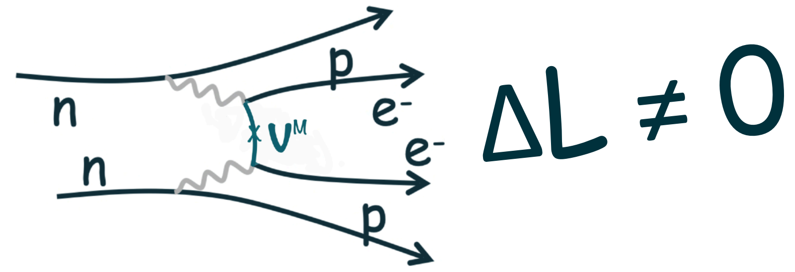
- Adapts to changing run conditions
- Allows ID of new populations during commissioning
- Could improve separability by using more waveform information

Disadvantages

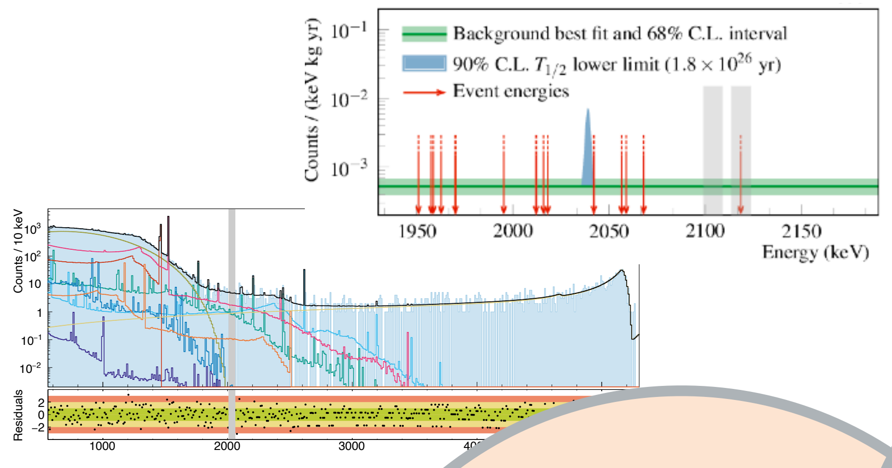
- **no uncertainty estimation**
- **Classification 0 or 1 for class identity**

waveform of a physical event





Bayesian parameter estimation and uncertainty quantification in Nuclear Science with focus on (Double) Beta decay



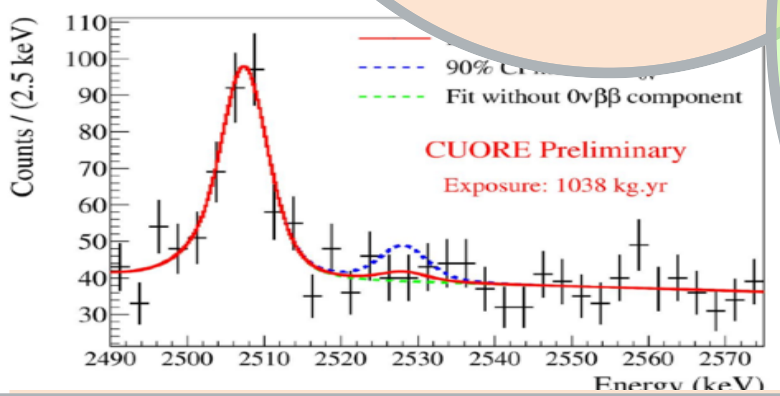
0nbb decay

LEGEND

LEGEND Background model

spectral fit with pdfs over several sub-datasets

CUPID

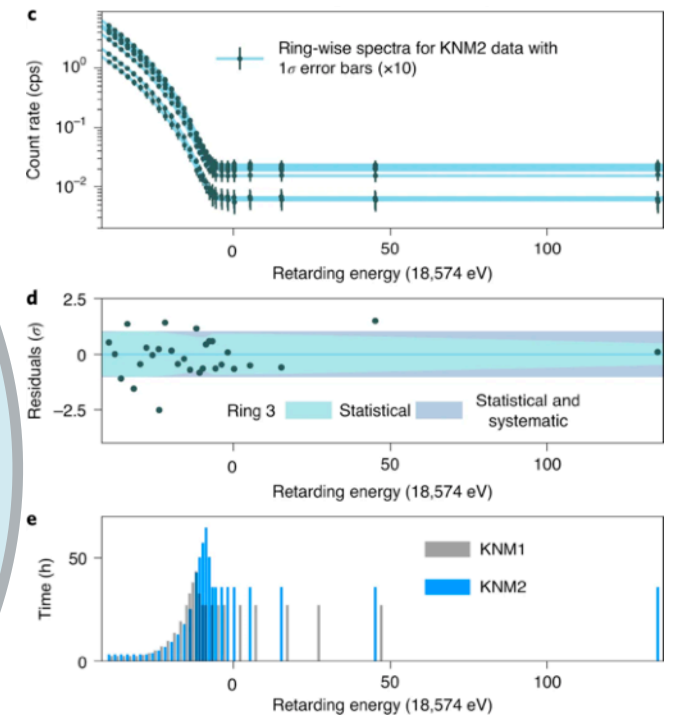


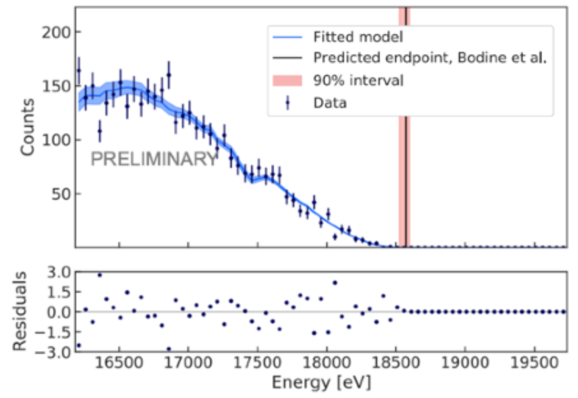
Beta decay - Neutrino mass

KATRIN

spectral modeling of the beta decay with all associated detector systematics

Project8



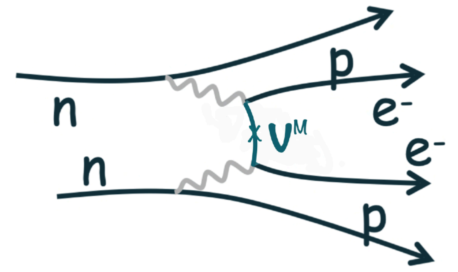


Bottlenecks:
- Increase of sub-datasets
- Marginalization over $O(10^6)$ nuisance parameters describing detector systematics and bkg

Need:
- More performant parameter estimation tools and analysis strategies that will handle large datasets
- fit which incorporates additional informations into the likelihood (psd, veto signals,…

Bottlenecks:
- increasingly high dimensional data due to large number of detector systematics
- “Long" calculation time of detector response time

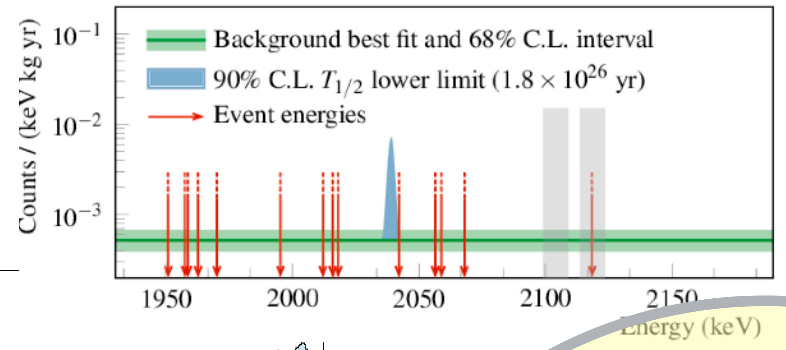
Need:
- differentiable model
- improved sampling tools e.j. gradient-based sampling
- multi-fidelity ML techniques

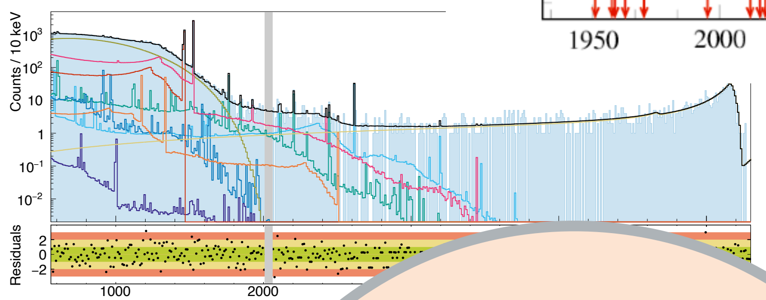


Bayesian parameter estimation and uncertainty quantification in Nuclear Science with focus on (Double) Beta decay

Neutrinoless double beta decay

Beta decay - Neutrino mass





LEGEND Background model

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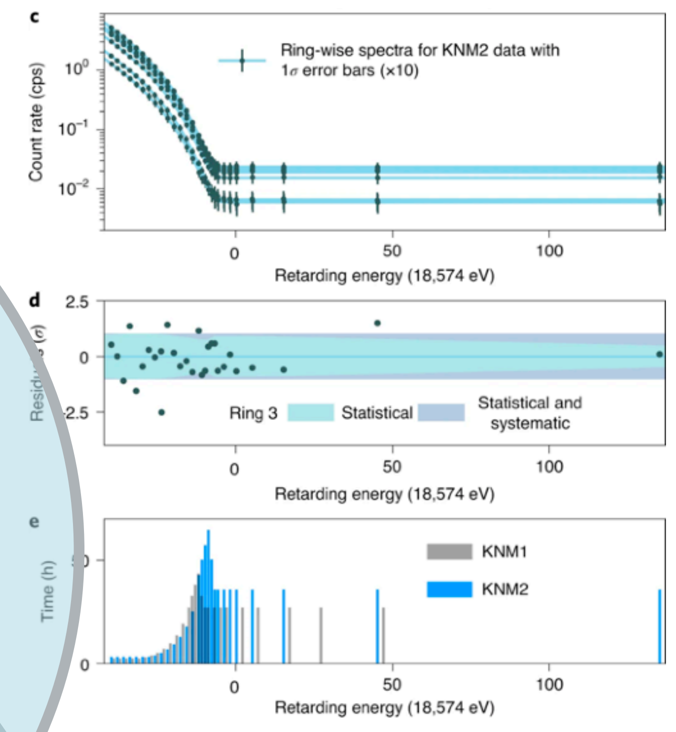
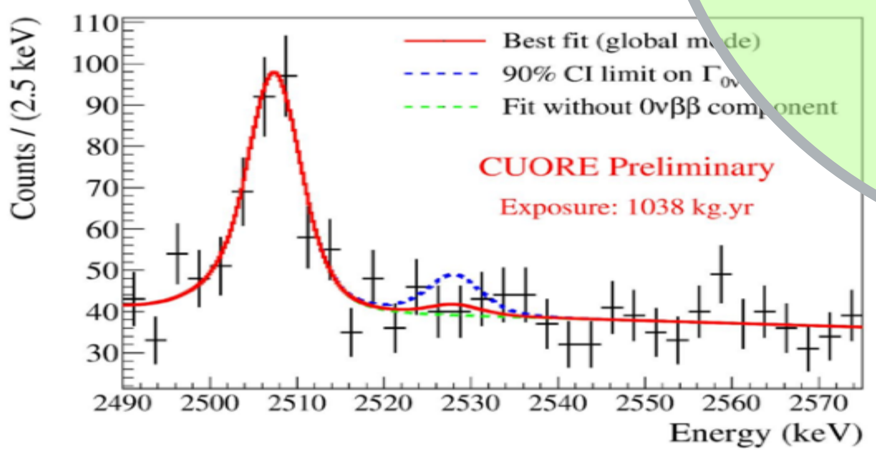
Bottlenecks:

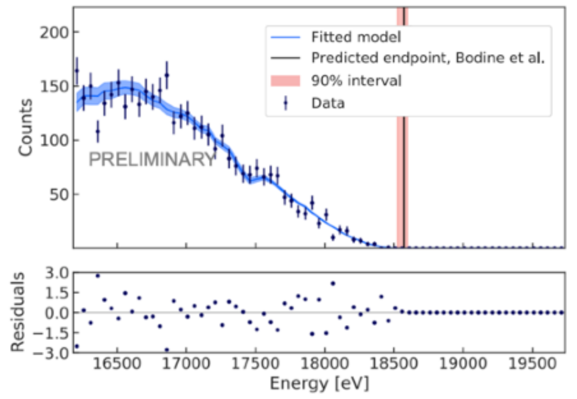
- Large number of datasets
- Large number of nuisance parameter

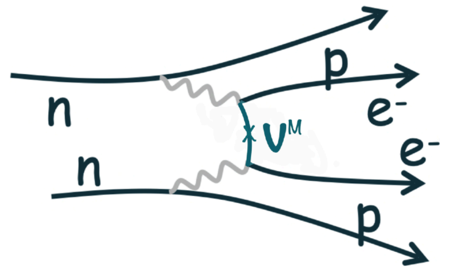
Need:

- More performant parameter estimation tools and analysis strategies
- Likelihoods which incorporates additional informations
- Potential ML-based dimensionality reduction
- "Advanced" likelihood sampling techniques
- Multi-dimensional sampling

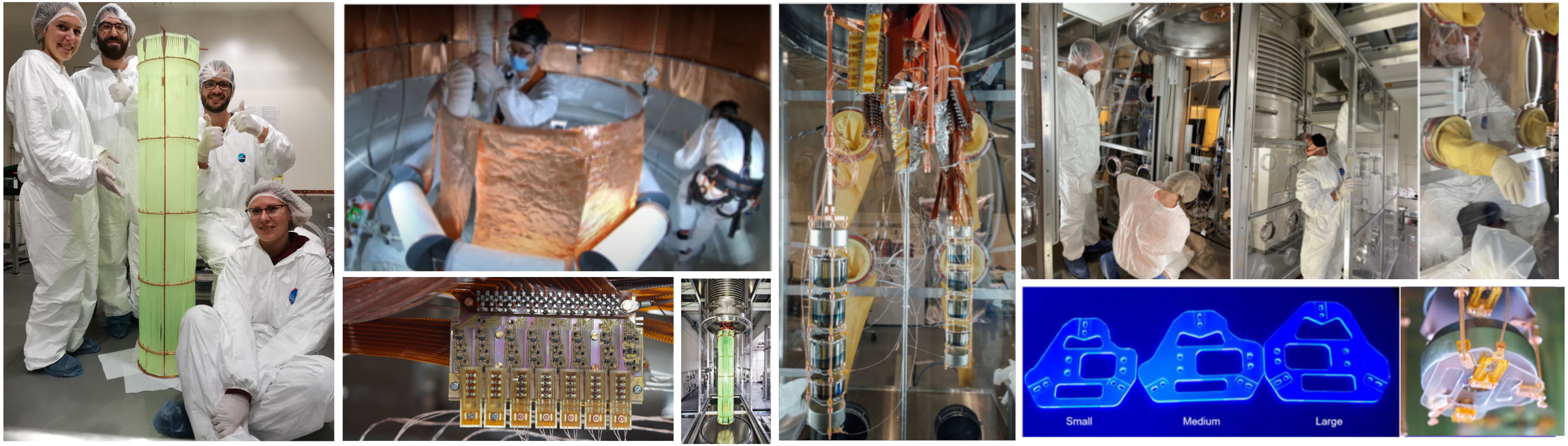








$\Delta L \neq 0$



Thank you for your attention!
Question?