Improving GEANT4's Neutron Physics for Modeling of Cosmogenic Isotope Production in LEGEND

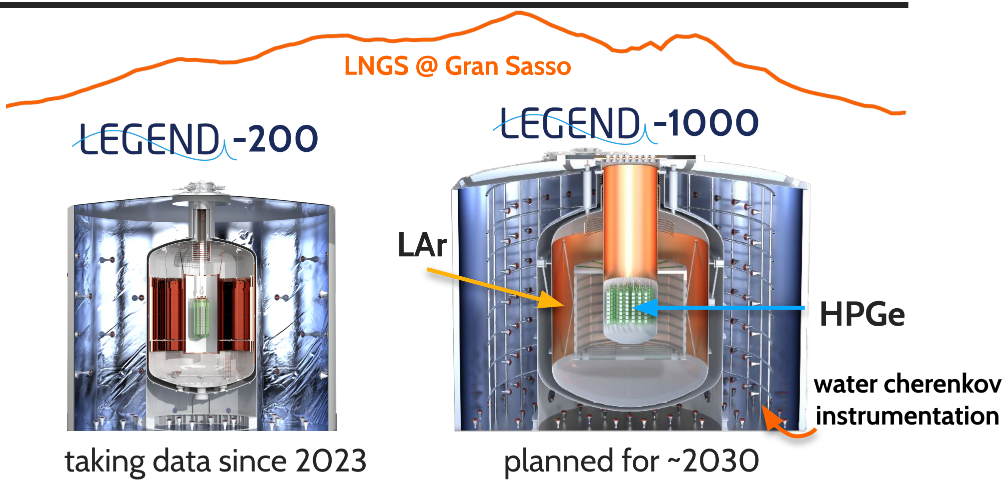
Moritz Neuberger (TUM) - VIEWS24 - Vienna 27.5.2024

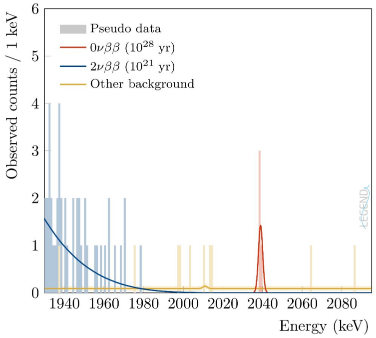
The LEGEND experiment ...

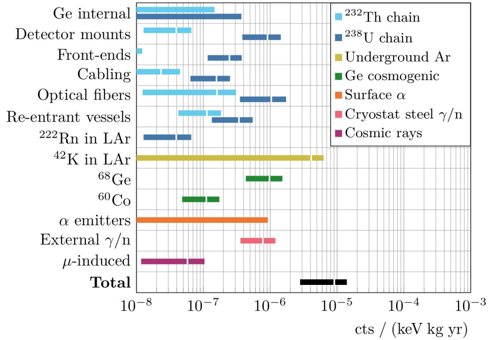
... searches for $0\nu\beta\beta$ in ^{76}**Ge** using enriched high-purity Germanium (**HPGe**) detectors immersed in liquid argon (**LAr**) and instrumented with a light readout.

Our signal is a narrow peak at $Q_{\beta\beta}$ over a (almost) flat background.

We concentrate today on **muon-induced background.**







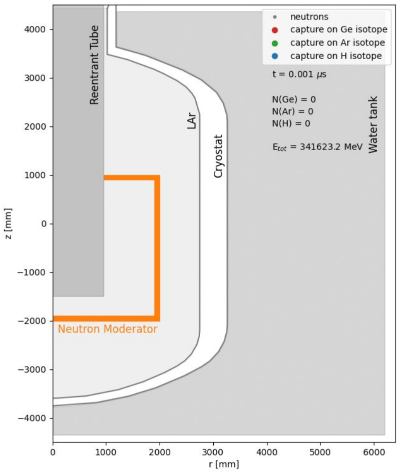
Muon-induced isotope production in LEGEND

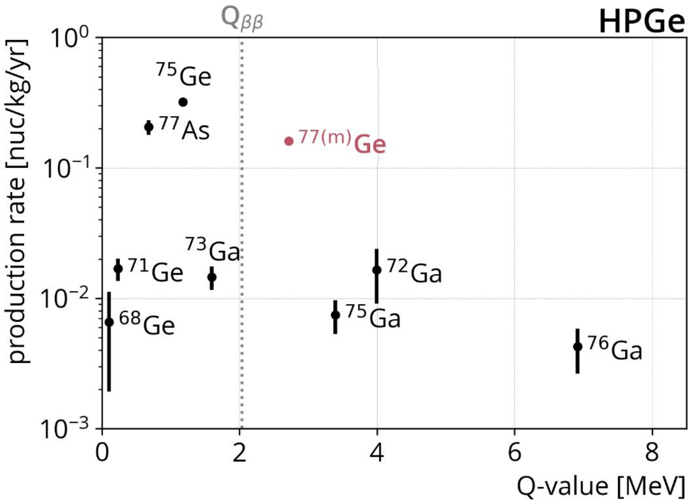
Decay of in-situ muon induced isotopes can cause background for LEGEND-1000.

The only relevant contributor to the background is **$^{77(m)}$Ge** [1,2].

Its production rate has not yet been found experimentally, **so we rely on Geant4 simulations.**

Previous simulation analyses exist [3,4].

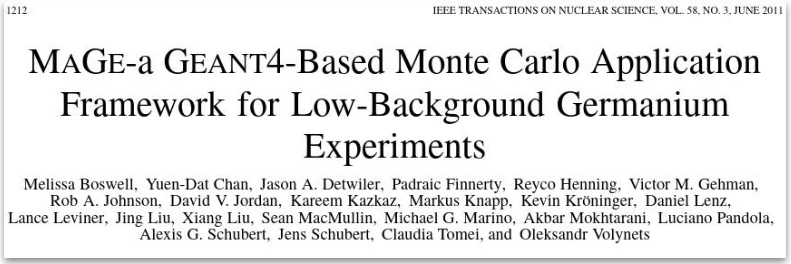




There is a need for a new simulation with a better understanding of the **systematic uncertainty** that also considersn **new experimental data.**

[1] L. Pandola et al., Nucl. Instrum. Meth., A570:149–158, 2007
[2] Christoph Wiesinger et al., Eur. Phys. J. C 78, 597 (2018)
[3] Clay Bartons PhD thesis, https://orcid.org/0000-0002-4698-3765
[4] M Neuberger et al., 2021 J. Phys.: Conf. Ser. 2156 012216

MaGe [10.1109/TNS.2011.2144619]



1212 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 3, JUNE 2011

MAGE-a GEANT4-Based Monte Carlo Application Framework for Low-Background Germanium Experiments

Melissa Boswell, Yuen-Dat Chan, Jason A. Detwiler, Padraic Finnerty, Reyco Henning, Victor M. Gehman, Rob A. Johnson, David V. Jordan, Kareem Kazkaz, Markus Knapp, Kevin Kröninger, Daniel Lenz, Lance Leviner, Jing Liu, Xiang Liu, Sean MacMullin, Michael G. Marino, Akbar Mokhtarani, Luciano Pandola, Alexis G. Schubert, Jens Schubert, Claudia Tomei, and Oleksandr Volynets

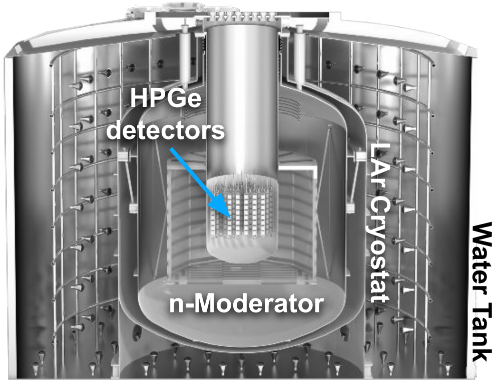
Developed for the **MAJORANA** and **GE**RDA experiments.

Advantages:

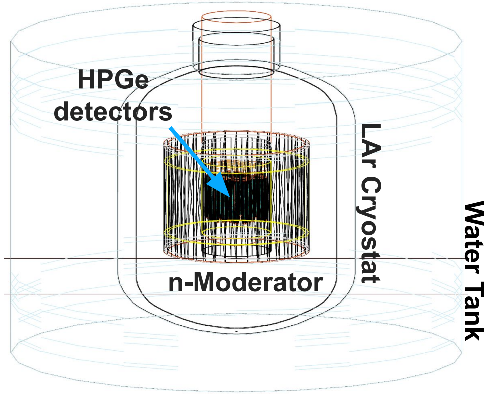
- LEGEND-1000 geometry implemented
- Customization of geometry, physics and output scheme via macro commands

Currently using **G4.10.5**, but upgrade in progress.

LEGEND-1000:



LEGEND-1000:
(as implemented in MaGe)



MUSIC and MUSUN [10.1016/j.cpc.2008.10.013]

Muon simulation codes MUSIC and MUSUN for underground physics

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Department of Physics and Astronomy, University of Sheffield, Sheffield S3 7RH, UK

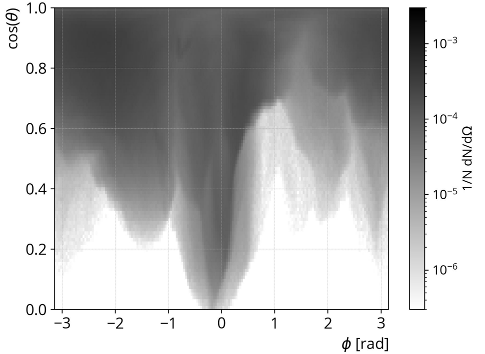
A R T I C L E I N F O A B S T R A C T

MUSIC (MUon SImulation Code) simulates the muon transport through matter.

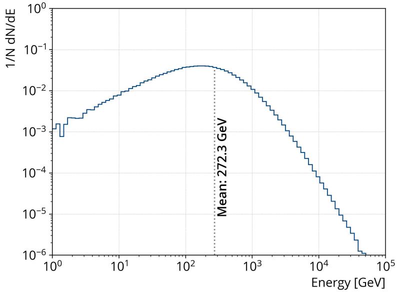
MUSUN (MUon Simulations UNderground) uses the output of MUSIC to sample muons in underground laboratories.

Since there are several versions of both codes the author finds impractical to submit all of them to the code library. Any specific version can be obtained by request to v.kudryavtsev@sheffield.ac.uk. There is a possibility to adapt the codes to specific needs of a user as was done on several occasions in the past.

Muon flux, angular distribution and energy of LDV in **Hall C** well reconstructed.



With LEGEND-1000 in **Hall A**, we estimate an **uncertainty in the muon flux of 3%** (from comparison of Borexino and LVD flux measurements).



MUSUN sampling settings

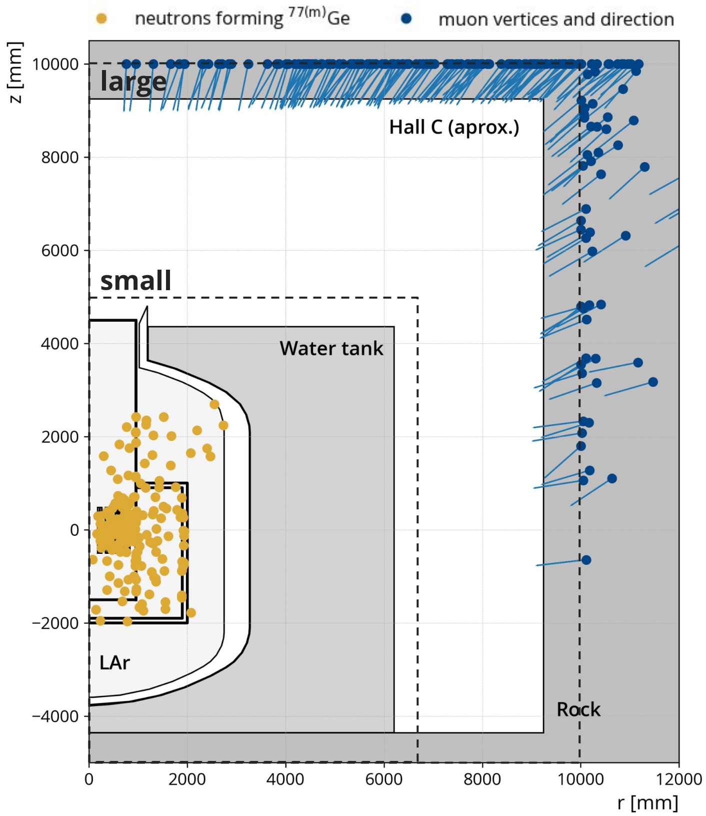
Musun samples position, energy and direction on a box of variable size.

Two options:

1. a **large** box inside the wall,
2. a **small** box around the water tank.

Difference in production rate **<5%.**

This is because the vast majority of neutrons forming $^{77(m)}$Ge are produced inside the LAr cryostat and neutrons from the wall are caught in the water tank.



Which hadronic physics list?

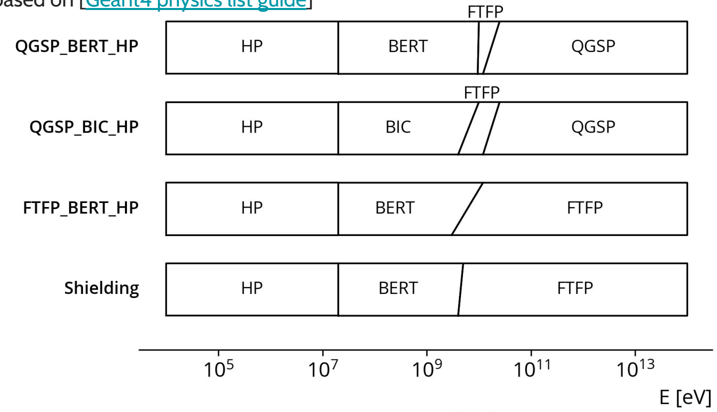
Differences in the physics list play a role in the **muon shower modeling.**

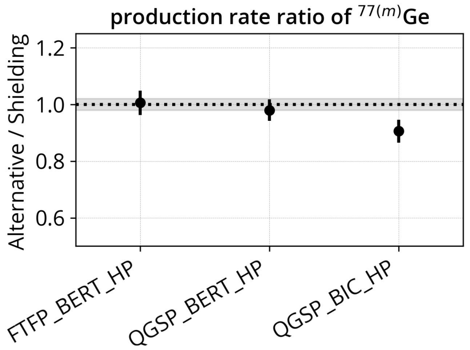
Our base physics list is **Shielding**, as it is *recommended for use in neutron transport.*
[Geant4 physics list guide]

Other physics lists agree within **10%.**

To do: Also test **EM physics list.**
So far **G4EmLivermorePhysics** has been used.

Relevant hadronic physics lists in Geant4 10.5:
based on [Geant4 physics list guide]





Which evaluated nuclear data library?

Neutron high-precision model (**NeutronHP**) is based on evaluated nuclear data libraries [link].

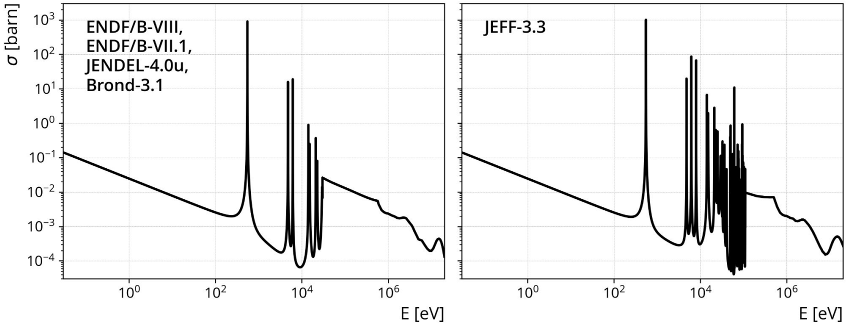
Several libraries are available in the Geant4 format [here].

Geant4 provides standard libraries:

- **G4NDL-4.5** is based on ENDF/B-VII.1
- **G4NDL-4.7** is based on JEFF-3.3 (>= G4 11.1)

Library	Versions available in G4NDL format [here]
ENDF/B	**VIII.0**, VII.1, VII.0, VI.8
JEFF	**3.3**, 3.2, 3.1, 3.0
JENDL	**4.0u**, 4.0, 3.3
CENDL	31
BROND	3.1, 2.2

^{76}Ge(n,γ) cross sections:

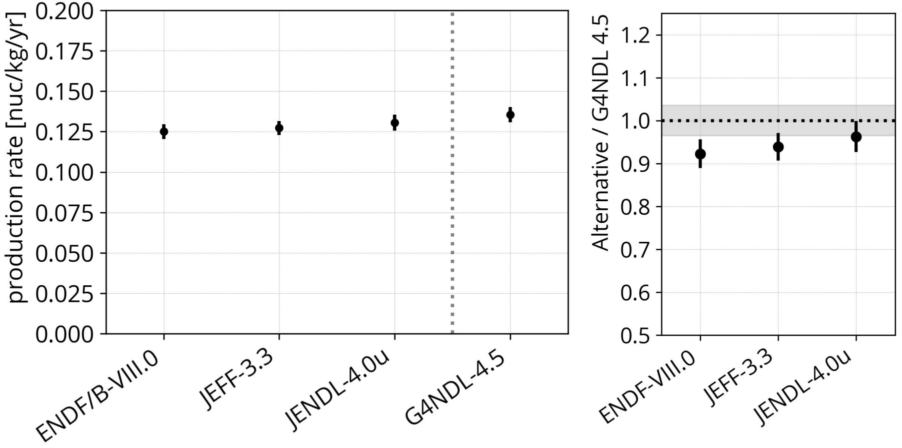


Comparing evaluated nuclear data library

We can check for dependence on the library selection by setting `G4NEUTRONHPDATA` to the appropriate folder and running the simulations.

With our base selection of **G4NDL-4.5**, the production rate is consistent up to **10%** between libraries.

But we are not done yet...



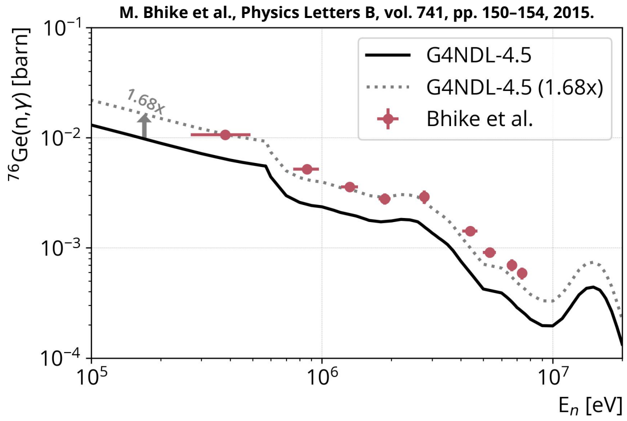
Updating the ^{76}Ge(n,γ) cross section (Part 1)

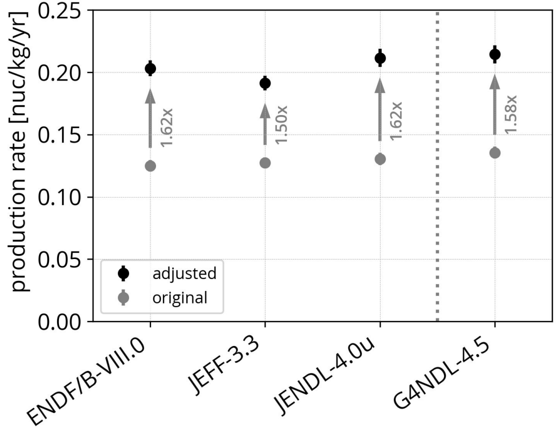
A measurements of the ^{76}Ge(n,γ) cross section [1] at high energies deviate significantly from the evaluated data.

To account for this, we manually adjust the cross section by **scaling the values** in `Capture/CrossSection/32_76_Germanium` **by 1.68x.**

The production rate with these new cross sections scales as expected.

[1] M. Bhike et al., Physics Letters B, vol. 741, pp. 150–154, 2015.





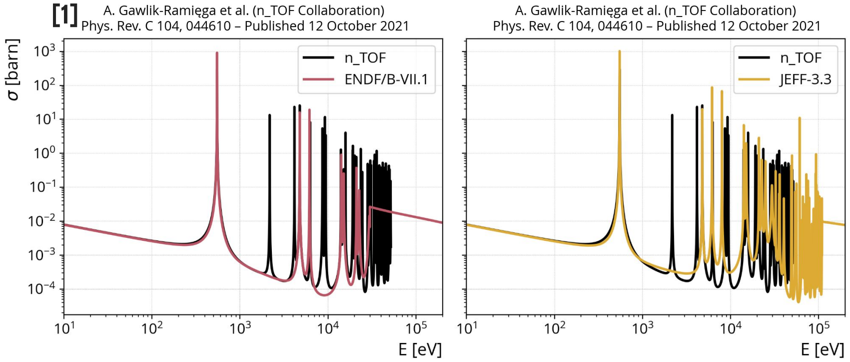
Updating the $^{76}Ge(n,\gamma)$ cross section (Part 2)

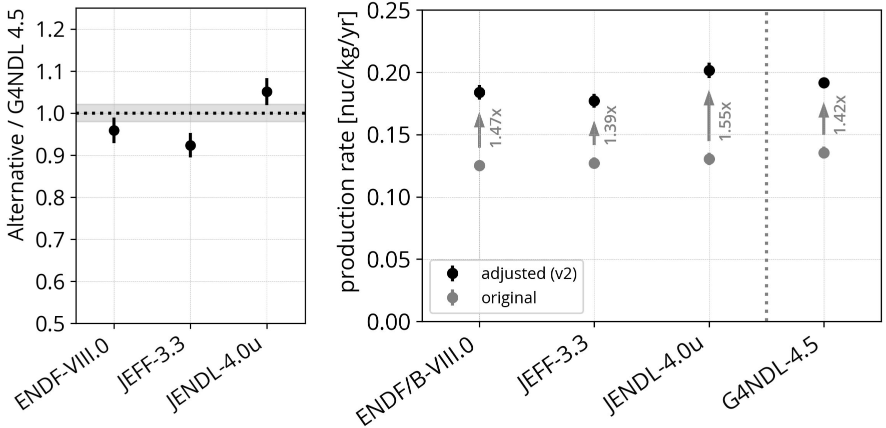
The **n_TOF** collaboration recently made a measurement of the $^{76}Ge(n,\gamma)$ cross section up to 52 keV [1].

To account for the **new resonances** they found, we **replaced the corresponding values** in the G4NDF files.

After the adjustments, the values are still within **10%** of G4NDL-4.5.

[1]





Comparing simulation vs data

In GERDA, the production rate was estimated by simulation to be 0.21 nuc/kg/yr [1].

The systematic uncertainties between simulation and data were estimated by comparing the simulation and data from other experiments:

Cause	Uncertainty
Neutron production (ZEPLIN)	25% [2]
Evaluated nuclear data library	20% [3]

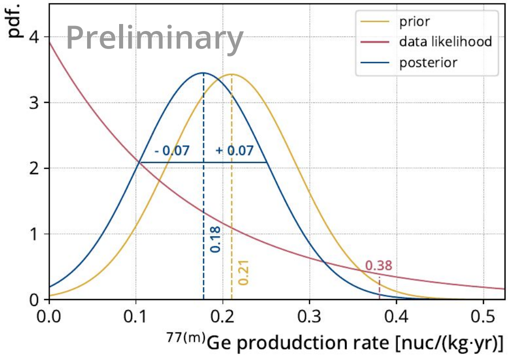
[1] Christoph Wiesinger et al., Eur. Phys. J. C 78, 597 (2018). https://doi.org/10.1140/epjc/
[2] L. Reichhart et al., Astroparticle Physics, vol. 47, pp. 67–76, 2013.
[3] B. Pritychenko, Nuclear Data Sheets, vol. 123, pp. 119–123, 2015.
[4] M. Neuberger for the GERDA experiment, PoS TAUP2023 (2024) 278

Recently, the GERDA data was searched for the decay of ^{77}Ge via an isomeric state in ^{77}As.

No candidate events were found and an upper limit of < 0.38 nuc/kg/yr (90%CL) on the production rate was estimated [4].

With Bayesian update, the GERDA simulation estimate is scaled by:

0.85±0.35



Production rate estimate + uncertainty

Cause	Relative uncertainty contribution
Statistical	<2%
Systematic	
Simulation - Model Choice	
Muon rate	3%
Muon sampling surface	<5%
Physics list	10%
Evaluated neutron data library	10%
Simulation vs Data	35%
Total	38%

Using **Shielding, G4EmLivermorePhysics**, and the **modified G4NDL-4.5**:

$^{77(m)}$Ge production rate estimate: **0.165 ± 0.074 nuc/kg/yr** (after scaling)

Outlook

We want to **model the production topology of $^{77(m)}$Ge**, as this can be used to **define rejection techniques** for its decay via **delayed coincidences** [1].

In addition, we plan to:

- use **thermal neutron data libraries**
- use **new gamma-cascade model** (see Eric's talk)

Search in LEGEND-200:

We will likely see a **positive signal of $^{77(m)}$Ge decays by the end of the year or early next year.**

Simulation vs data uncertainty down to <25% at the end of LEGEND-200.

[1] M Neuberger et al., 2021 J. Phys.: Conf. Ser. 2156 012216

Summary

We develop a muon-induced background simulation model and explore the systematic uncertainties connected with it.

So far, we checked:

- Muon sampling
- Hadronic physics list
- Evaluated nuclear data library
  - additionally adjusted the ^{76}Ge(n,γ) cross section with new data
- Comparison simulation vs data

In the long run, we will switch to

[link]

Advantages:

- lightweight (MaGe is very bloated)
- setup-agnostic (geometry via GDML)
- modern Geant4 methods / tools

Backup

Signal and Background in LEGEND-1000

We search for events around $Q_{\beta\beta}$ after applying all background suppression.

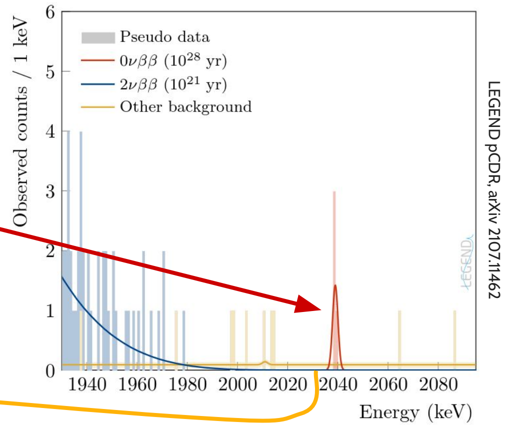
We estimate:

$$\underset{\text{\#background events}}{N_b} = \underset{\text{exposure [kg × yr]}}{\mathcal{E}} \times \underset{\text{energy window [keV]}}{\Delta E} \times \underset{\text{Background Index}}{BI}$$

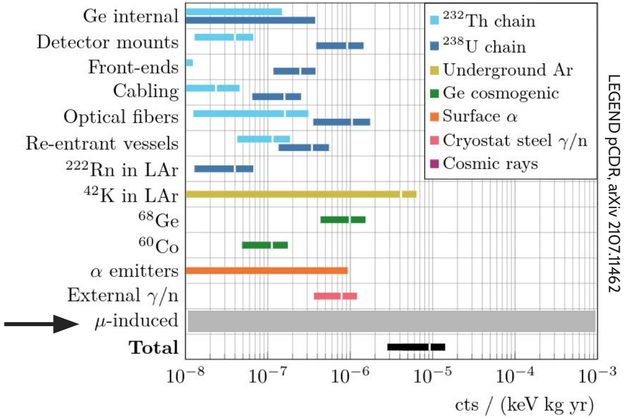
For LEGEND-1000, with **$\mathcal{E}$ = 10 ton × yr** and **ΔE = 2.5 keV**, we expect **N_b < 0.25 cts** with:

$$BI_{goal} < 10^{-5} \text{ cts/keV/kg/yr}$$

Compare with LEGEND-200: < 2 × 10^{-4} cts/keV/kg/yr



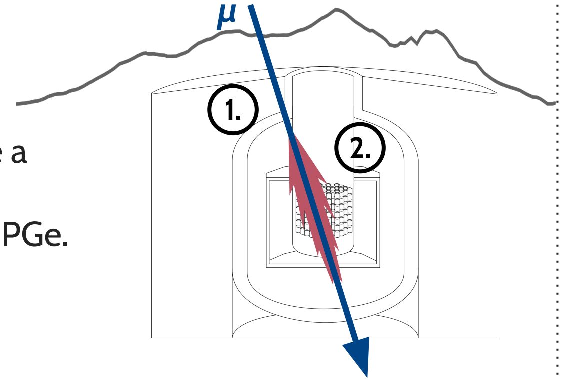
today we focus on this



Types of muon-induced background:

Prompt:

Muons can produce a particle shower and deposit energy in HPGe.



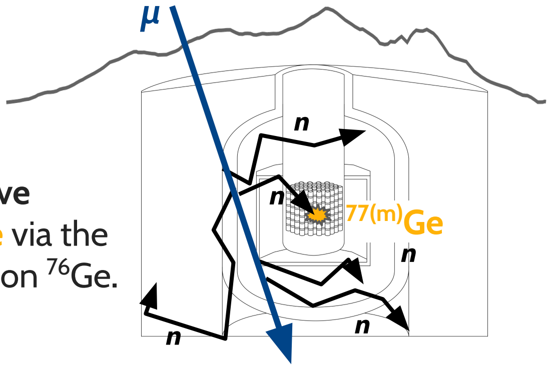
We can strongly suppress them by requiring an anti-coincidence with

1. the water cherenkov instrumentation and
2. the LAr instrumentation.

$BI_{prompt} < 7.1 \times 10^{-8}$ cts/keV/kg/yr (✓)

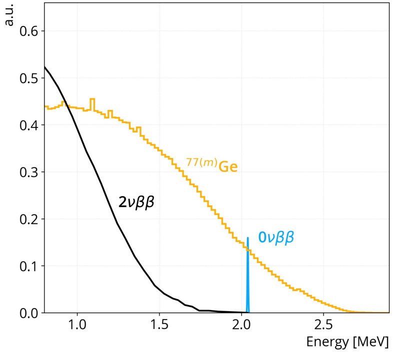
Delayed:

Muons can produce **long-lived radioactive isotopes**, e.g. $^{77(m)}$Ge via the capture of neutrons on ^{76}Ge.

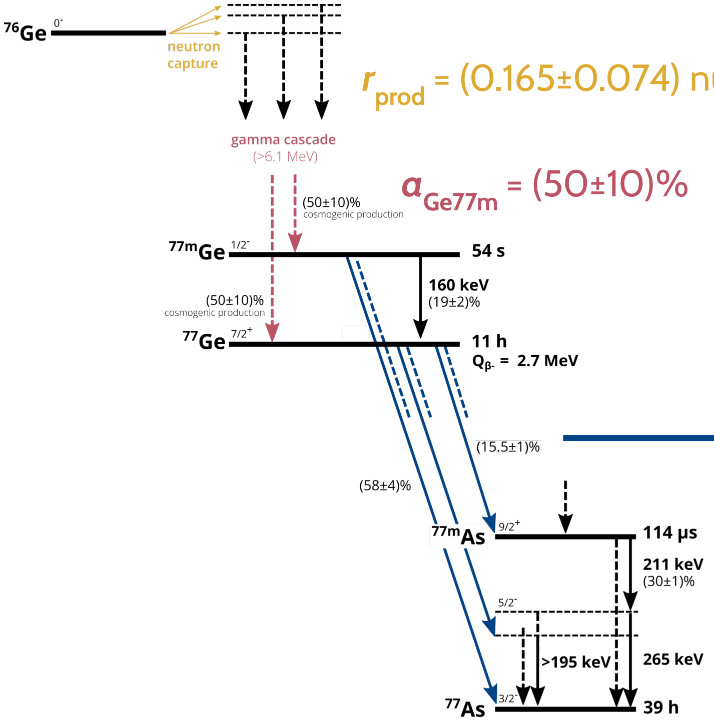


$^{77(m)}$Ge (short for ^{77}Ge and ^{77m}Ge) has Q_β = 2.7 MeV, which is higher than ^{76}Ge's $Q_{\beta\beta}$ = 2.039 MeV.

Therefore, its decay can cause background.



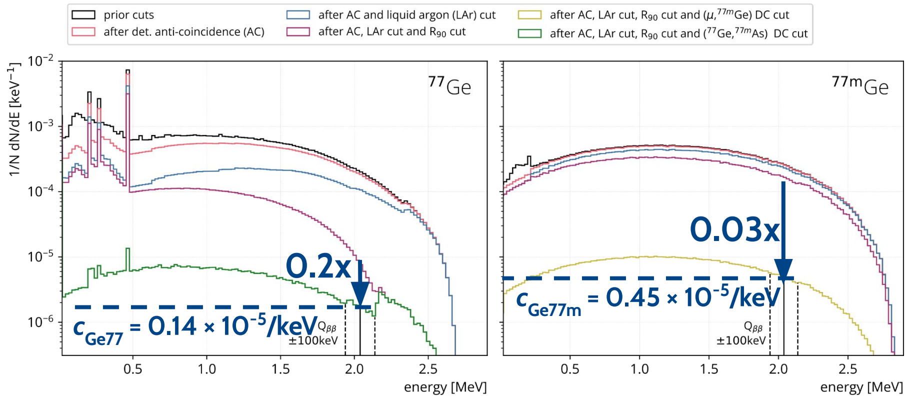
Final background contribution



r_{prod} = (0.165±0.074) nuc/kg/yr

a_{Ge77m} = (50±10)%

$$BI_{delayed} = r_{prod} \times [\, a_{Ge77} \times c_{Ge77} + a_{Ge77m} \times c_{Ge77m} \,]$$



$BI_{delayed}$ ~ 5.5 × 10^{-7} cts/keV/kg/yr ~ 5.5% BI_{goal}

the reduction in the 0νββ survival efficiency is small (-3%).

✓

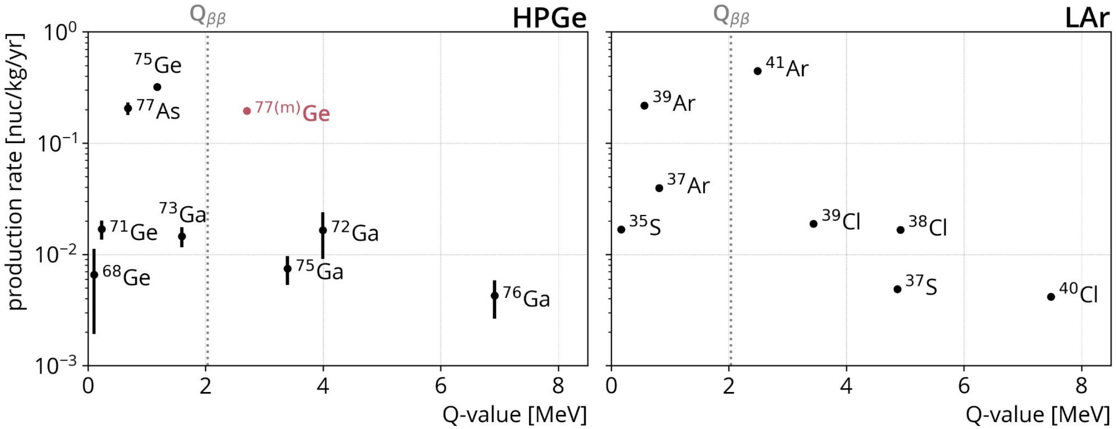
Muon-induced isotope production in LEGEND

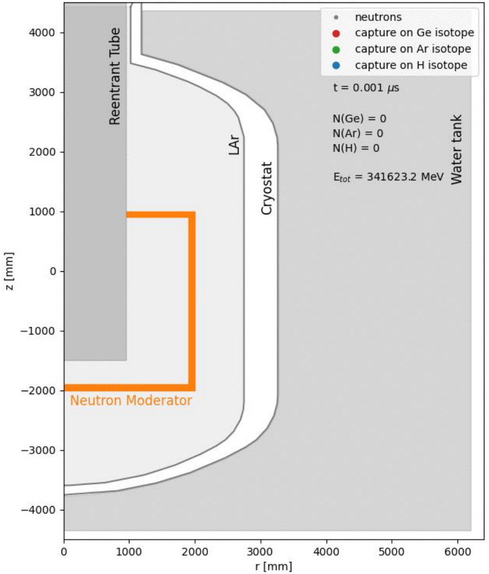
Decay of in-situ muon induced isotopes can cause background for LEGEND-1000.

$^{77(m)}$**Ge** was previously found to be the only relevant contributor [1]. It has $Q_\beta > Q_{\beta\beta}$ and is produced frequently enough.

[1] L. Pandola et al., Nucl. Instrum. Meth., A570:149–158, 2007

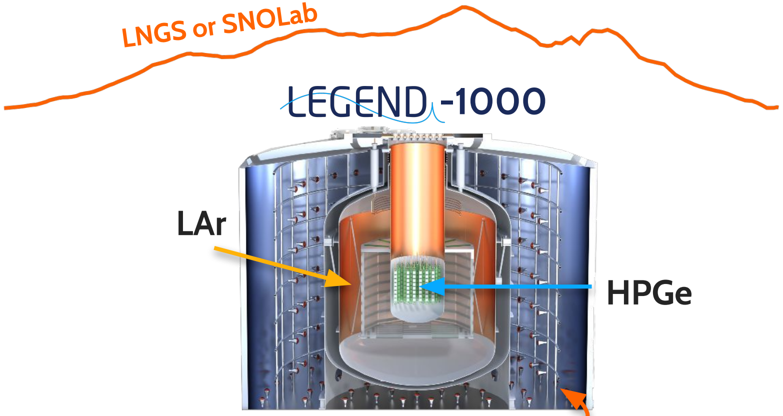
Its production rate has not yet been found experimentally, **so we rely on Geant4 simulations.** This is particularly relevant for the **LNGS** site.





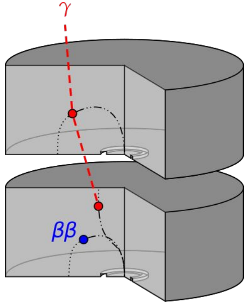
The LEGEND experiment ...

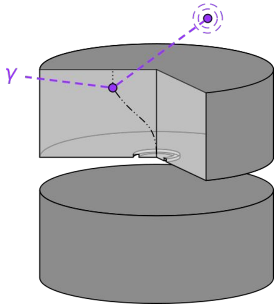
... searches for $0\nu\beta\beta$ in ^{76}**Ge** using enriched high-purity Germanium (**HPGe**) detectors immersed in liquid argon (**LAr**) and instrumented with a light readout.

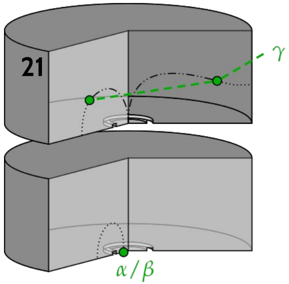


LEGEND uses three background suppression techniques:

1. **HPGe** anti-coincidence
2. **LAr** anti-coincidence
3. **Pulse Shape discrimination**







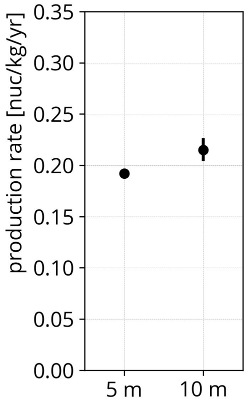
Illustrations by Christoph Wiesinger

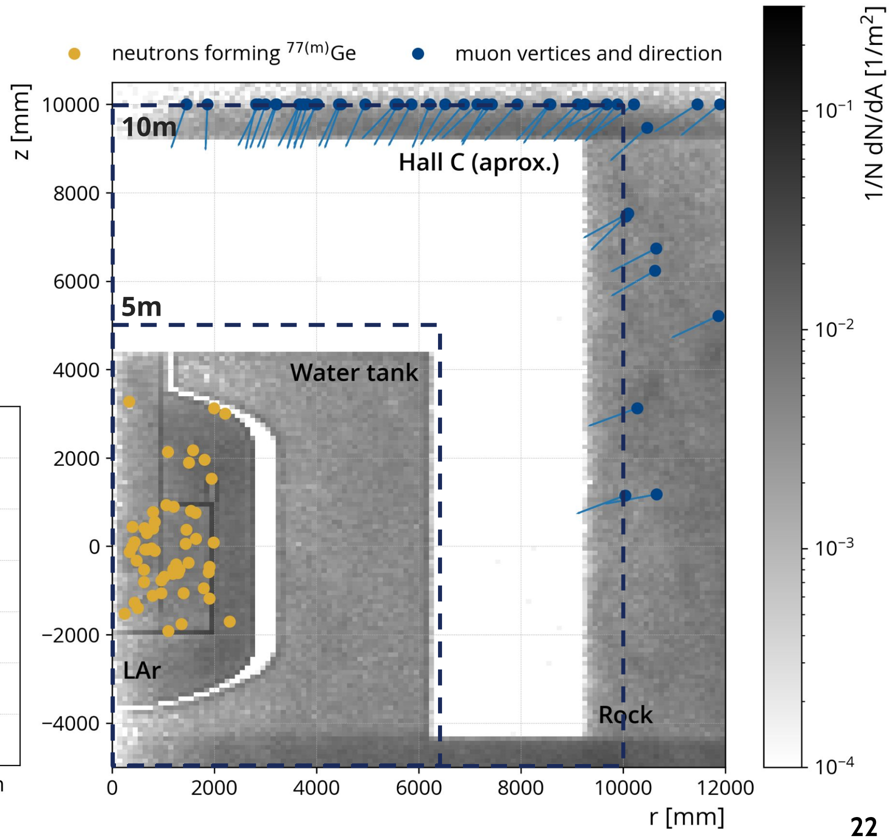
MUSUN sampling settings

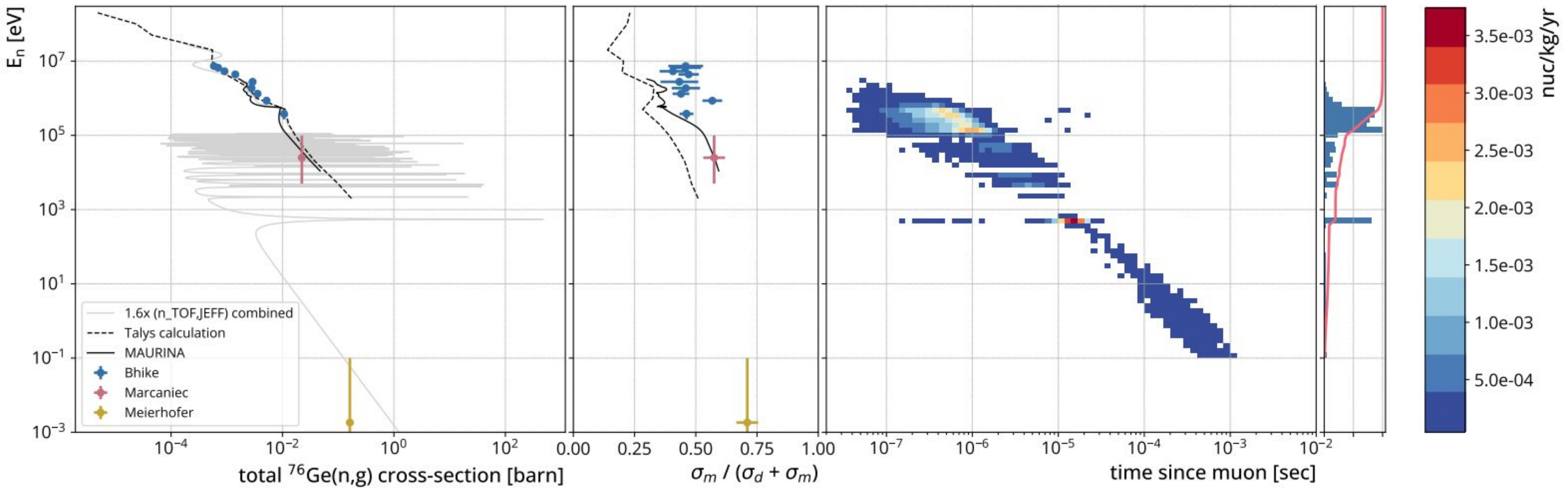
Musun samples position, energy and direction on a box of variable size.

The vast majority of neutrons forming $^{77(m)}$Ge are produced inside the LAr cryostat (see right).

This motivates us to use a 5m half-width box around the water tank to save computation time.







E_n [eV]
1.6x (n_TOF,JEFF) combined
Talys calculation
MAURINA
Bhike
Marcaniec
Meierhofer
total ^{76}Ge(n,g) cross-section [barn]
$\sigma_m / (\sigma_d + \sigma_m)$
time since muon [sec]
nuc/kg/yr