

The Simulation of Neutrinoless $\beta\beta$ Decay Experiments

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Outline

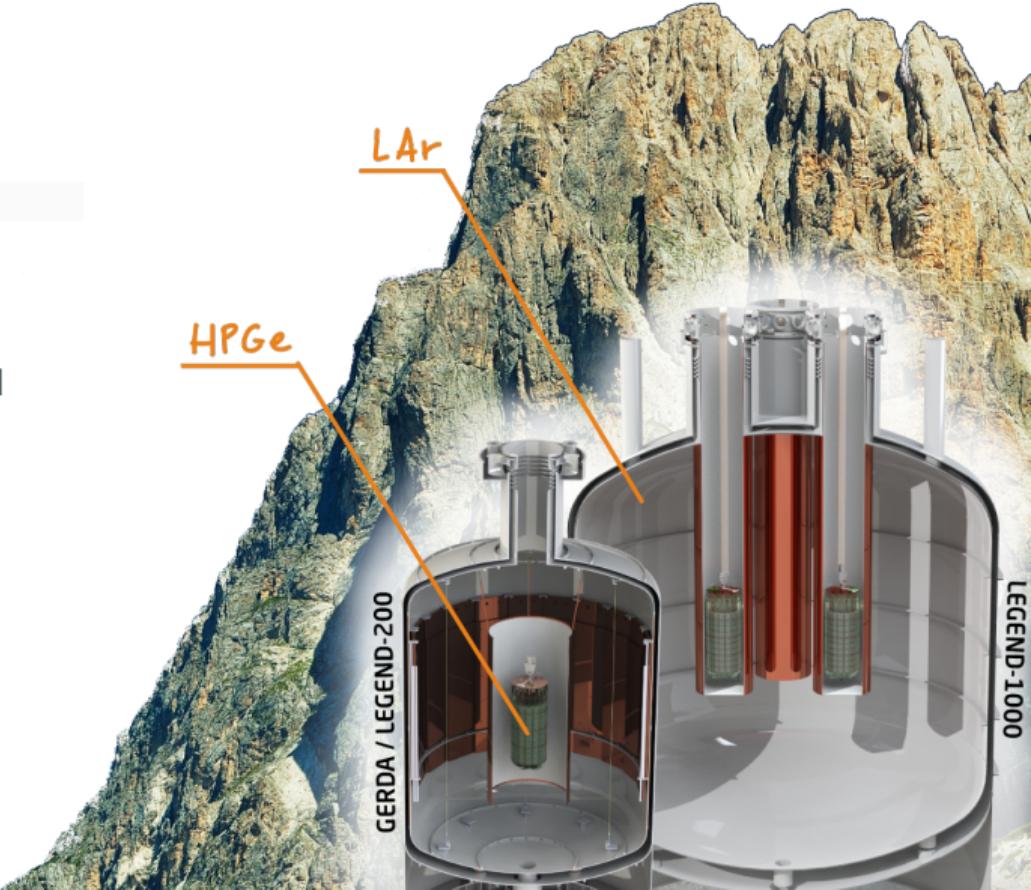
I will focus on the simulation of $0\nu\beta\beta$ ^{76}Ge experiments (I collaborate to GERDA  and LEGEND )
→ many concepts are experiment agnostic

- The physics case: the role of a GEANT4 simulation when searching for $0\nu\beta\beta$
- Get double beta decay physics into GEANT4
- Simulating backgrounds
 - Radioactive decays
 - *in situ* cosmogenics
- Simulation of particle detectors
 - HPGe detectors
 - Liquid argon detector

Underground physics with HPGes

In a nutshell

- HPGes enriched in ^{76}Ge ($\beta\beta$ emitter): source = detector
- Liquid argon (LAr) detector: passive and active shield
- Čerenkov water tank: muon veto
- Underground: cosmic ray backgrounds reduction
- Material radiopurity



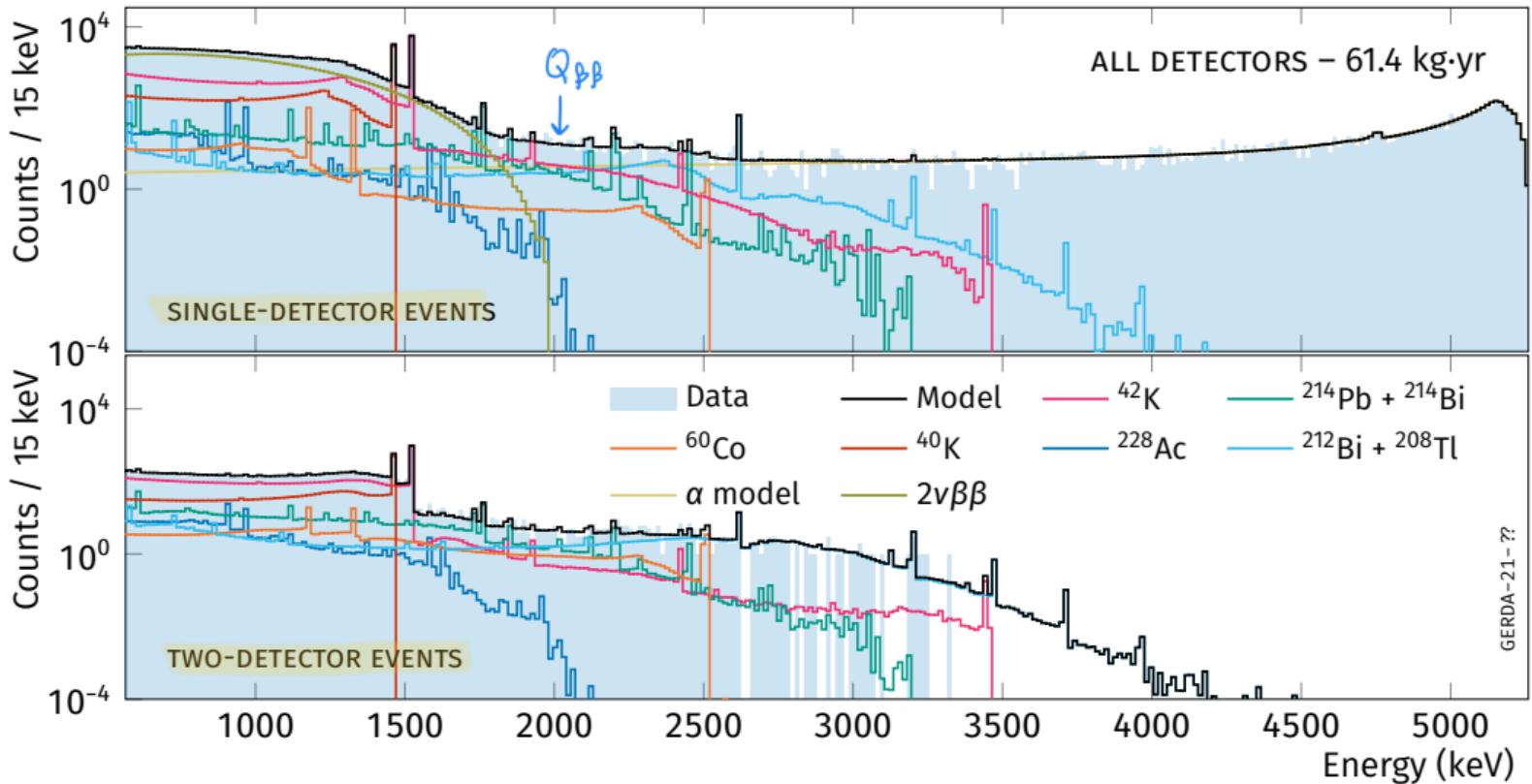
What do we need a GEANT4 simulation for?

To simulate

- Main experiment: GERDA (Phase I & Phase II), LEGEND-200, LEGEND-1000
 - Background projections (LEGEND)
 - Experimental design phase (LEGEND)
 - $2\nu\beta\beta$ spectral analysis
 - ...
- HPGe characterization test stands
 - Active volume determination

The physics realms

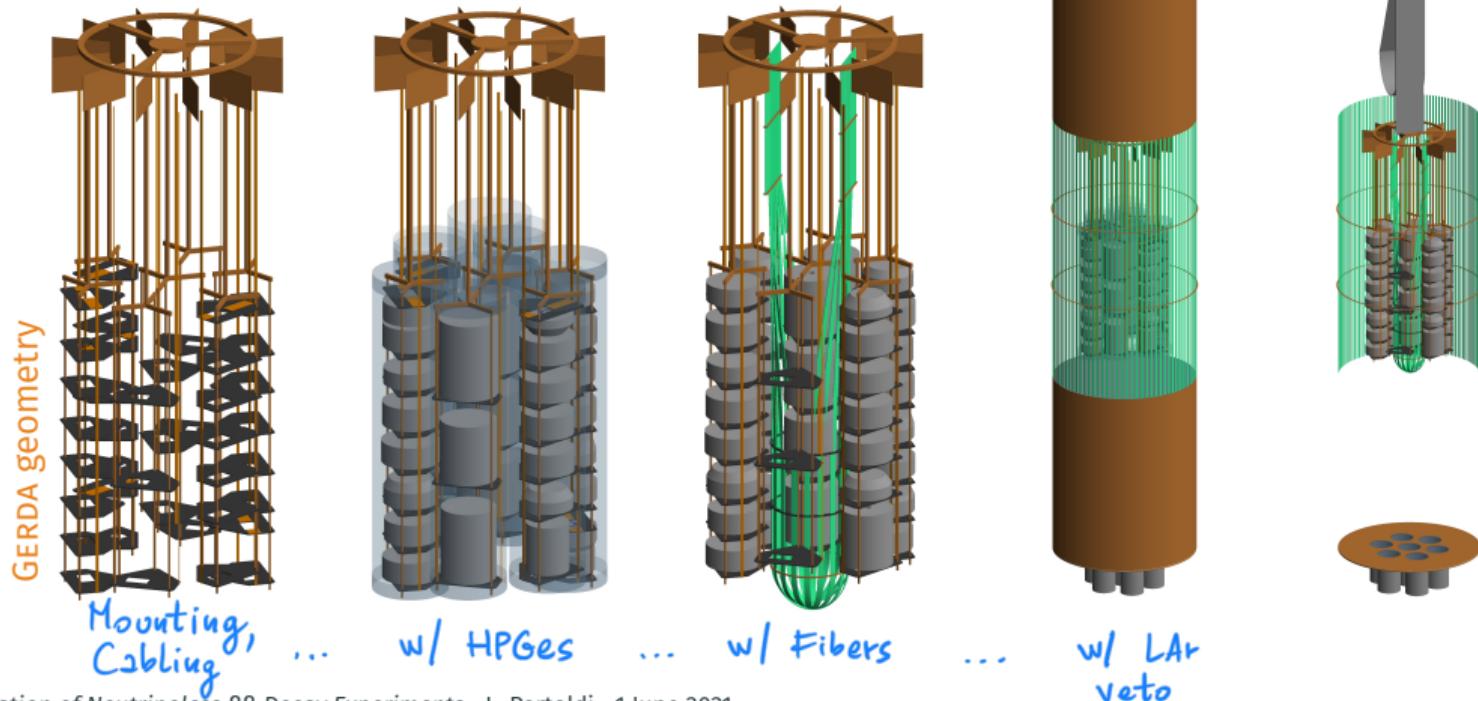
- Double Beta decay physics
- Radioactive decays
- μ -induced showers
- (*in situ*) neutron activation
- Optical physics (LAr)



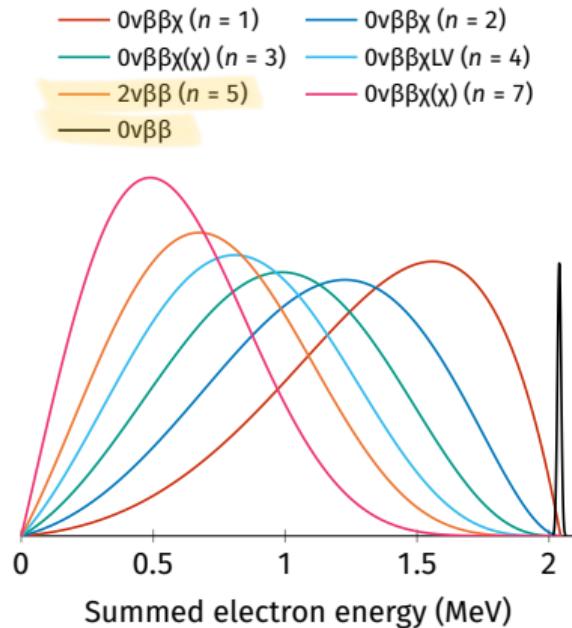
MAGE: MAJORANA GERDA simulation framework

MAGE: a GEANT4-based simulation framework

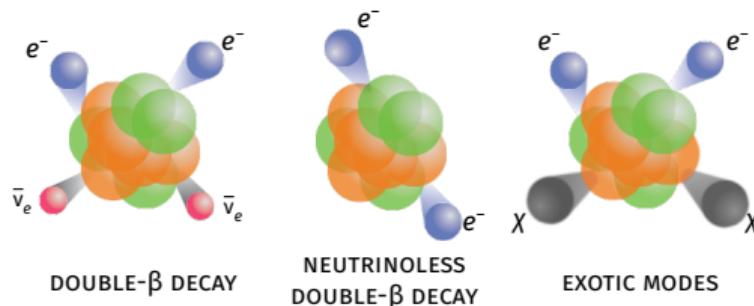
IEEE Trans. Nucl. Sci. 58 (2011) 1212-1220



Double beta decay (precision) physics

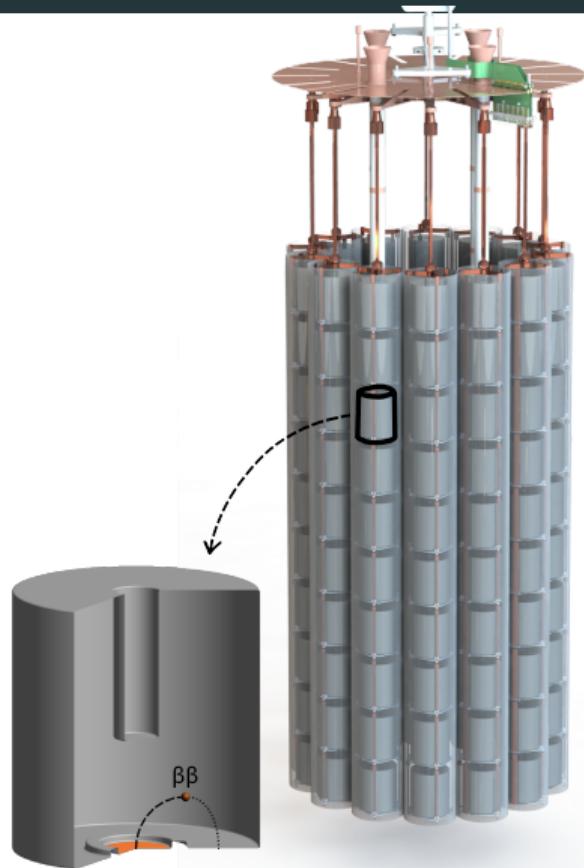
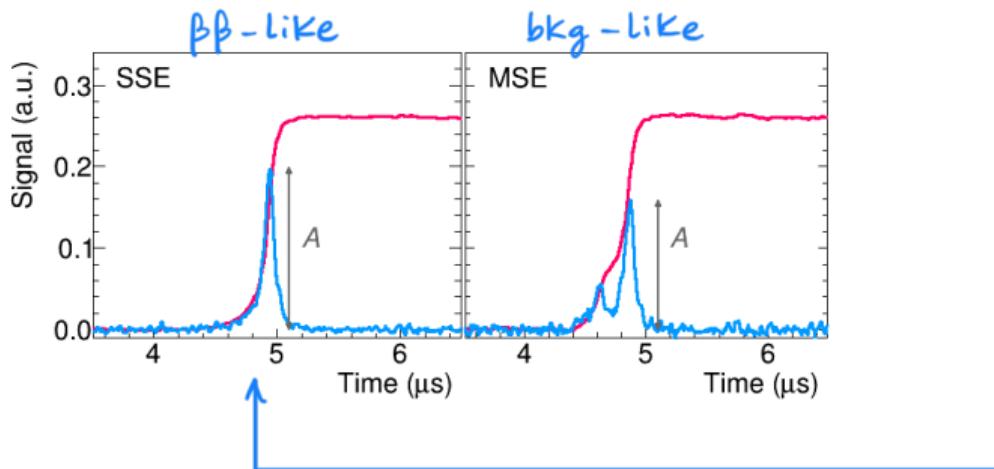


- Neutrinoless $\beta\beta$ decay (**0v $\beta\beta$**): lepton-violating process
- Two-neutrino $\beta\beta$ decay (**2v $\beta\beta$**): standard process
- **Exotic modes**: excited states, Majoron emission, Lorentz violation, sterile neutrinos, baryon decay...



Double Beta decay in germanium

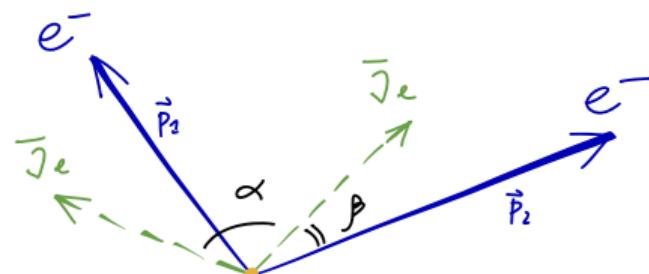
- Localized event (~ 1 mm) \mapsto single-site
- No energy deposited outside the crystal



GEANT4 and double beta decay (yesterday)

$\beta\beta$ decay is a complex process

- Not natively supported in GEANT4, must rely on external tools
- **Decay0** (Fortran77) by V. Tretyak used to generate primary decays [3, 10]
- Extended support for exotic modes (Majorons, Lorentz violation...)
- Output parsed by GEANT4 application (custom G4PrimaryGenerator)



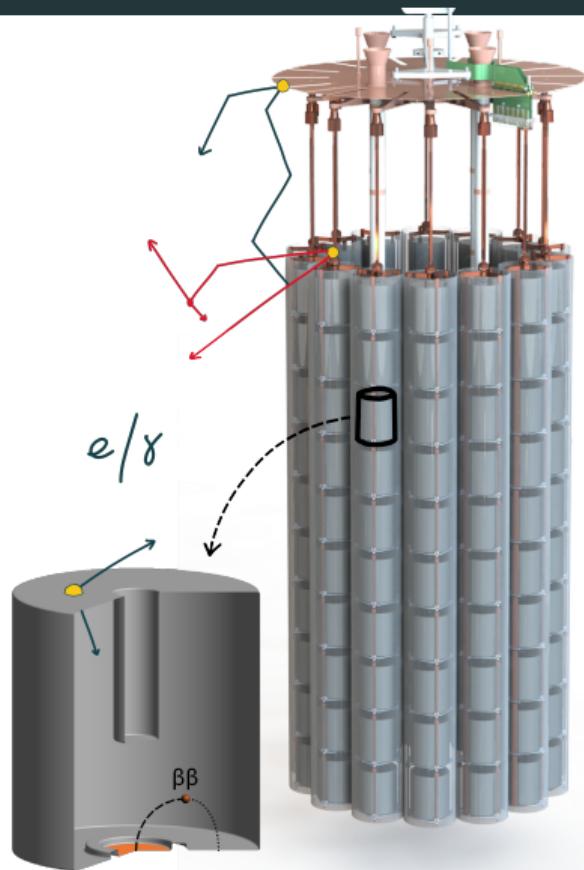
GEANT4 and double beta decay (today)

SUPERNEMO-led attempt to modernize: [BxDecay0](#) ↗ [BxCppDev/bxdecay0](#)

- C++ port of the original Decay0
- Maintained in sync with the Fortran program
- Ships with a handy **GEANT4 interface** (through a PrimaryGeneratorAction class and its associated messenger) ↞ easy to integrate in your GEANT4 app
- Used/supported by SUPERNEMO and LArSoft (DUNE) collaborations

Radioactive decays

- Standard **physics list**:
 - G4EmStandardPhysics
 - G4EmExtraPhysics
 - G4DecayPhysics
 - G4RadioactiveDecayPhysics
- **Angular correlations** usually turned on via
G4DeexPrecoParameters/G4NuclearLevelData
- Choose between different models for low-energy EM processes (Penelope, Livermore...)



High Q-value (> 2 MeV), critical for $0\nu\beta\beta$ region

- Cosmogenic
 - ^{42}K in LAr (above ground)
 - ^{60}Co and ^{68}Ge in germanium (above ground)
 - ^{77}Ge and ^{77m}Ge (*in situ*)
- Natural radioactivity
 - ^{228}Th and ^{238}U decay chains in materials
 - HPGe surface α events
 - External γ rays and neutron background

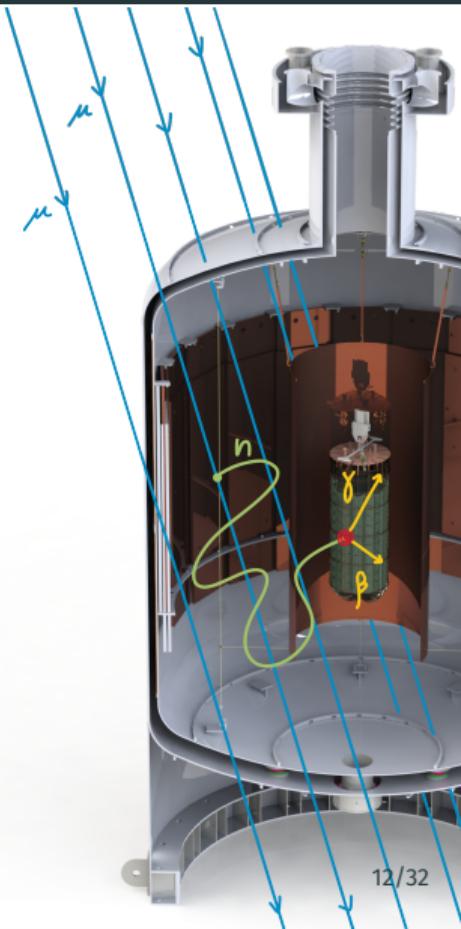
Lower Q-value

- ^{40}K , ^{60}Co in construction materials
- Low energy: ^{39}Ar , ^{42}Ar , ^{85}Kr in LAr

[prompt] Muons are vetoed by instrumenting the Čerenkov water tank.
Simulations to design it and determine veto efficiency [9]

[delayed] Spallation neutrons can activate germanium ($^{77}\text{Ge}/^{77m}\text{Ge}$).
Simulations are crucial in order to:

- Predict background level for given setup
- Study potential mitigation strategies
 - Passive reduction: cryostat size, neutron absorbers, etc.
 - Active reduction: delayed coincidence cuts



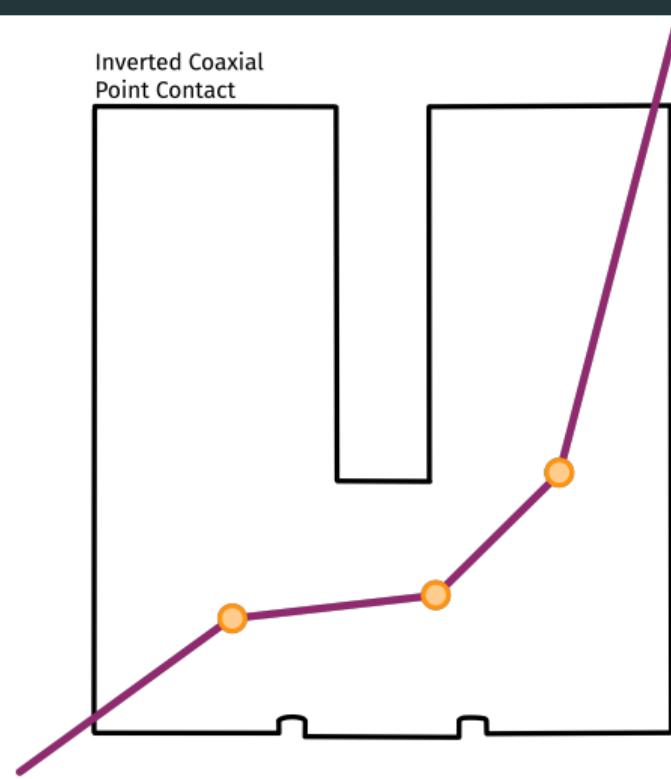
- GEANT4 or FLUKA? Our GEANT4 simulations seems to be compatible with GERDA data.
- Muon distribution at laboratory as starting point. Custom primary generators for:
 - MUSUN generator [7]
 - Mei and Hime formulas [6]
- Simplified experimental geometry (detectors, cryostat, water tank)
- Identify the activated isotopes (in germanium and LAr) with timing info

Movie time! https://docs.google.com/presentation/d/1ZK18Rj61mJGcG7TjEp9_f1AhZDhv9XD18_qAfphHW-0/edit?usp=sharing

HPGe detector simulation

HPGe implementation in the GEANT4 app is a block of germanium...

- HPGe modeled as a **G4GenericPolycone**
- Every HPGe is unique \mapsto specs as **JSON** input
- Hits saved to disk



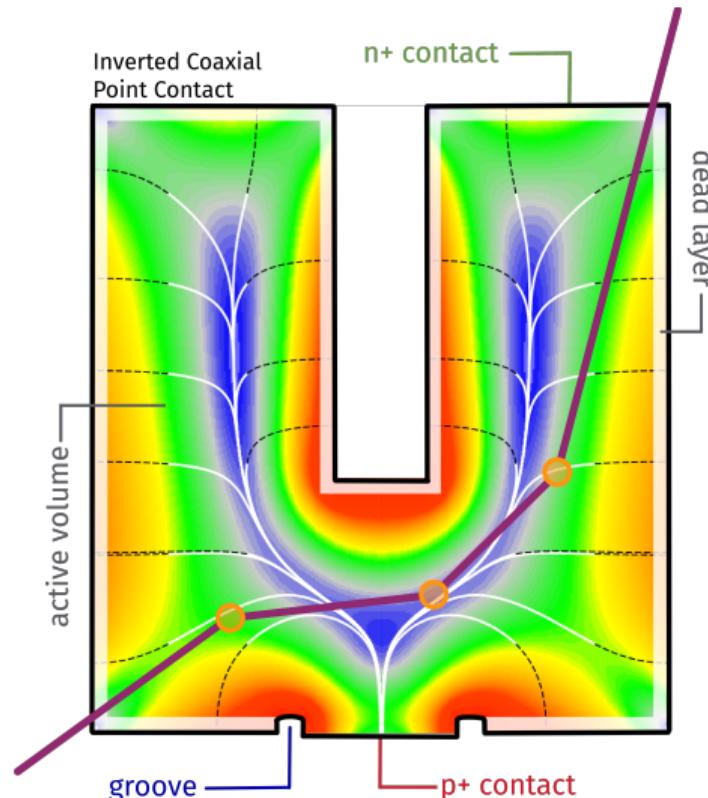
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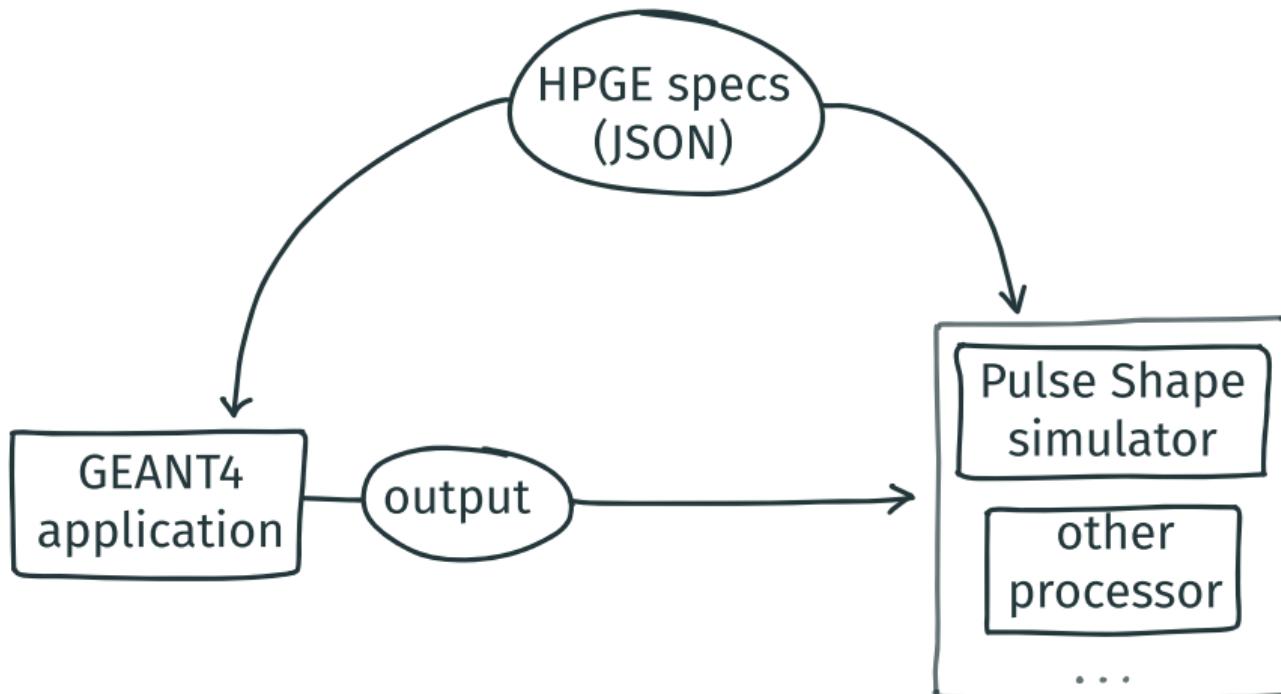
...but an HPGe detector is in reality a complex object!

- Energy resolution
- Active volume model (n^+ lithiated surface)
- Weighting potential distribution \mapsto charge carrier motion \mapsto waveform

\mapsto applied “offline” with dedicated applications
(post-processors)

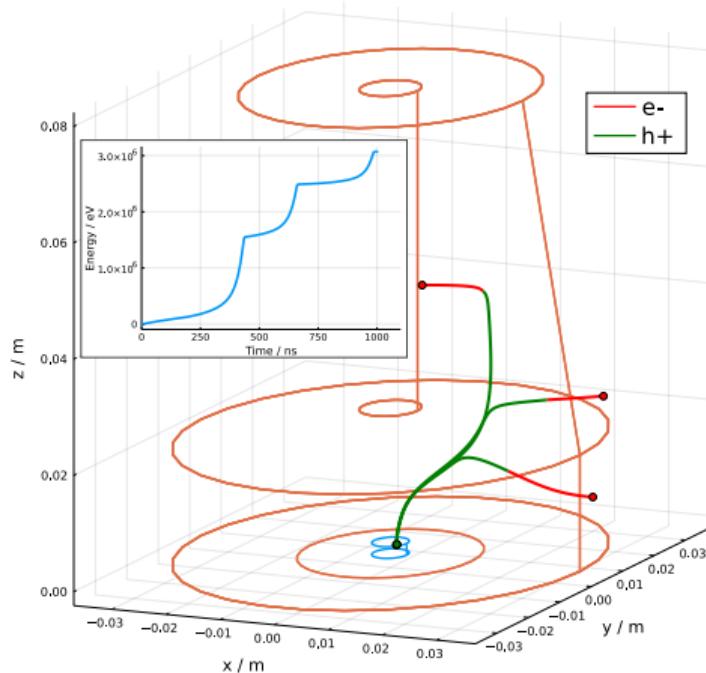


Externalizing the HPGe detector model



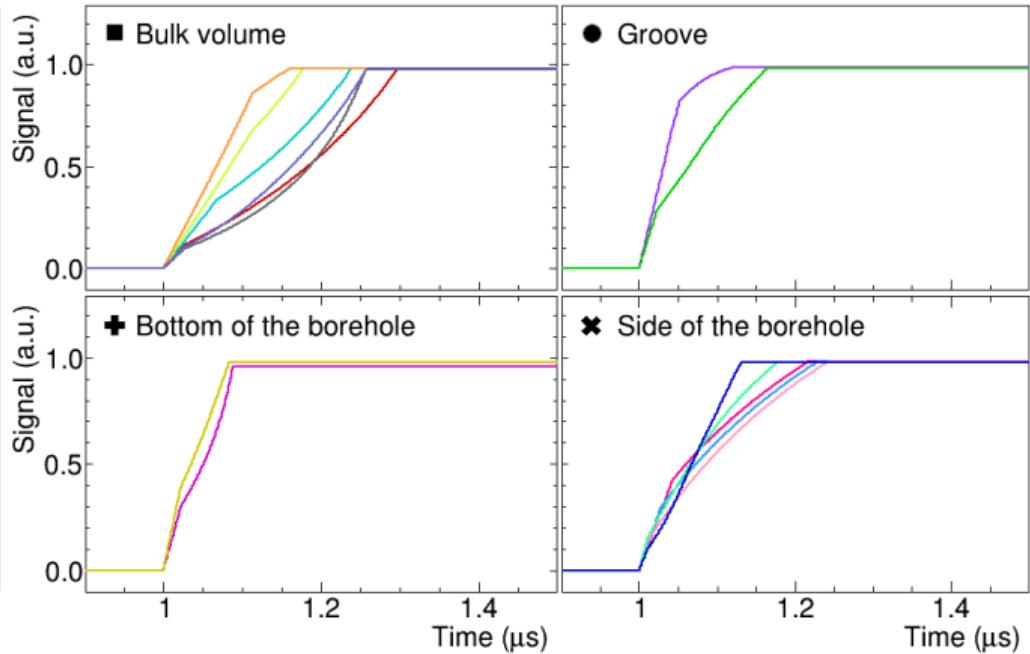
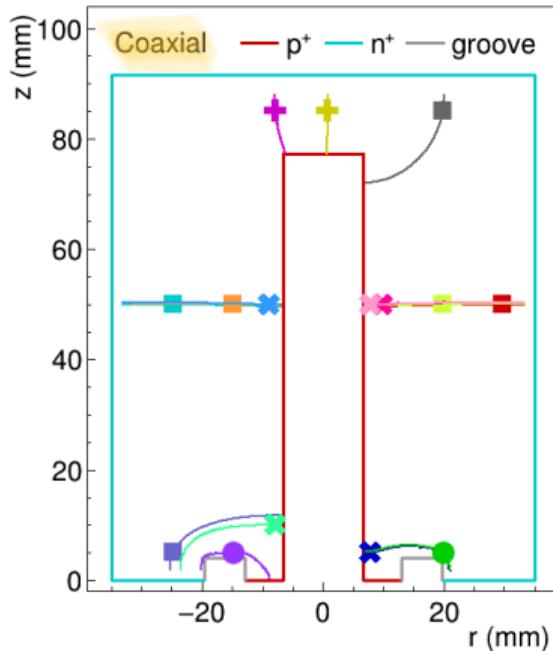
Pulse shape simulation R&D

- siggen (by David Radford)
⌚ [radforddc/icpc_siggen](#)
- ADL (Agata Detector Library)
EPJA 52, 70 (2016)
- SolidStateDetectors.jl
⌚ [JuliaPhysics/SolidStateDetectors.jl](#)



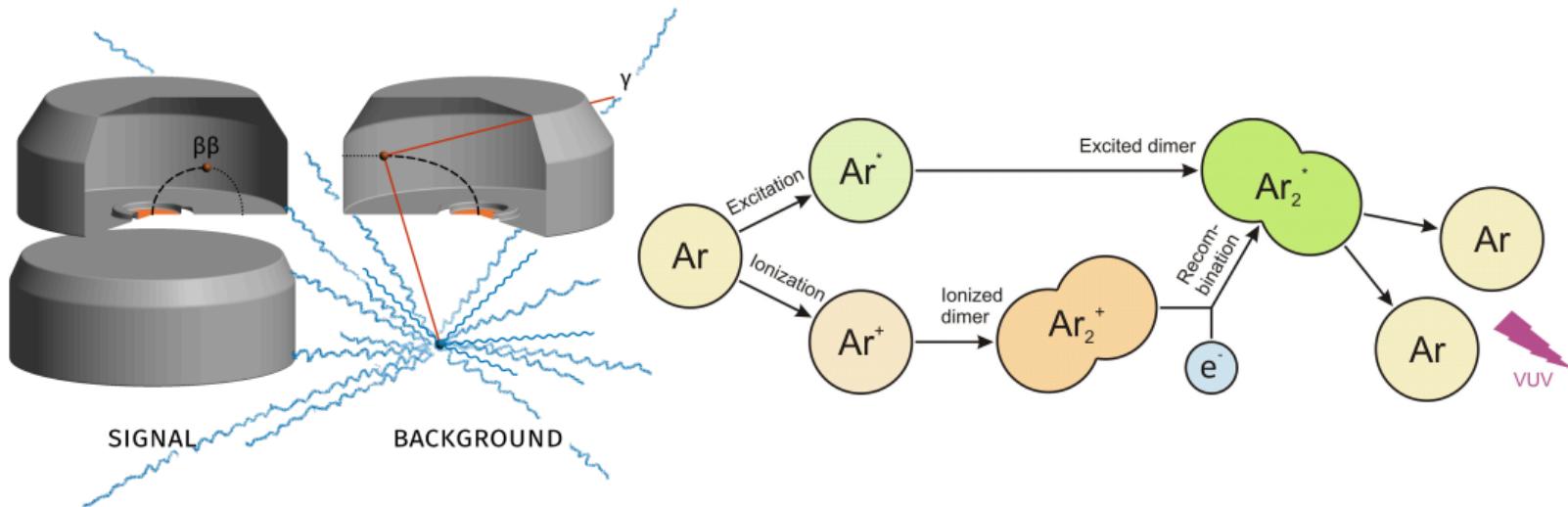
[from
the SolidStateDetectors.jl documentation]

Pulse shape simulation R&D



The Liquid Argon Detector

Background rejection through the liquid argon light collection system



LAr as a *cooling medium*, passive and **active shield** against backgrounds

LAr veto cut: HPGe triggers with coincident LAr light are removed from the analysis

The liquid argon detector instrumentation

How to practically detect this scintillation light?

- Double-cladding WLS green **fibers** read-out by SiPMs
- **TPB** coating of surfaces to shift the VUV light
 - Fibers, nylon “mini-shrouds”, copper shrouds, PMT glass
- **Reflective surfaces** (VM2000 from 3MTM, Tetratex[®], copper, germanium)
- (only GERDA) PMTs

All this needs to be carefully implemented in the GEANT4 app



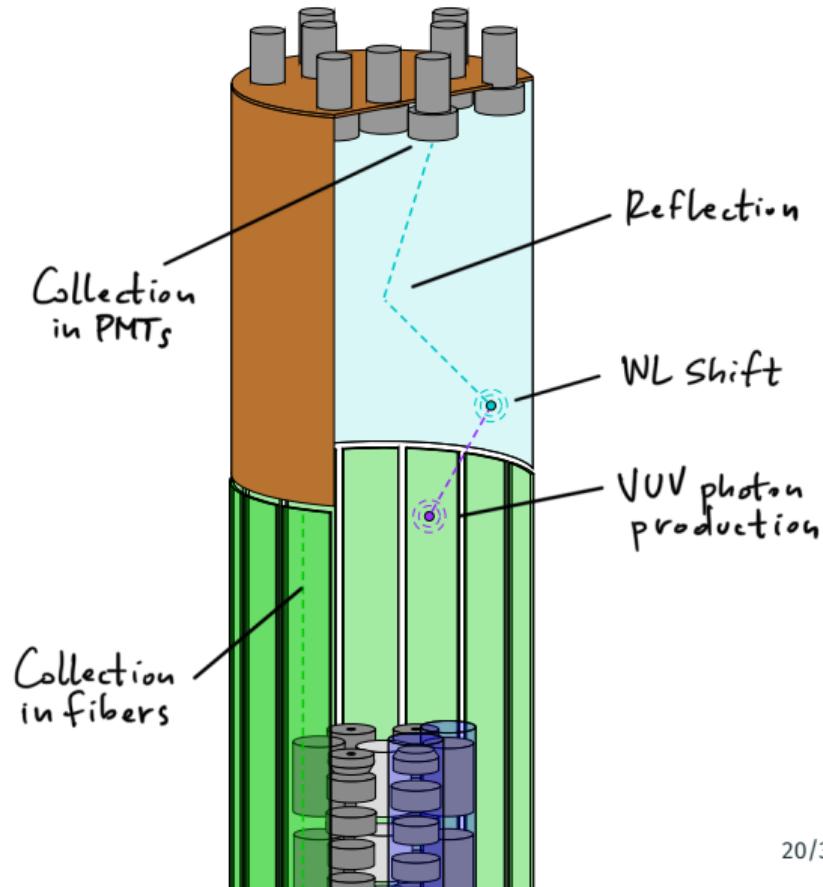
Optical physics in GEANT4: physics list

Photon-generating processes

- G4Scintillation
- G4Cherenkov (only when simulating the water tank)

Photon-tracking processes

- G4OpAbsorption
- G4OpBoundaryProcess
- G4OpRayleigh
- G4OpWLS



Extended support for optical physics processes in GEANT4 [\[manual\]](#)

- LAr scintillation spectrum: Gaus($\mu = 128, \sigma = 2.9$) nm [8]
- LAr photon yield: unknown, set conservative 28 ph/keV based on [4, 2] and 1 μ s triplet lifetime measured in GERDA. Quenching implemented [4]
- LAr refractive index [1], scattering length [5]
- LAr attenuation length: purity-dependent, measured at ~30 cm in GERDA
- TPB shifting: specs depend on layer thickness, substrate, temperature, deposition method.
Measured by us or best literature values
- WLS fibers: as in vendor tech specs sheet
- Reflectors: reflectivity measured by us or best literature values

Problem: huge number of photons to track on the CPU (RadioactiveDecay)

- Tracking of single VUV photon: $50 \text{ ev/sec}^1 \mapsto O(10) \text{ ph/keV}$

Mitigation: custom G4UserStackingAction to track photons only if a hit in germanium occurs

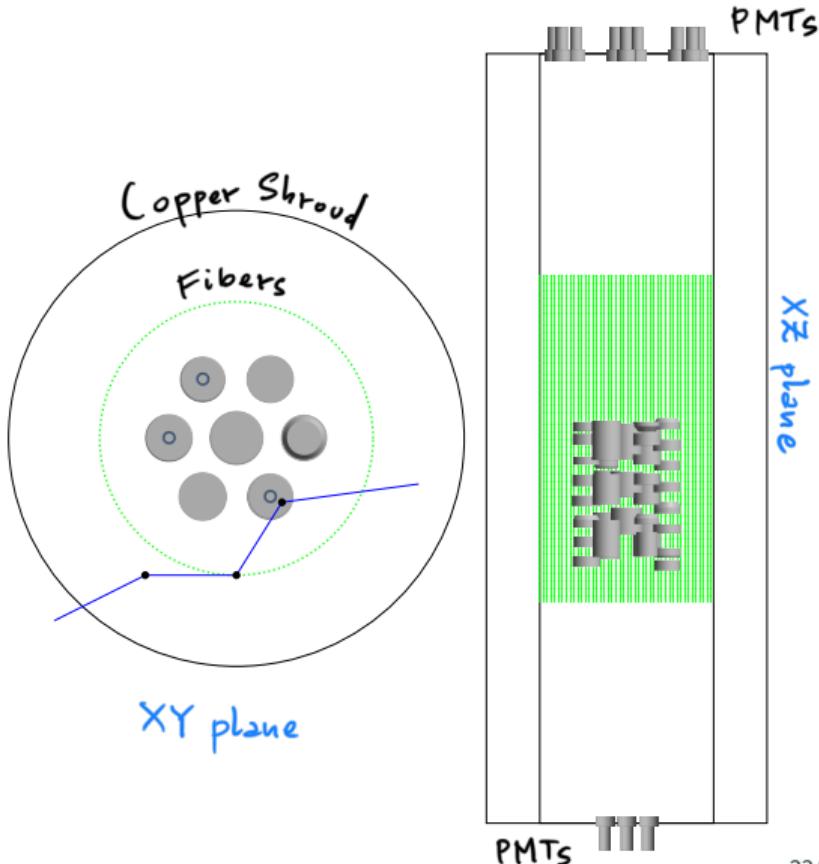
- CPU time becomes reasonable: ^{214}Bi calibration run: 30 ev/sec

...but still significantly time-consuming

¹strong dependence on the starting point

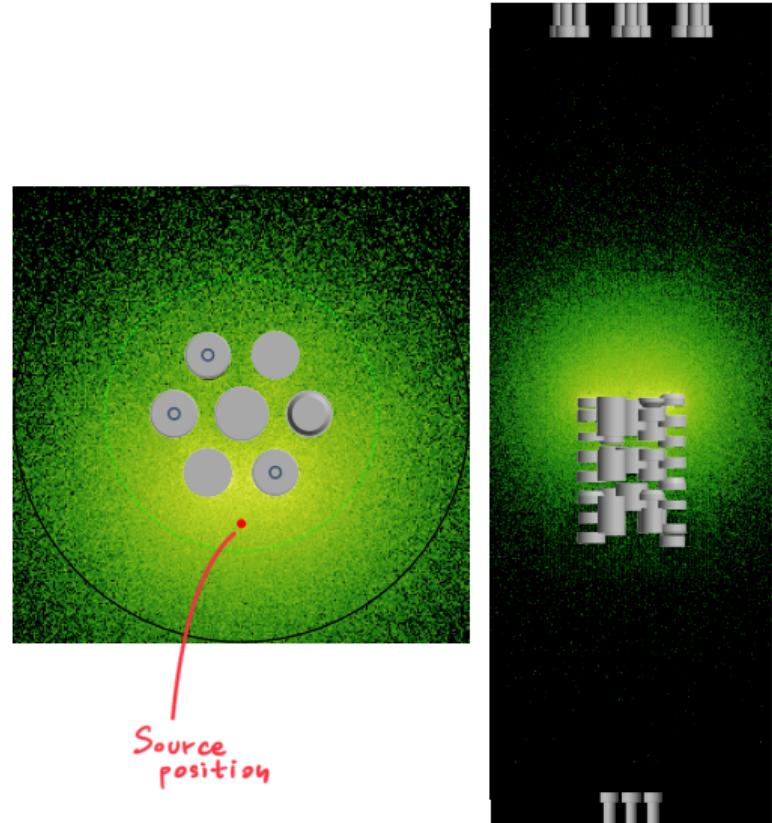
Externalizing the LAr detector model

- Optical physics is turned **off** in “regular” simulations (similarly to the HPGe detector case)
- Hits in LAr are saved to disk
- Example: ^{226}Ra calibration source



Externalizing the LAr detector model

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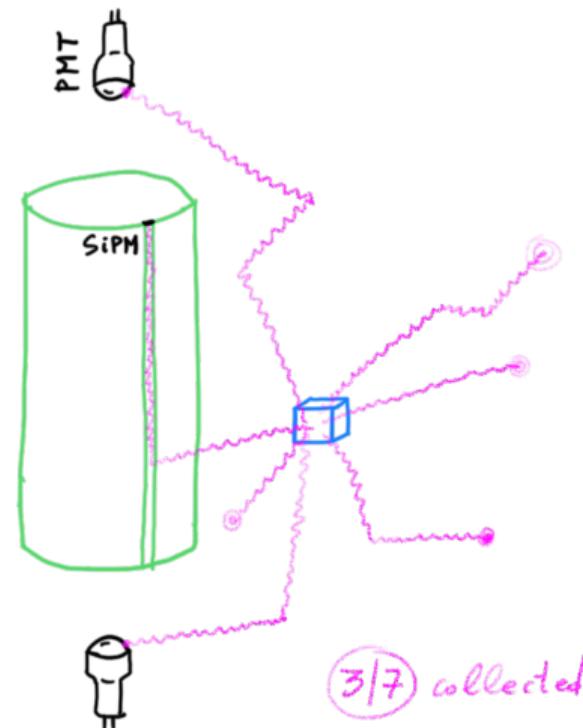


Determining the LAr veto model: probability map approach

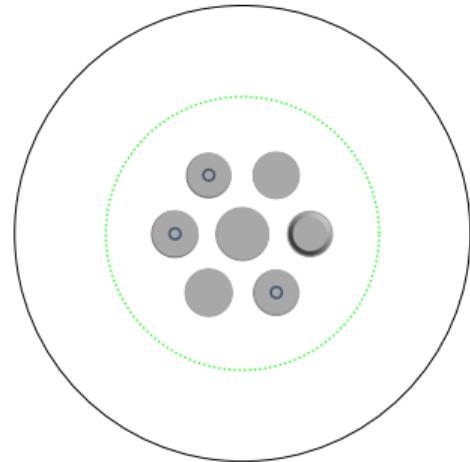
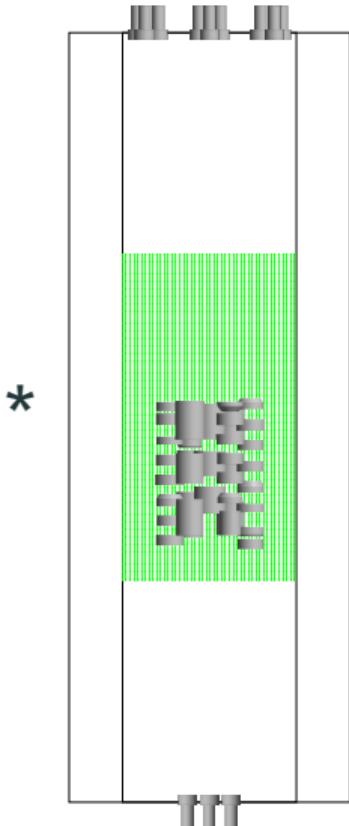
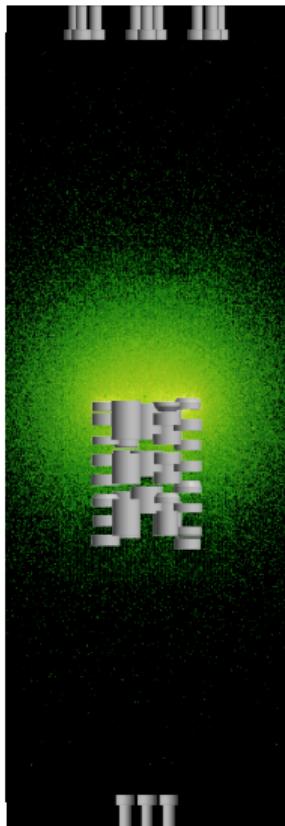
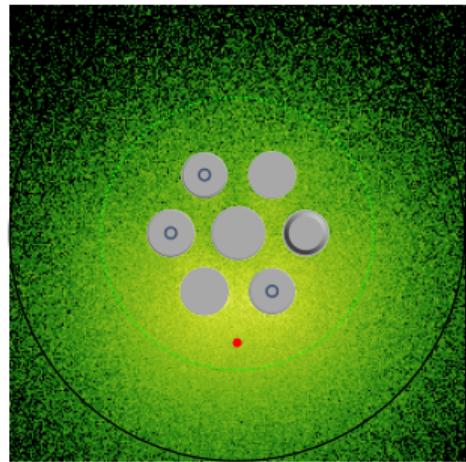
Tracking optical photons is computationally intensive, can we do it just once? **Probability map**

- Simulate 128 nm photons in LAr
- Partition the LAr volume in voxels ($\sim 3^3 \text{ mm}^3$)
- Calculate LAr veto detection probability for a photon in a voxel

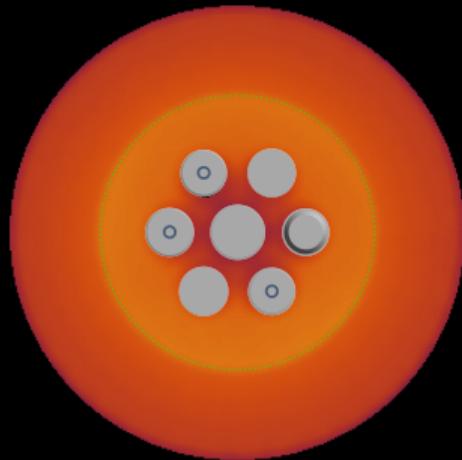
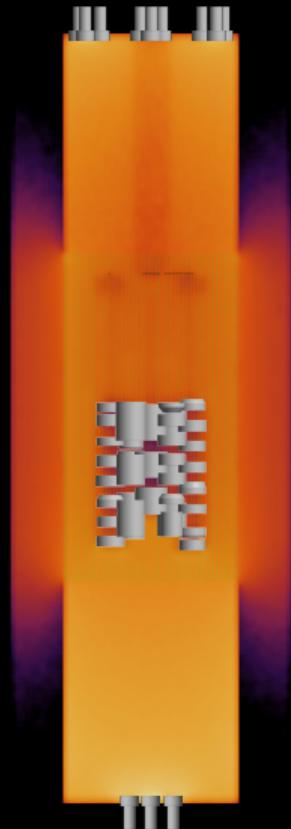
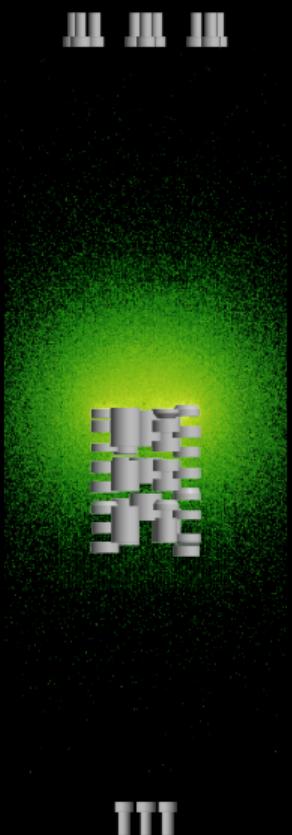
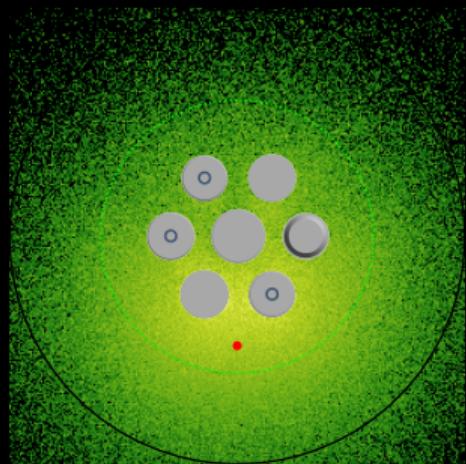
Effectively encapsulates the LAr veto model

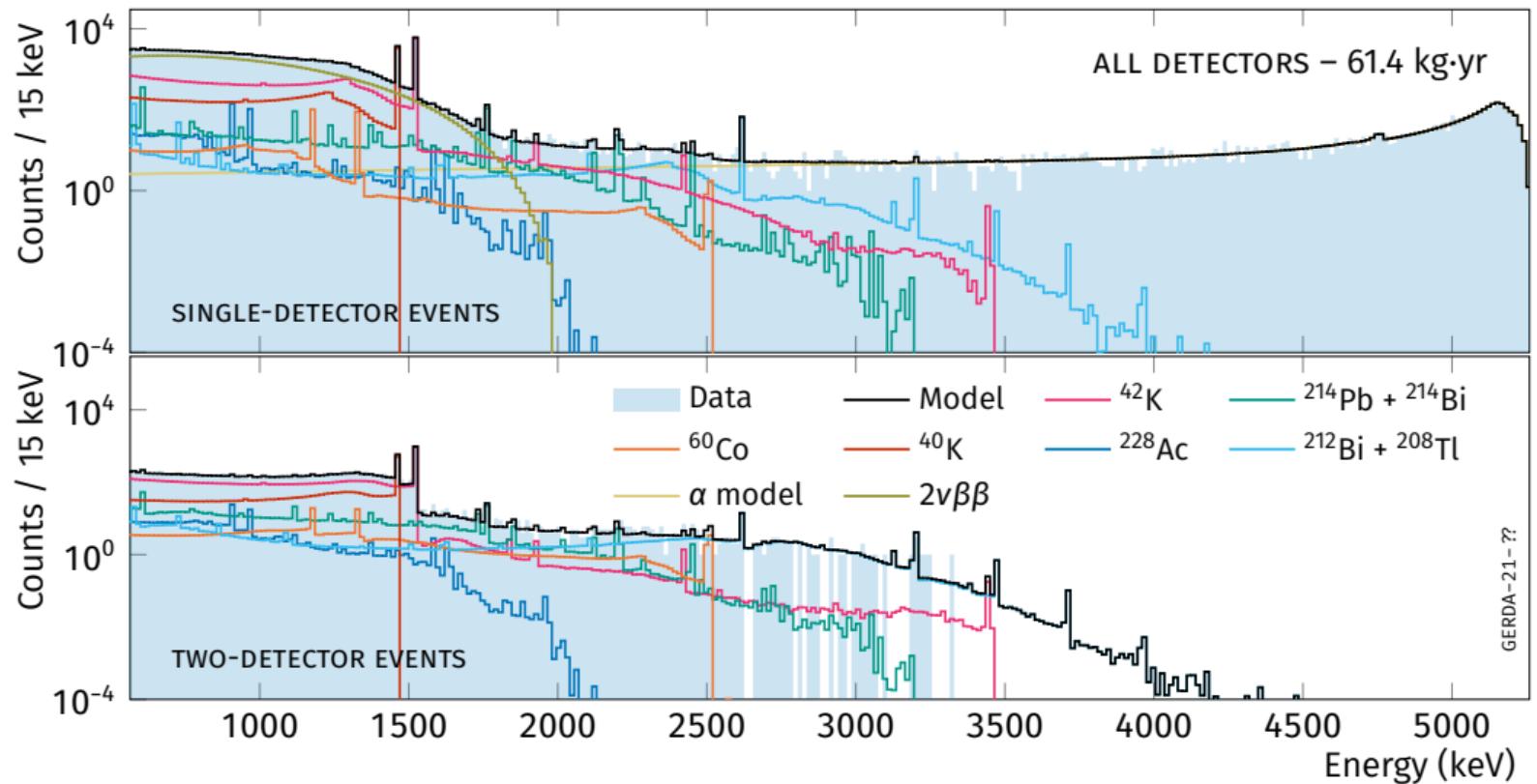


The probability map approach (lights on)

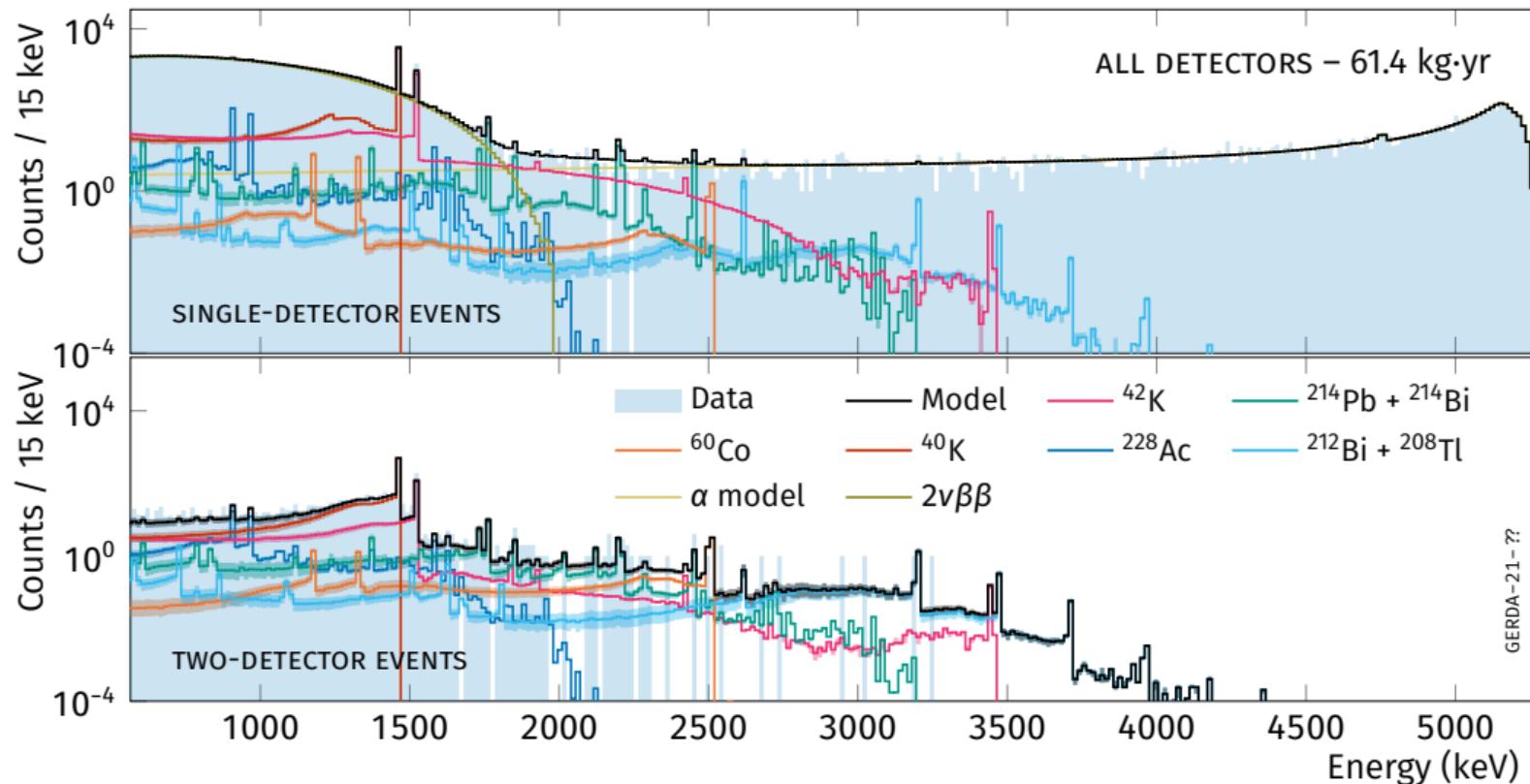


The probability map approach (lights off)





GERDA background decomposition after the LAr veto cut (preliminary)



The probability map approach: future

- With this voxel size, probabilities are quite low
- Several thousands of CPU hours are generally needed to produce a map

How to scale up? GPU!²

Opticks: GPU Optical Photon Simulation for Particle Physics using NVIDIA OptiX

Integrates NVIDIA GPU ray tracing, accessed via NVIDIA OptiX, with GEANT4 toolkit based simulations. Demonstrated x1500 speedup compared to GEANT4 (single-threaded)

- [simoncblyth/opticks](#) → stable releases
- [hanswenzel/G4OpticksTest](#) → integration in GEANT4 app demo

² Maybe electromagnetic interactions can be offloaded to the GPU too? [apt-sim/AdePT](#)

Outlook

A complete detector simulation is fundamental to

- Model the background of a running experiment (GERDA)
- (then) search for new physics
- Predict the background in the region of interest for $0\nu\beta\beta$ (LEGEND)

Challenges for future GEANT4-based frameworks

- Reduce disk space requirements (scorers, biasing)
- Speed up EM and optical simulations (GPU?)
- Integrate pulse shape simulations routines
- GEANT4 keeps improving, exploit new features

References i

- [1] A. Bideau-Mehu et al. *J. Quant. Spectrosc. Radiat. Transf.* 25 (5 1981), pp. 395–402. DOI: [10.1016/0022-4073\(81\)90057-1](https://doi.org/10.1016/0022-4073(81)90057-1)
- [2] T. Doke et al. *Nucl. Instrum. Meth.* A269 (1988), pp. 291–296. DOI: [10.1016/0168-9002\(88\)90892-3](https://doi.org/10.1016/0168-9002(88)90892-3)
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References ii

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- [10] URL: https://www.dropbox.com/sh/nky7k414bqevhv7/AACnr_ncW5mJdY7huq9EaxcCa?dl=0