Enabling Rare Event Discovery with Surrogate Modeling and Simulation AI Agents

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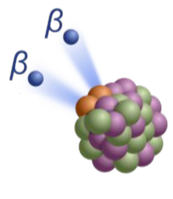
LEGEND

Large Enriched Germanium Experiment for Neutrinoless ββ Decay

LEGEND: Large Enriched Germanium Experiment for Neutrinoless ββ-Decay

Mission: Develop a phased, **^{76}Ge based ββ-decay experimental program** with discovery potential at a half-life beyond 10^{28} y

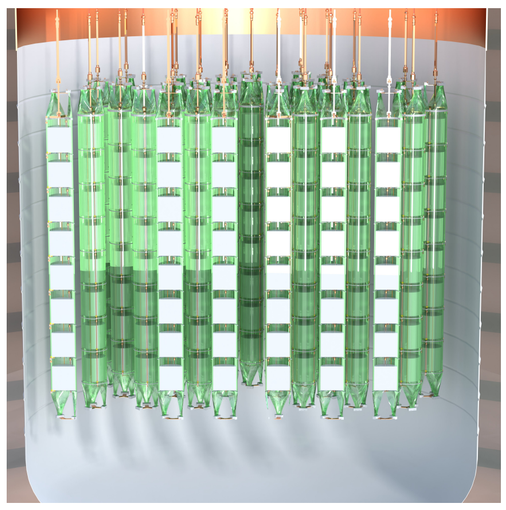
Strategy: Build an **array of high purity germanium detectors enriched in ^{76}Ge** as source and detector of the decay; operate **background free**



Neutrinoless ββ-decay (0νββ)

Phased Deployment:

1. **LEGEND-200**: currently operating 140 kg of detectors; discovery sensitivity goal $T_{1/2} > 10^{27}$ y.[1]
2. **LEGEND-1000**: will operate 1000 kg of detectors. Discovery sensitivity goal $T_{1/2} > 10^{28}$ y.[2]
   - Successful CD1 review; awaiting funding

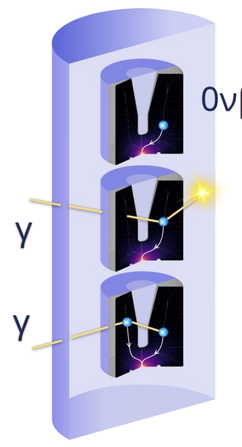


CAD Rendering of LEGEND-1000 detector array

Background free goal: achieve background index $< 2 \times 10^{-4}$ cts/keV-kg-y

Detectors **deployed in liquid argon**. Use scintillation light to **actively veto** backgrounds that are not contained in a detector

LEGEND rejects >99% of backgrounds to 0νββ



Reject backgrounds not confined within ~1 mm

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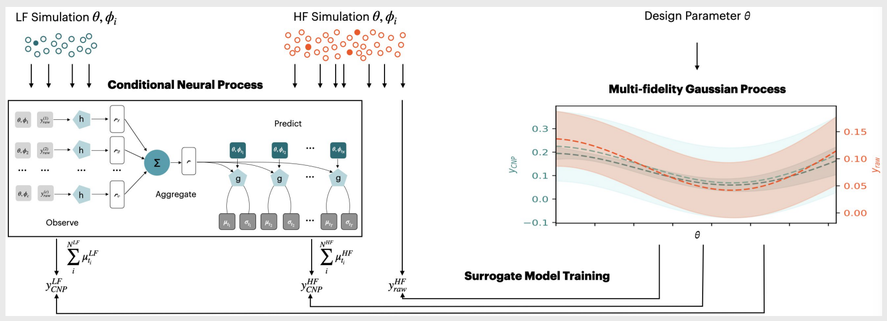
Purpose: to ensure LEGEND-1000 is background free we aim to **optimize the detector design** for maximal light collection over the full liquid Argon volume based on simulations

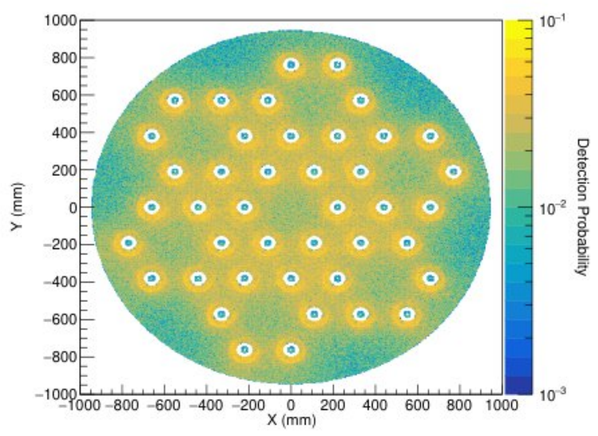
Problem: **Optical simulations** are a computationally expensive bottleneck. LEGEND produces maps of the photon detection probability over the volume, and the cost of constructing the maps hinders optimization tasks

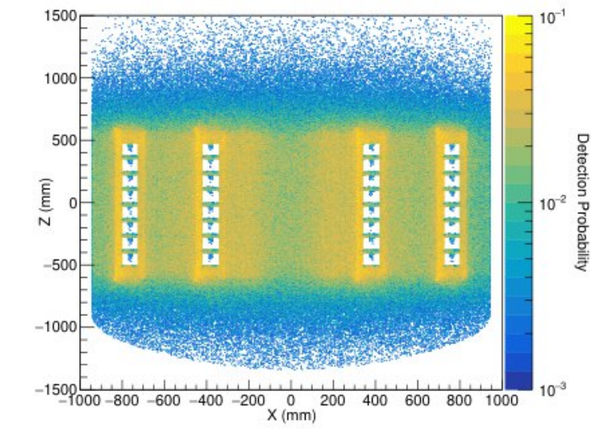
Goal: **accelerate optical map construction by two orders of magnitude** using a GPU-accelerated surrogate model assisted by an AI agent, and integrating into the LEGEND analysis pipeline



RESuM uses conditional neural process (CNP) and multi-fidelity Gaussian process (MFGP) to produce uncertainty-aware surrogate model; achieve similar precision with fewer resources![3]

Objective 1: Develop a **Rare Event Surrogate Model (RESuM)[3]**, an uncertainty-aware model, to construct optical maps using **>10x fewer simulated photons** than existing, voxelized techniques





Slice of LEGEND-1000 optical map generated using slow voxelized method[4]

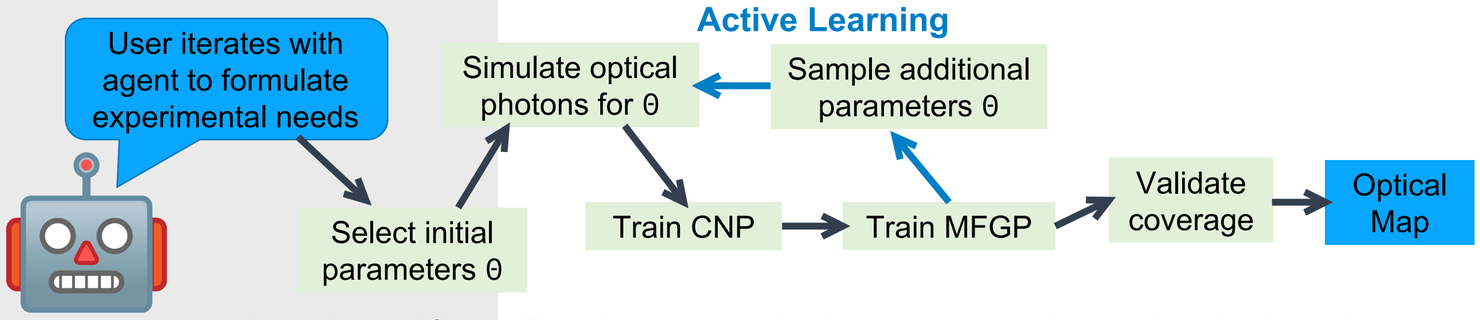
Objective 2: **Integrate the RESuM map** and training process into the LEGEND simulation framework, remage[5], and **generate training and validation data** using the LEGEND-1000 design geometry

Application	Runtime (s)	Speed-up
Geant4	478.990	1x
Celeritas CPU - Event	116.251	4.12x
Celeritas CPU - Track	6.739	71.1x
Celeritas GPU	0.485	988x

Benchmark comparison of simulated optical transport in liquid argon sphere using A100 GPU and single AMD Epyc 7532 CPU[7]

Objective 3: Accelerate optical simulation using GPUs by **integrating the Celeritas[6] monte-carlo code** for Geant4 into LEGEND optical simulations, for >800x speedup vs single-CPU (**reduce node-for-node wall time by >10x**)

Objective 4: Develop a large language model-based **AI agent to orchestrate** the construction of a map, enable **active learning**, and accelerate the **training of researchers** in the construction of maps



Agentic workflow will orchestrate optical map construction and active learning

Towards Genesis Phase II

We are interested in collaborating with a consortium geared at revolutionizing our use of particle transport simulations for physics experimental design and analysis, nuclear engineering, medical imaging, and other applications, by developing tools including surrogate models, differentiable simulations, agentic automation of complex processes, etc. **Reach out to collaborate!**

References

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2. N. Abgrall et al (LEGEND Collaboration). "The Large Enriched Germanium Experiment for Neutrinoless ββ Decay: LEGEND-1000 Preconceptual Design Report." arXiv:2107.11462 (2021)
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