Machine learning based design optimization for the search of neutrinoless double-beta decay with LEGEND

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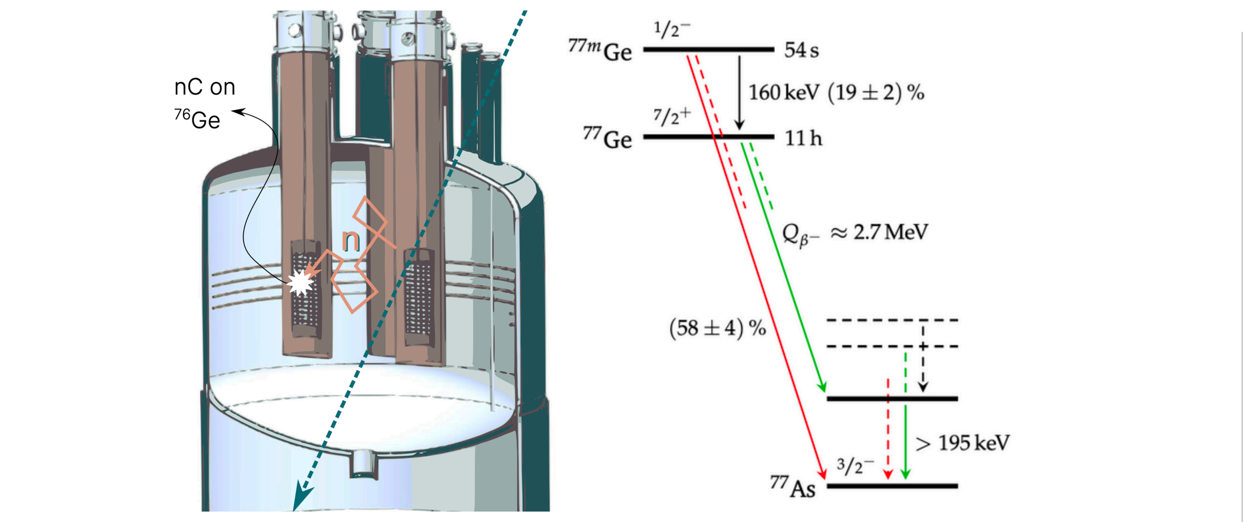
The **Large Enriched Germanium Experiment for Neutrinoless ββ decay** (**LEGEND**) searches for the neutrinoless double beta decay in the ^{76}Ge isotope. The proposed LEGEND-1000 phase will consist of 1000 kg of enriched High Purity Ge detectors, designed to achieve a discovery sensitivity of 10^{28} yr going beyond the inverted-ordering neutrino mass region.

Muon-induced background



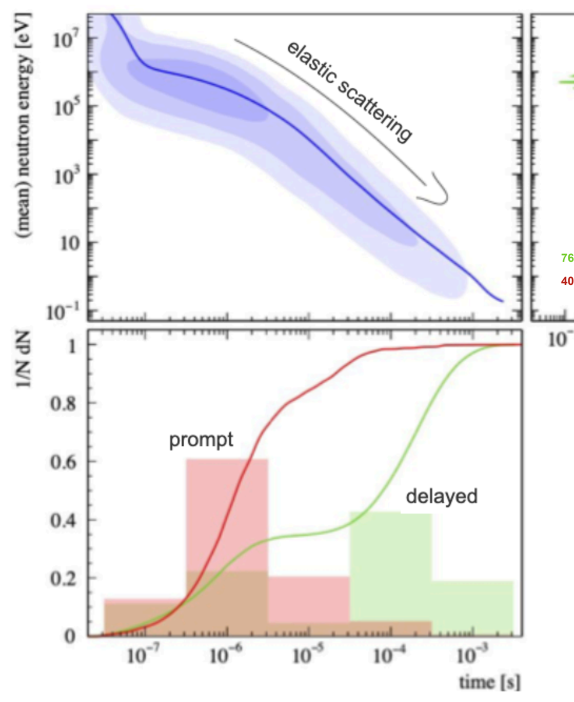
- Prompt interactions of shower constituents discriminated with >99% [0]
- $^{77(m)}$Ge produced by neutron capture on ^{76}Ge
- Delayed decays of ^{77}Ge and metastable ^{77m}Ge are dominant cosmogenic background [1,2]

Total background index goal of LEGEND-1000 is 10^{-5} cts/keV/kg/yr [5]. How large is the muon-induced background at LNGS?

Location	Depth [km.w.e]	$^{77(m)}$Ge background contribution (w/o new cuts) [cts/(keVkgyr)]
SNOLab (Ref. Site)	6	$(2.0 \pm 0.5)\cdot 10^{-7}$ [5]
LNGS (Alt. Site)	3.5	$2\cdot 10^{-5}$ [0]

Adding a passive shielding into the LAr with neutron absorber materials, such as e.g. polymethylmethacrylat (PMMA), the production rate of ^{77}Ge depends on various material properties, e.g. neutron yield, cross-section, as well as the positioning of the absorber,…

Neutron flux reduction



Neutron moderators can reduce the ^{77}Ge production by slowing down the neutrons and increasing their likelihood to be captured on ^{40}Ar instead of ^{76}Ge.

Neutron Moderator Design Optimization with ML based Active Learning

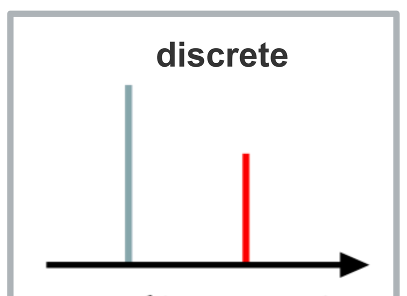
Traditional Monte Carlo simulations, may prove time-consuming and challenging when addressing full optimization across numerous parameter spaces. This renders conventional methods, such as grid searches, computationally infeasible. **Goal:** Build an emulator and find optimal design parameters

Design [Radius, Thickness, N panels, Theta, Length] → **Emulator** → **^{77}Ge production rate**

GEANT4 Monte Carlo Simulation

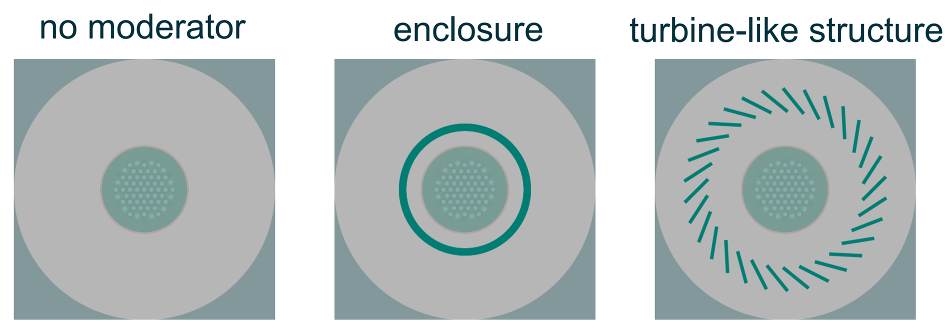
Run a few simulations at different parameters

- MC studies using a custom simulation module[3] to optimize the moderator screening effect
- Based on LEGEND-1000 and GERDA setup[3] implementation



$$f(x) = \begin{cases} 1, & \text{n captured,} \\ 0, & \text{n not captured} \end{cases}$$

- Solid neutron moderator design [3],[6]: enclosing tube (with thickness **d**) or turbine-like structure (with **n panels, thickness d, length L** and **angle** θ) at **radius r** (both designs can be described by the 5 parameters)



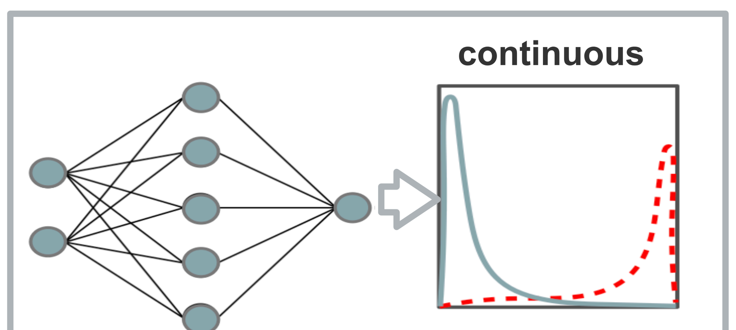
Two fidelity levels:

- **High fidelity (HF):** cosmic muons are propagated through the setup including their secondaries (very costly)
- **Low fidelity (LF)**: neutrons inside the LAr cryostat are simulated, the neutron input parameters are drawn randomly from the HF simulation

Conditional Neural Process (CNP)[7]

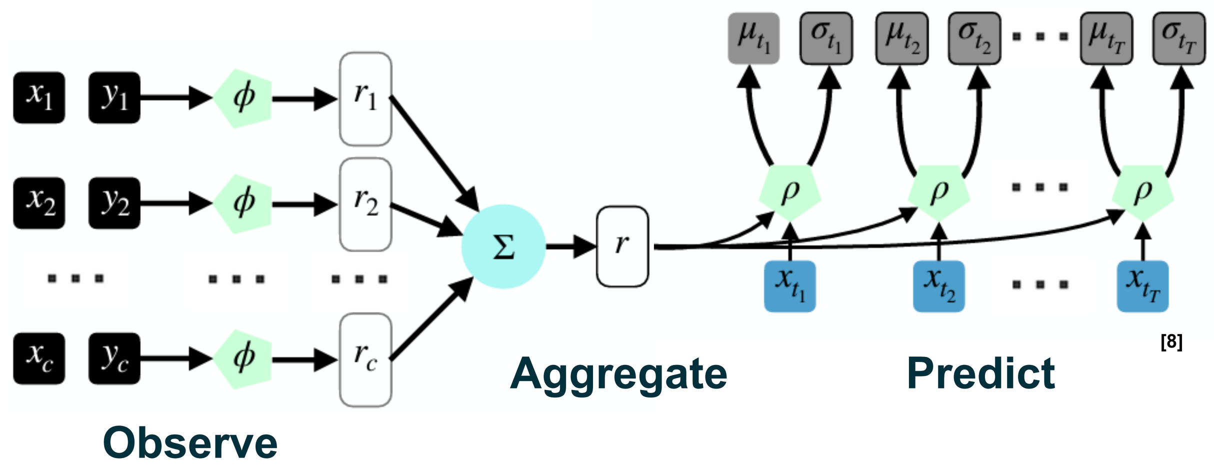
Train a predictive model using simulation data

neutrons, ^{77}Ge captures

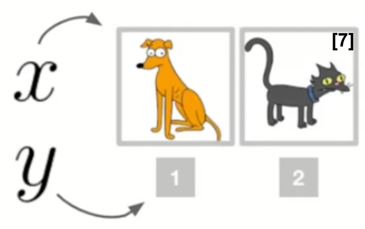


$f(x) \in [0,1]$

mean neutron capture prob. of each moderator

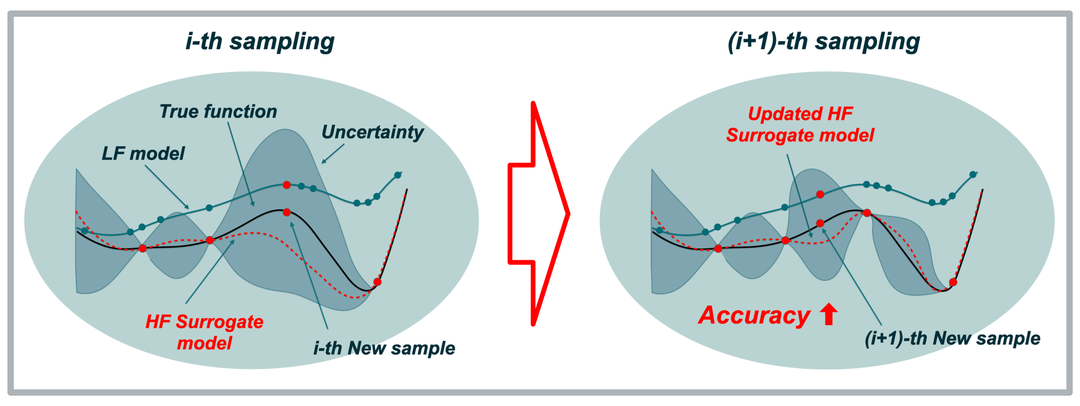


- Learn Contextual Features
- Maximize the Posterior Likelihood to Train
- Uncertainty prediction
- Small dataset size (where avoiding overfitting important)

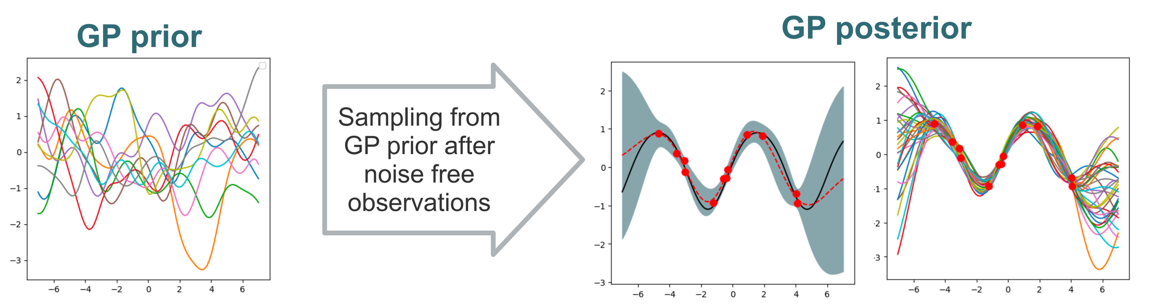


Surrogate Modeling via MF-GP

Predict simulation output at new parameters



- Gaussian Process: Bayesian method of prediction and uncertainty analysis combined with multi-level approach



- Combine fast LF simulations with costly HF simulations sharing basic features
- Multi-Fidelities (MF) ranked hierarchically by accuracy (t=0,…,T)

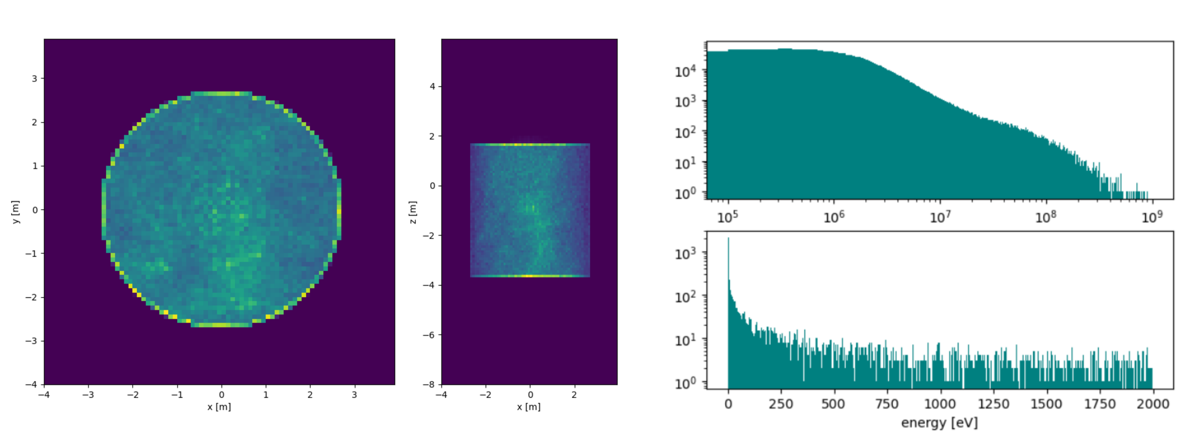
$$\eta_t(x) = \rho_{t-1}\,\eta_{t-1}(x) + \delta_t(x)$$

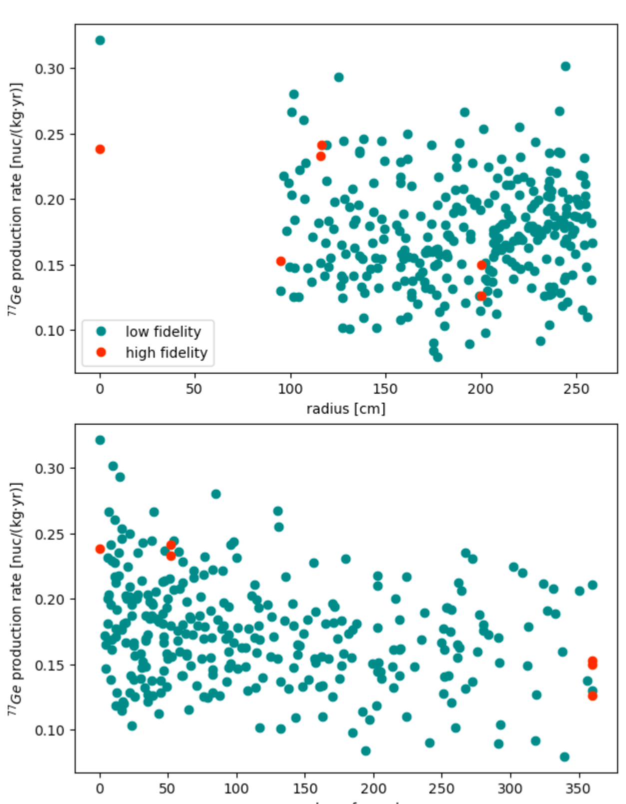
discrepancy term modeled by GP

similarity to lower fidelity (GP)

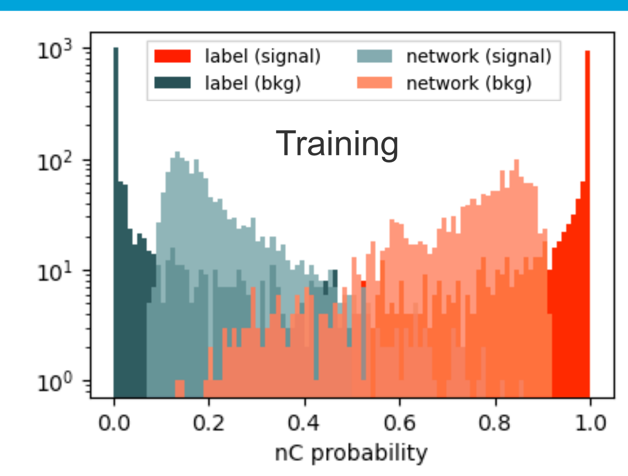
- Adaptive sampling by maximizing acquisition function (trade off between exploration and exploitation)

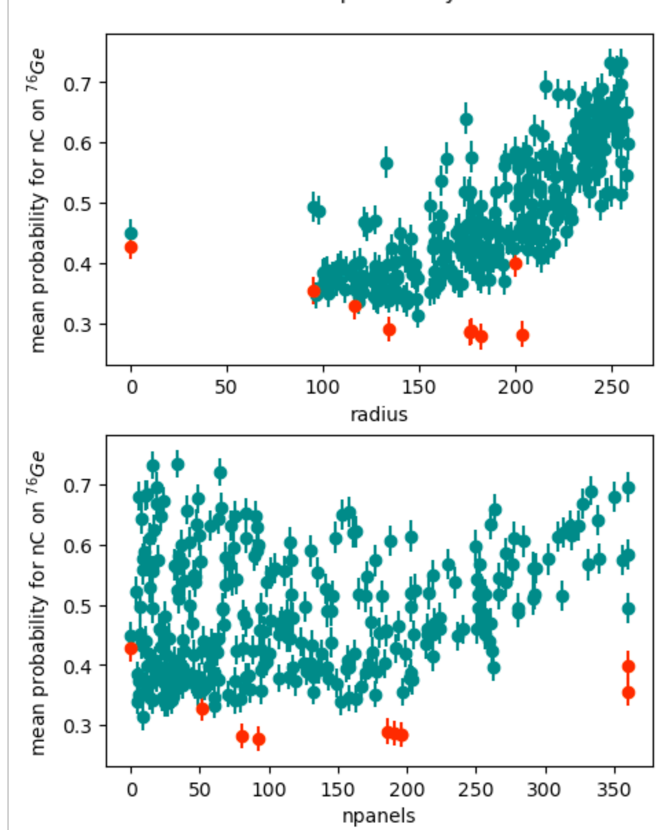
Apply active learning to neutron moderator design optimization



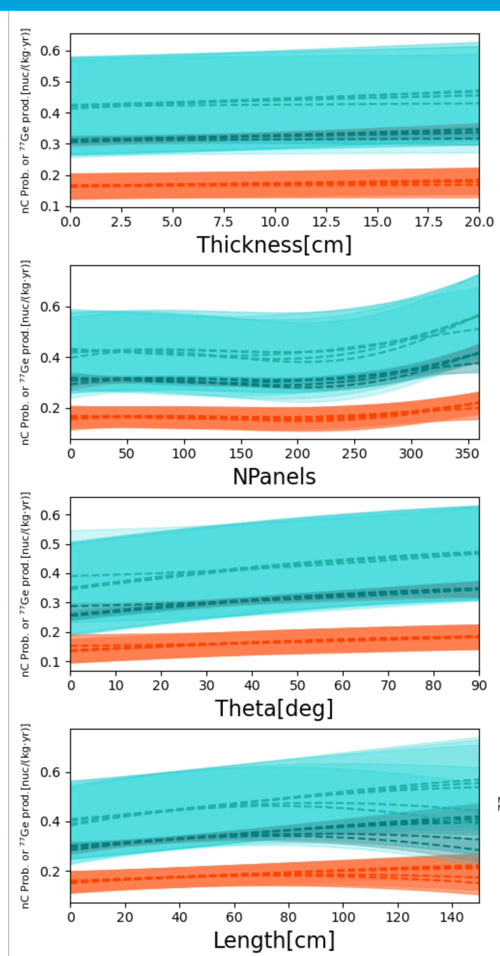


- 300 LF samples, randomly sampled while adhering to parameter constraints
- 4 initial HF samples
- Count total number of neutron captures on ^{76}Ge
- ^{77}Ge production rate over radius (t.l.) and number of panels (b.l.) shown as 1-dim projection

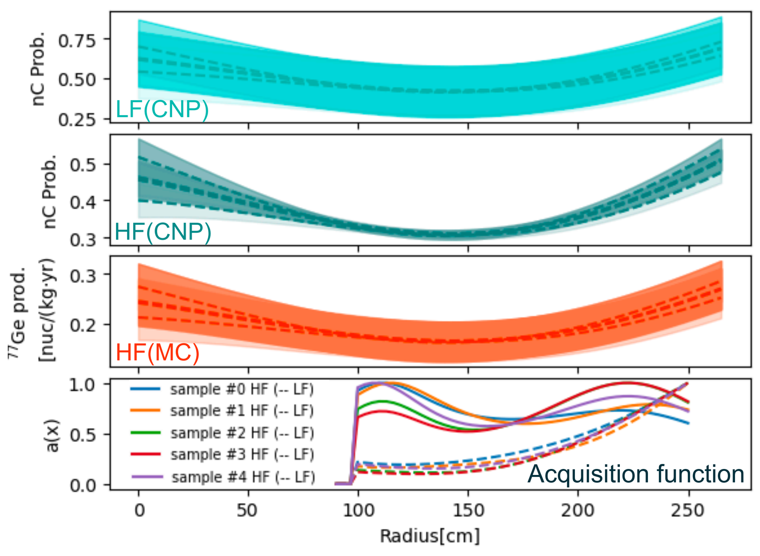


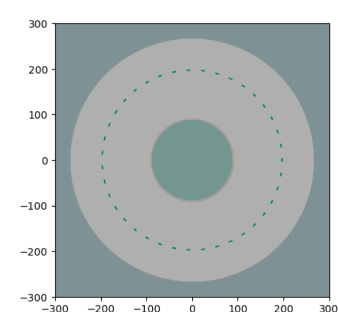


- Signal (red) vs background (blue) Classification
- Data augmentation used for imbalanced training data set
- CNP effectively learns from neutron physics parameters
- Separation between signal and background
- For each moderator design, a mean neutron capture probability with an uncertainty estimate can be derived
- Mean neutron capture probability over radius and number of panels is shown as 1-dim projection
- CNP learns underlying distribution



- Modeling of 5 dim space (r, t, θ, n, L) with 3 fidelities (HF(MC), HF(CNP) and LF(CNP))
- Model evolution shown as projection on r, t, n, θ and L at a random point in space
- Acquisition function: Integrated variance reduction with parameter constraints





Optimal design (b.r.) found with reduction by a factor of 1.7 and a ^{77}Ge production rate of 0.14 nuc/(kg·yr)

Summary

- Active and passive cosmogenic background reduction is contingent upon LEGEND-1000 selecting a shallower host site
- Various options for moderator designs are currently under active research and are being considered for implementation
- A solid shield design has been identified which holds the potential of reducing the neutron background by a factor of 1.7

Goal

- Demonstrate a technique on a small-scale application, which can be adopted for more complicated tasks of exploring alternate designs of detectors
- Approach can be used for many (shielding) simulation optimization tasks. There are many different multi-fidelity model approaches (hierarchically ranked, varying mesh size, staged,…) available

Future Improvements

- Integration of additional output constraints such as material dependence, additional background contribution, and cost considerations.
- Transfer Learning MF-GP model that makes informed decisions by incorporating expected improvements and considering the computational resources associated with each fidelity level

[0] K. Freund et al., Eur.Phys.J.C 76 (2016) 5, 298. [1] L. Pandola et al., Nucl. Instr. Methods A 570 (2007) 149 [2] C. Wiesinger et al., Eur. Phys. J. C (2018) 78:597 [3] https://github.com/drbenmorgan/warwick-legend
[4] C.J. Barton, PoS(ICHEP2020)195 [5] LEGEND-1000 pCDR (https://legend-exp.org/science/publications) [6] M. Neuberger, J. Phys.: Conf. Ser. 2156, 012216 (2022). [7] arXiv:1807.01613 [8] Richard E Turner [9] arXiv:211013293

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