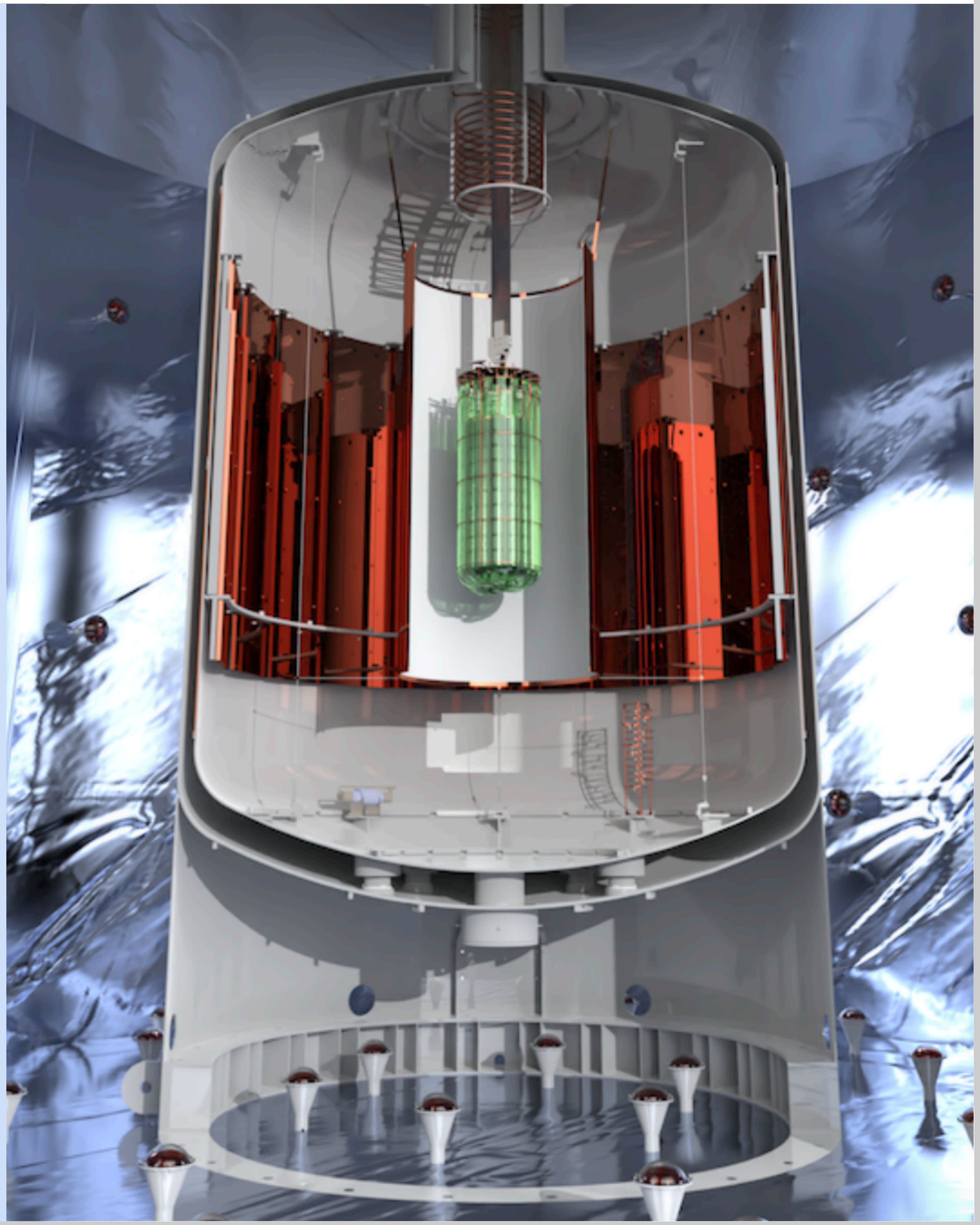
Machine learning based design optimization for the search of neutrinoless double-beta decay with LEGEND

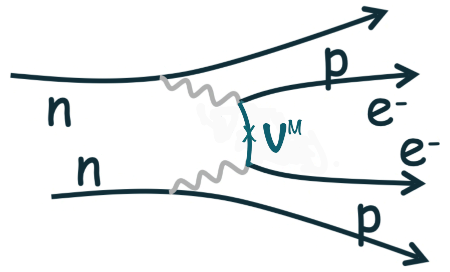
LEGEND

Large Enriched
Germanium Experiment
for Neutrinoless ββ Decay



Ann-Kathrin Schuetz (LBNL), Aobo Li (UCSD)
Lawrence Berkeley National Laboratory
on behalf of the LEGEND collaboration

4th MODE Workshop - September 23rd 2024



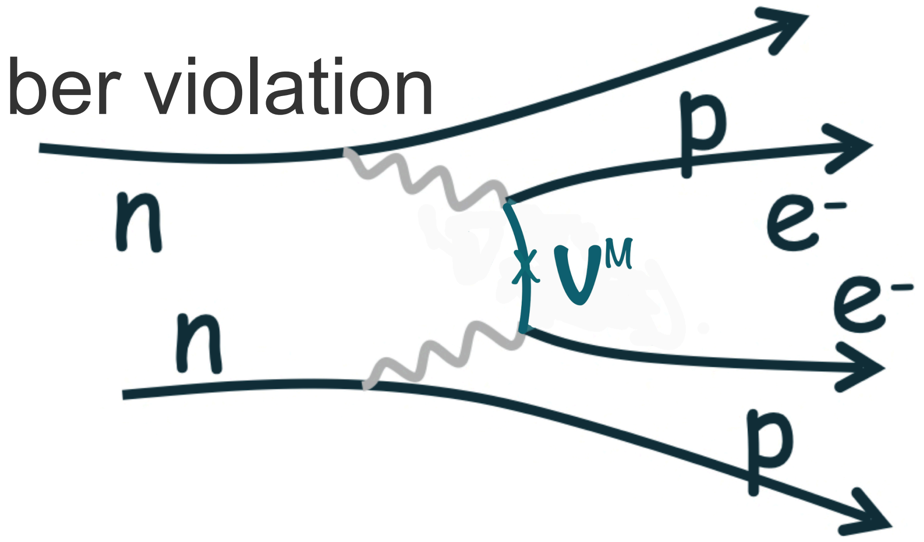
$\Delta L \neq 0$

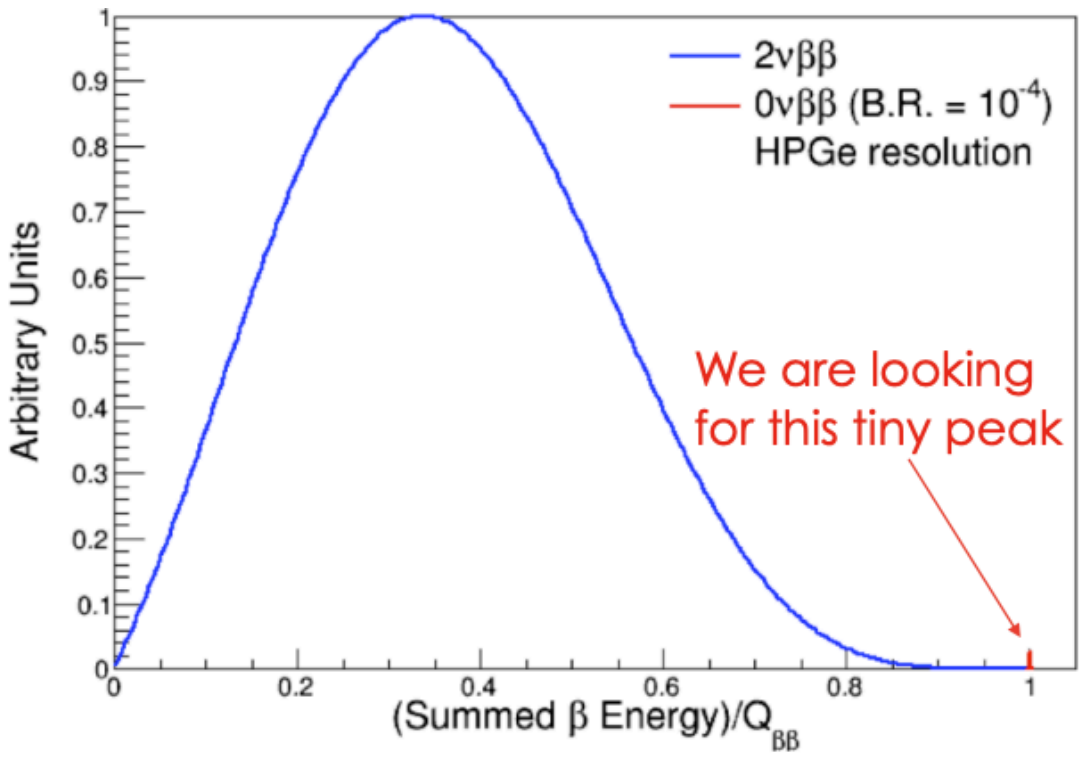
Example: Bayesian Inference and 0νββ decay

Experimental goal is to measure mono-energetic peak at Q_{bb}

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

Lepton number violation





measure sum energy spectrum of electrons

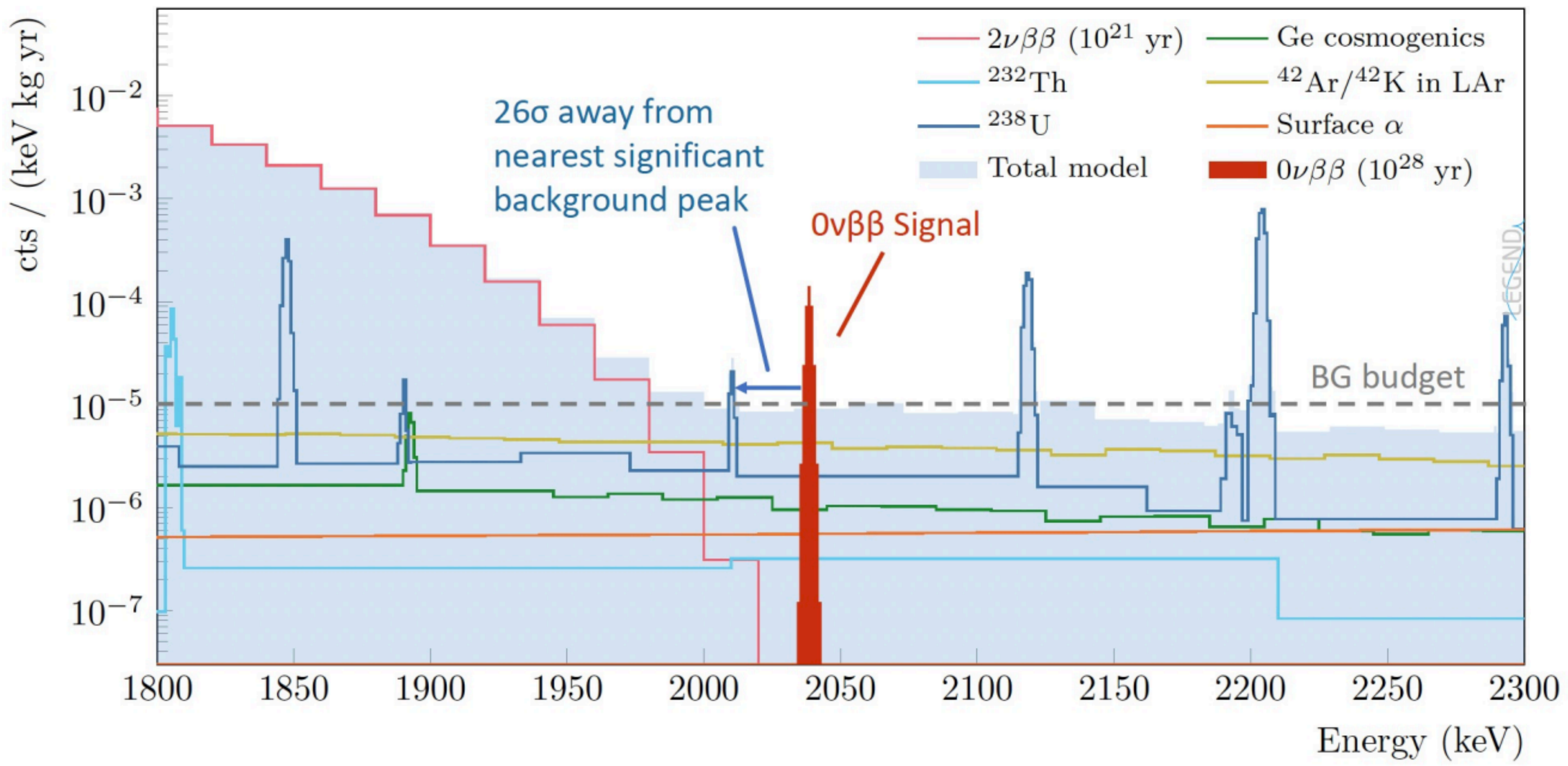
- 2νββ → continuum
- 0νββ → mono-energetic peak @ $Q_{\beta\beta}$

But this signal is buried under other backgrounds…

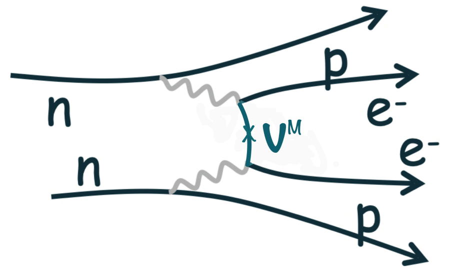
Experimental sensitivity:

background (BI) > 1:

$$T_{1/2}^{0\nu} \propto \varepsilon \cdot a \cdot \sqrt{\frac{M \cdot t}{BI \cdot \Delta E}}$$



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



$\Delta L \neq 0$

0νββ decay - Experimental sensitivity

$$T_{1/2}^{0\nu} \propto \varepsilon \cdot a \cdot \sqrt{\frac{M \cdot t}{BI \cdot \Delta E}}$$

Background index

LEGEND-1000 background goal:

$<10^{-5}$ cts/keV/kg/yr

$^{77(m)}$Ge background at LNGS:

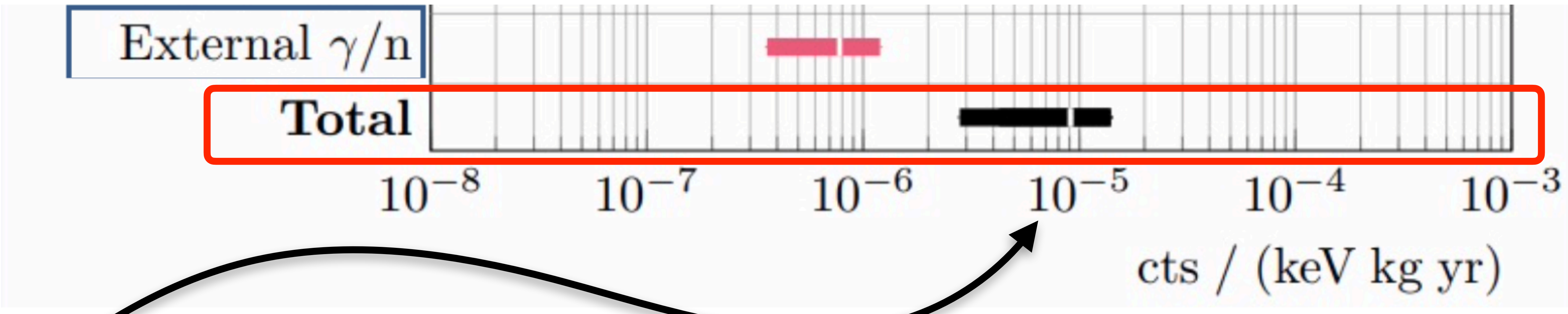
$>10^{-5}$ cts/keV/kg/yr

arXiv:2107.11462

BUT: many opportunities to reduce and actively suppress this background

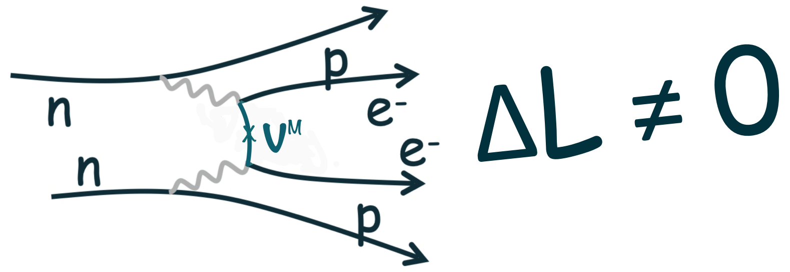
arXiv:1802.05040

Why do we have to reduce the cosmogenic background at LNGS?

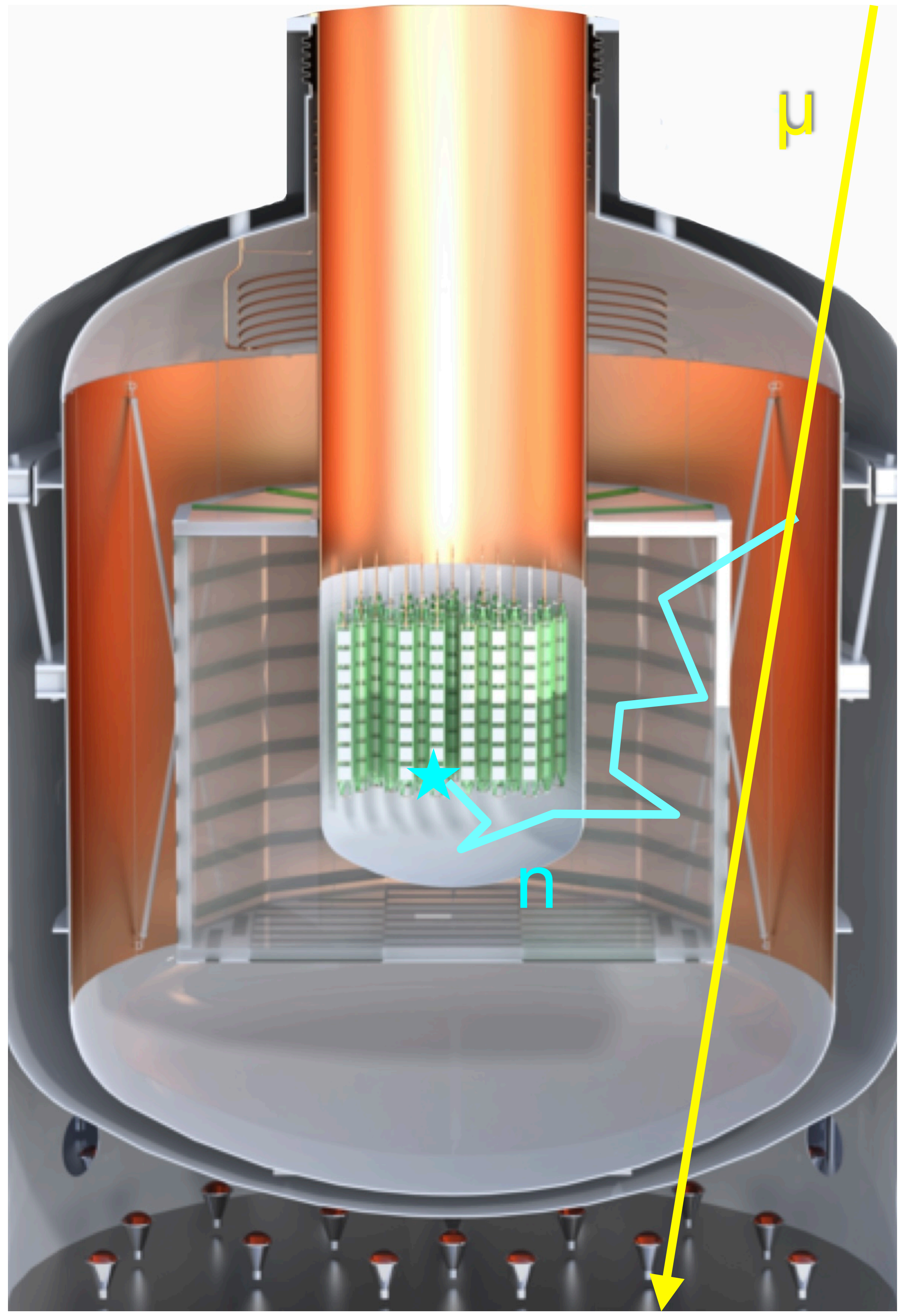


Location	Depth [km.w.e.]	$^{77(m)}$Ge background contribution (w/o new cuts*) [cts/keV/kg/yr]
SNOLab (Reference Site)	6	4.2×10^{-7} [0]
LNGS (Alternative Site)	3.5	2.7×10^{-5}

* standard background rejection are applied which strongly supresses ^{77}Ge



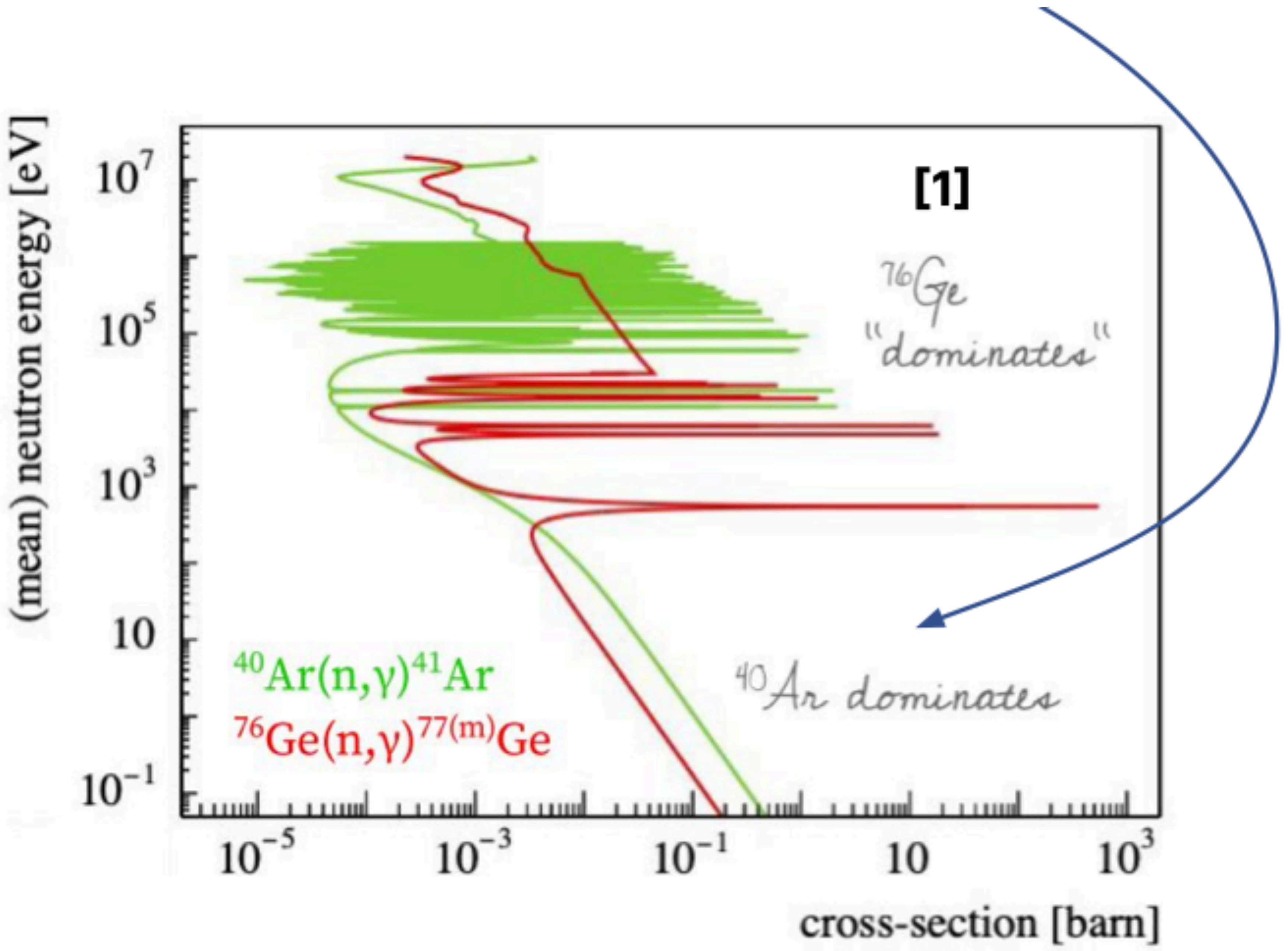
What options are there to reduce the impact of cosmogenic background?

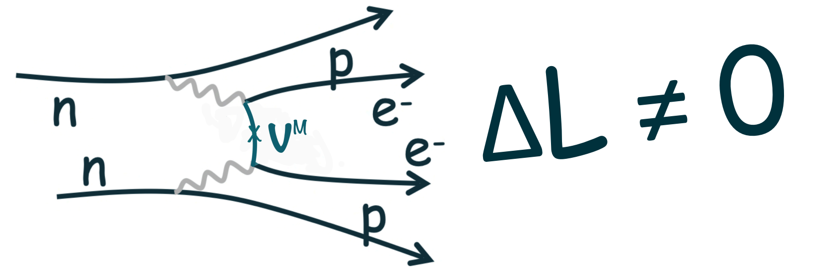


1. Reduce the muon flux → increase overburden.
2. Reduce the neutron flux around the detectors.
3. Tag the $^{77(m)}$Ge production and apply a delayed coincidence cut.

Reduce the neutron flux around the detectors - *Idea*:

add neutron moderators to slow neutrons down and increase their likelihood to be captured by LAr instead of ^{76}Ge.

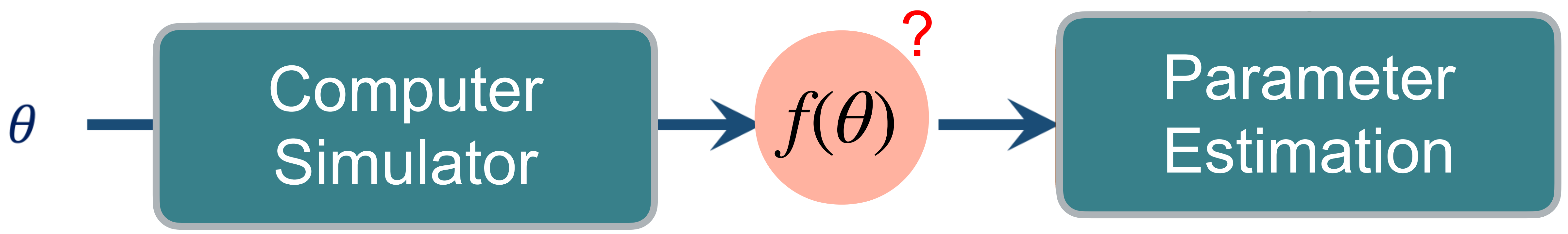


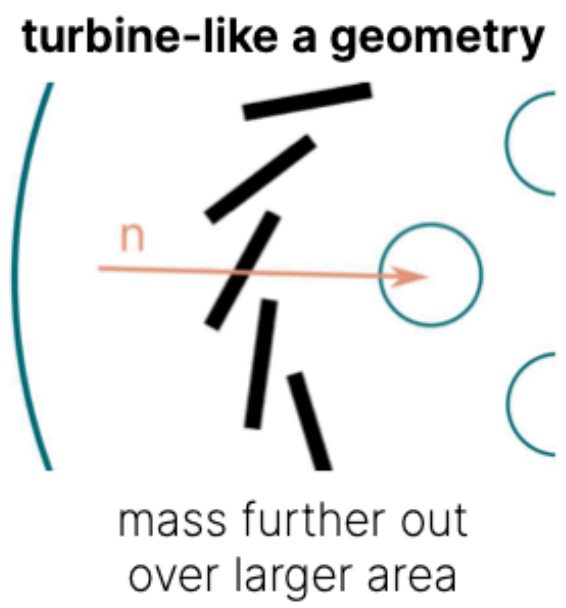


Optimal Design Parameters

How to find the optimal design parameter?

Run a few simulations at different parameters





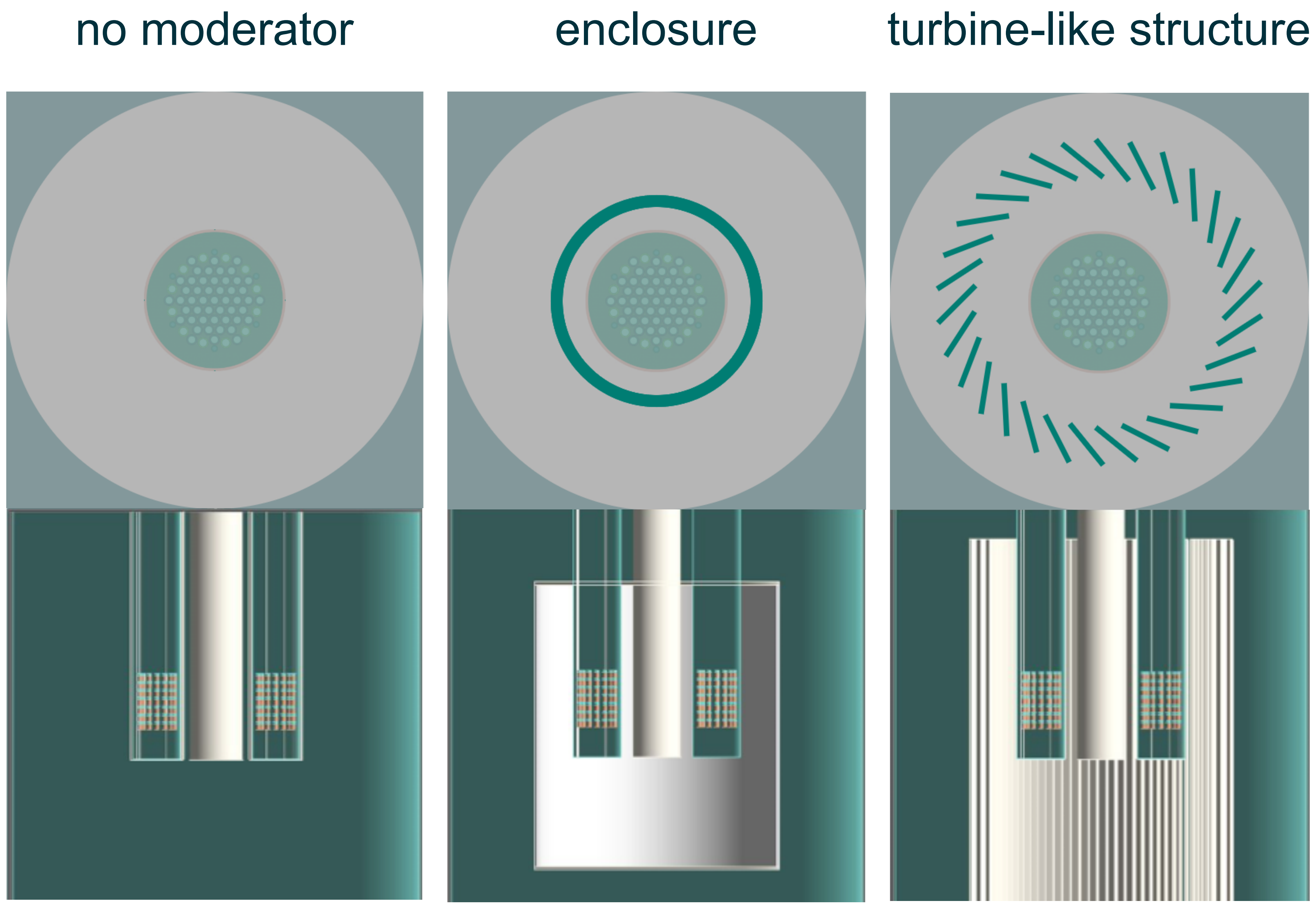
- MC studies using a custom simulation module[3] based on LEGEND-1000 and GERDA setup[3] implementation
- Solid neutron moderator design: enclosing tube or turbine-like structure
- 5 design parameters: Radius r, n Panels, Thickness d, Length L and Angle θ

➡ **High-dimensional parameter spaces**

➡ **High computational cost of Geant4 MC simulations (~200 CPUh)**

➡ **Traditional methods like grid searches are impractical**

Starting point: 4 high fidelity simulation data points only!!



Surrogate based on Gaussian Process

Regression task:

predict the value of y_n for a new value of x_n where $f : \{\theta_n\}^N \rightarrow \{y_n\}^N$ maps the input space to the output space

Let's start with a distribution of all possible functions that, could have produced our data (without actually looking at the data!).

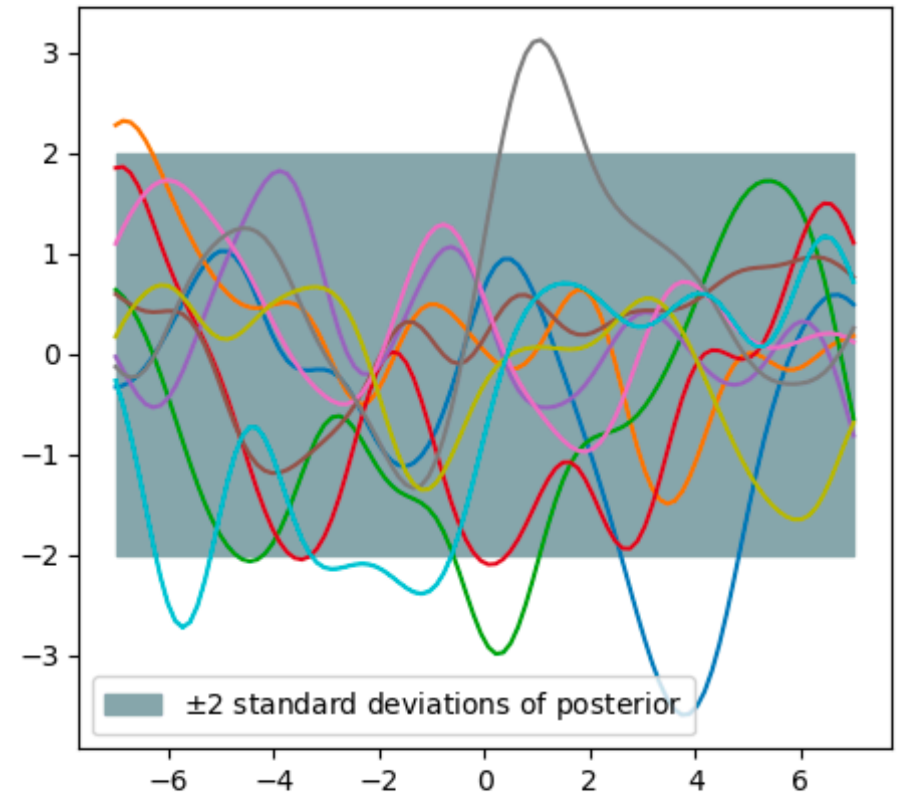
$$f(\cdot) \sim p(f(\cdot)) \sim \mathcal{N}(\mu(.), \sigma(.))$$

> ***A Gaussian process is a probability distribution over possible functions that fit a set of points.***

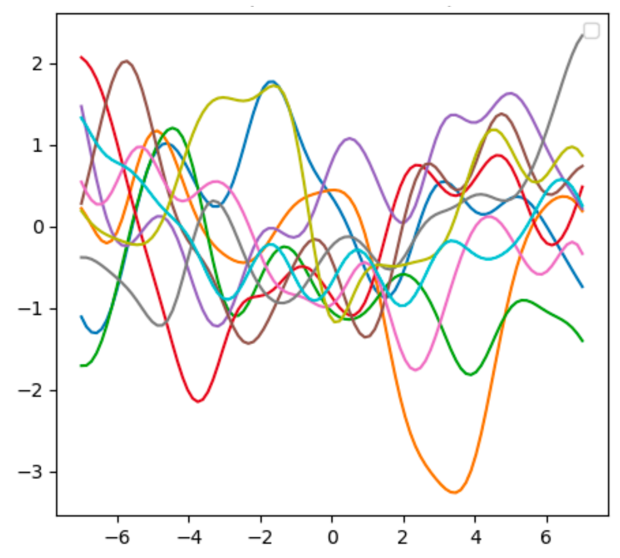
Gaussian Process

$$f(\theta) \sim GP(m(\theta), k(\theta, \theta'))$$

mean of posterior

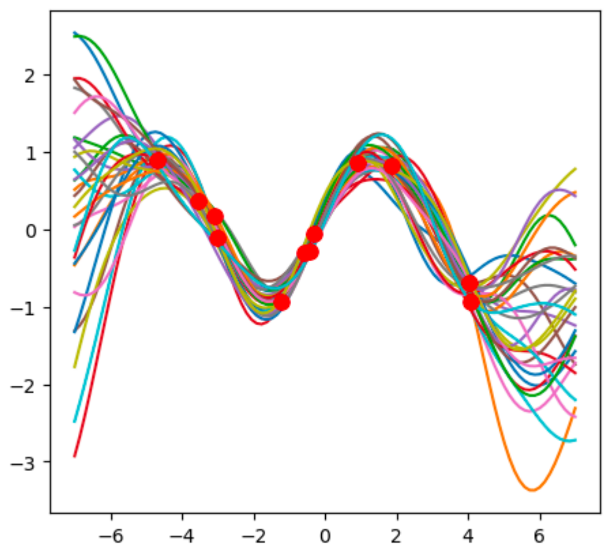


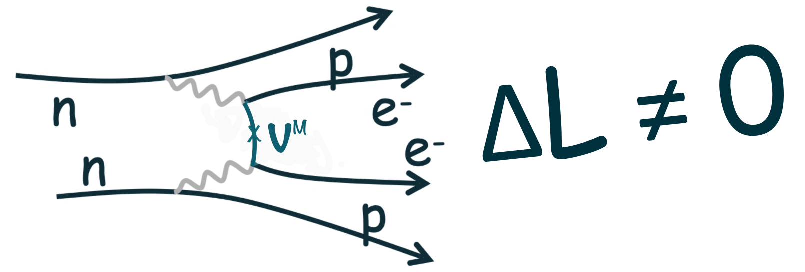
GP prior



data

GP posterior

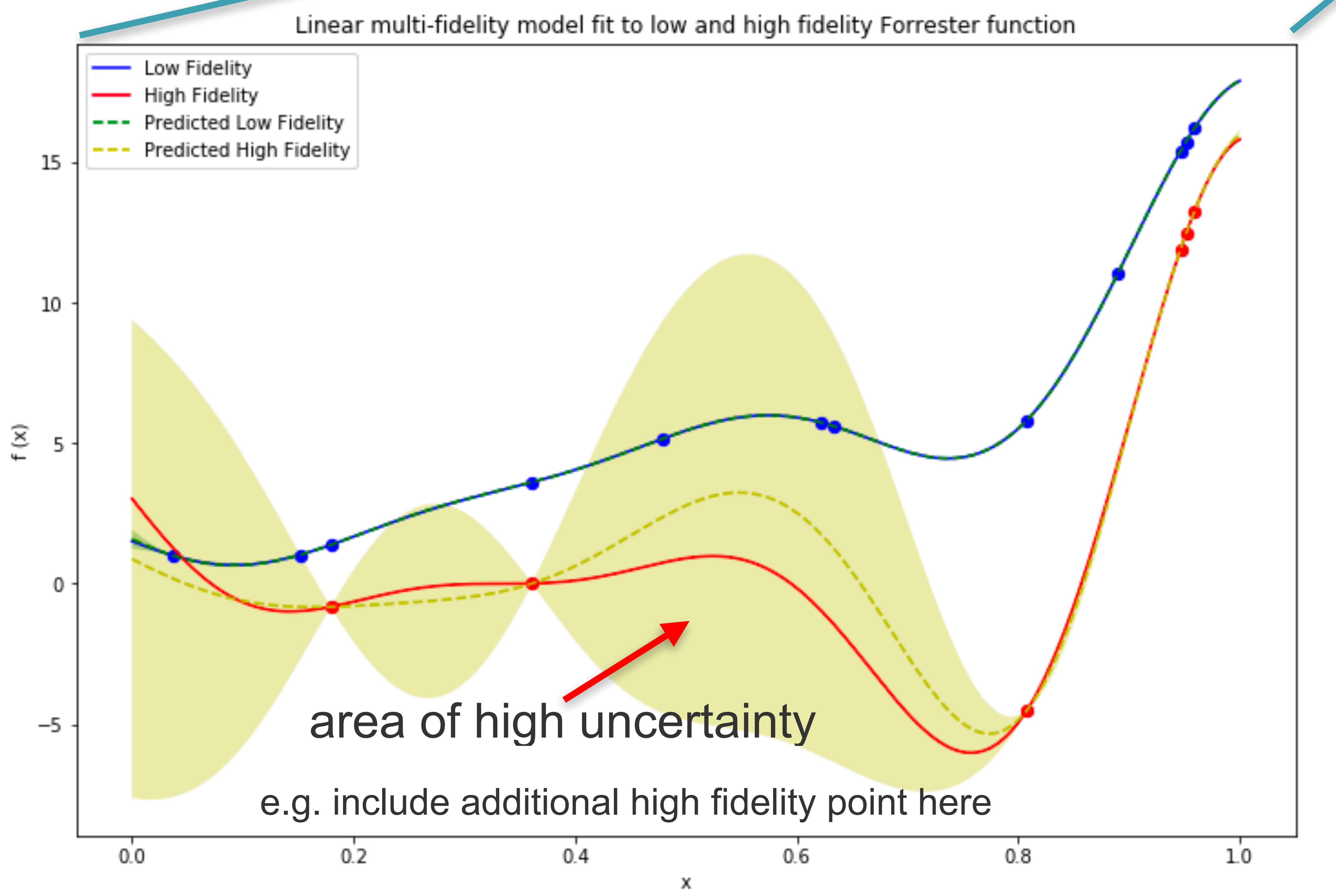




Surrogate with Multi-Fidelity (MF)

Design 1: [Mod. Thickness, …] → Emulator → ^{77}Ge Reduction efficiency

Design 2: [Mod. Thickness, …] → Emulator → ^{77}Ge Reduction efficiency



- combine **fast low-fidelity** simulations with **costly high-fidelity** simulations

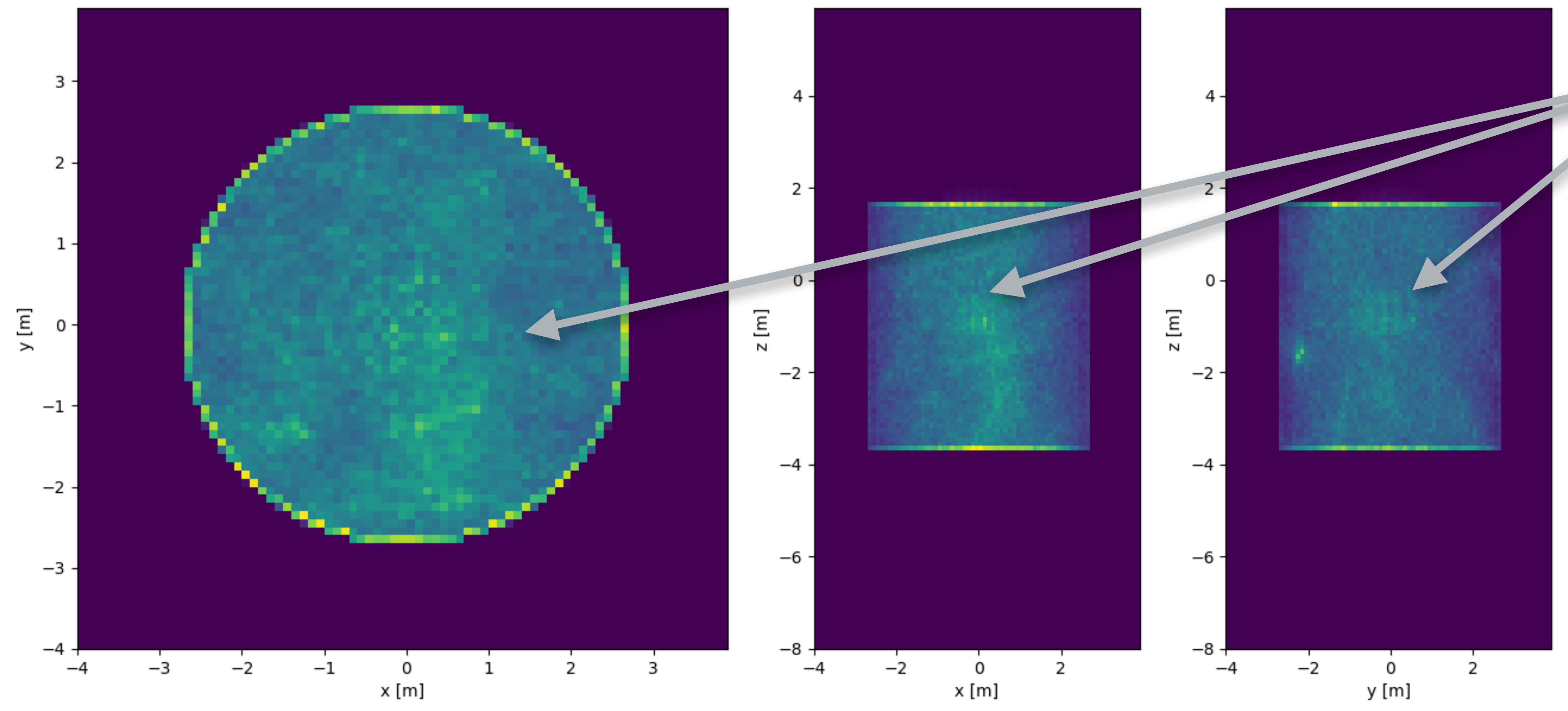
  ➡ **efficient method to decrease costly simulations when predicting the output of a system**

- simulator can be run at **different levels of complexity**, from most high level code to the most basic version
- each level **share some basic features** and include **most important features**
- **simple, fast versions** useful for preliminary investigations
- Bayesian methods of prediction and **uncertainty analysis** combined with multi-level approach

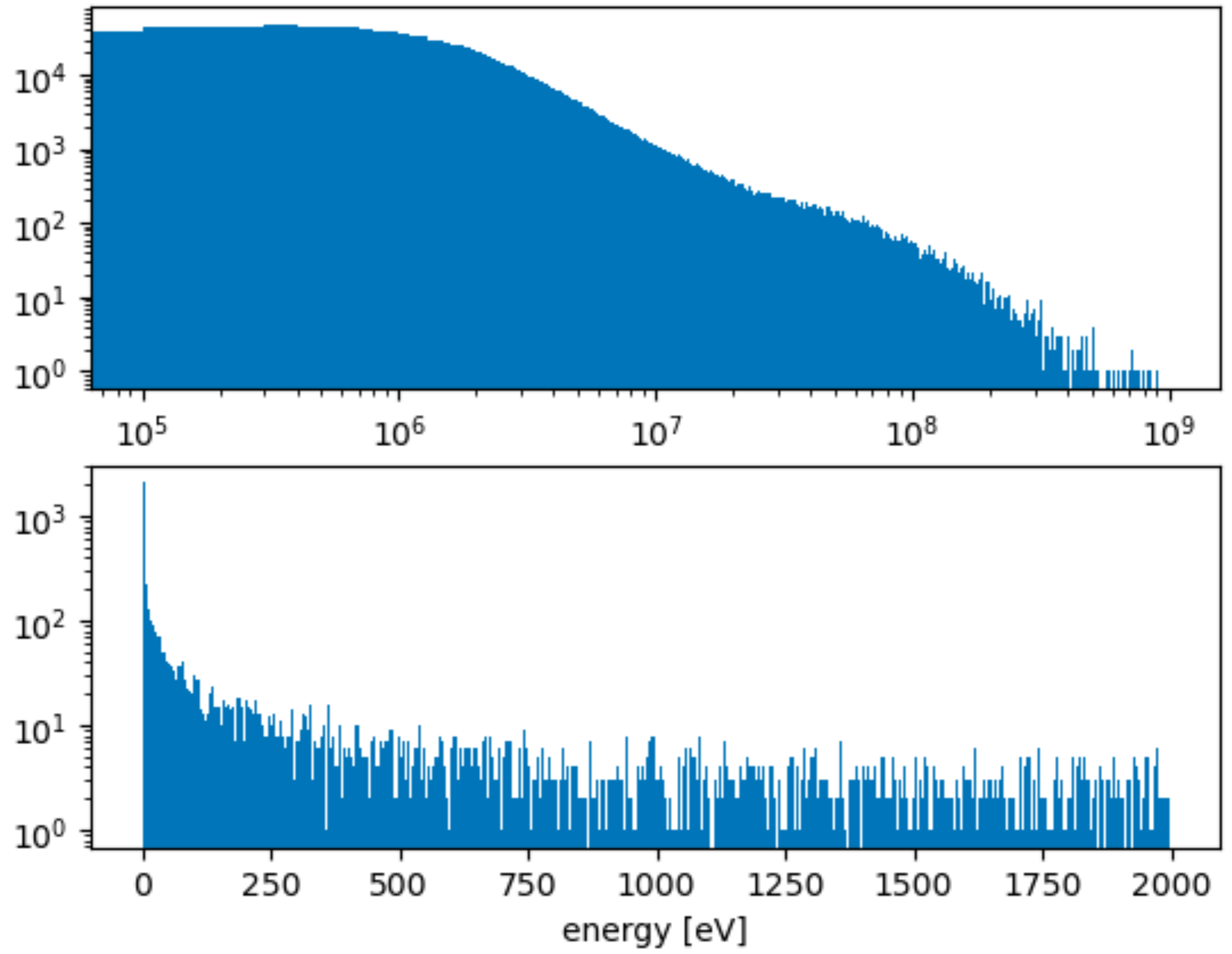
ΔL ≠ 0

HF & LF simulation: Neutron input locations

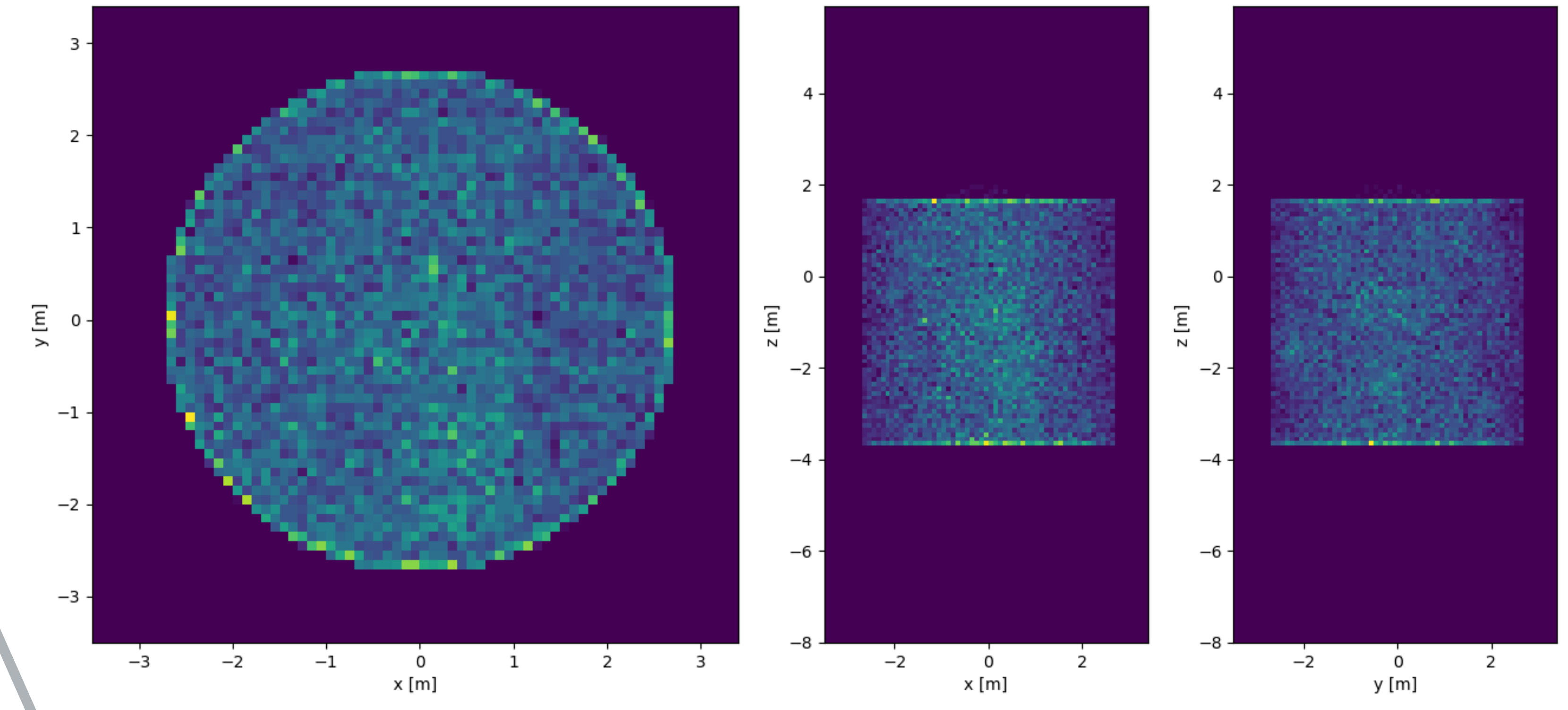
10000000 primary muons (high fidelity) ⇒ ~1300000 (~13%) secondary neutrons crossing the LAr cryostat (low fidelity)

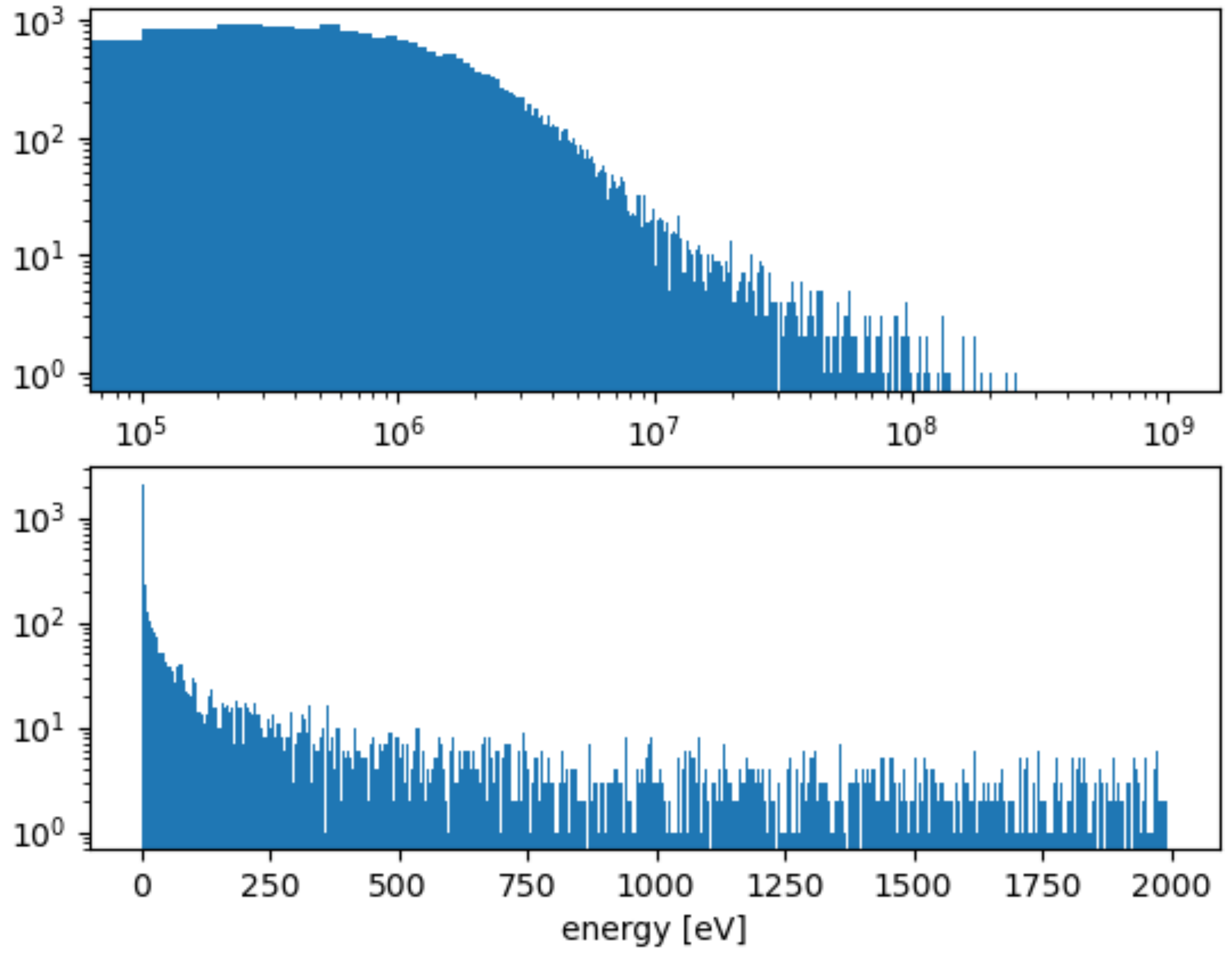


neutrons not homogeneously distributed → effect slightly washed out for randomly drawn starting points

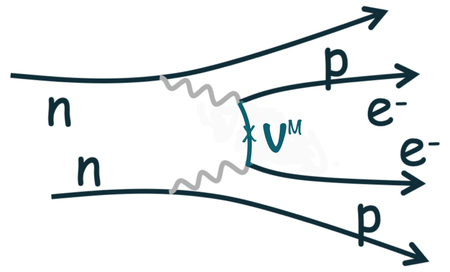


draw distributions with random starting points from high fidelity simulation w/o moderator



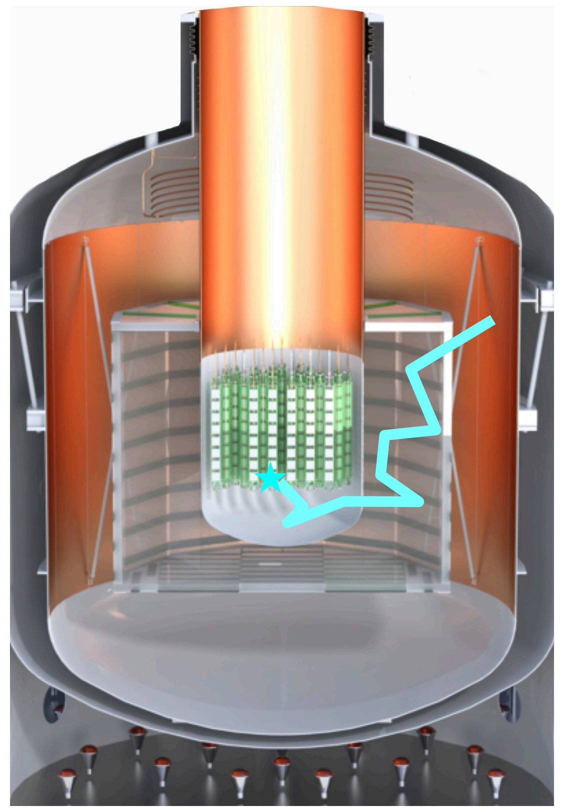


	HF	LF
Primary particle	Muon	Neutron
CPUh per neutron	$1.5\cdot10^{-4}$ ($2\cdot10^{-5}$ per muon)	$3\cdot10^{-6}$
Full detector geometry	✓	✓
Full neutron physics lists	✓	✓
Timing to primary and production info	✓	✗



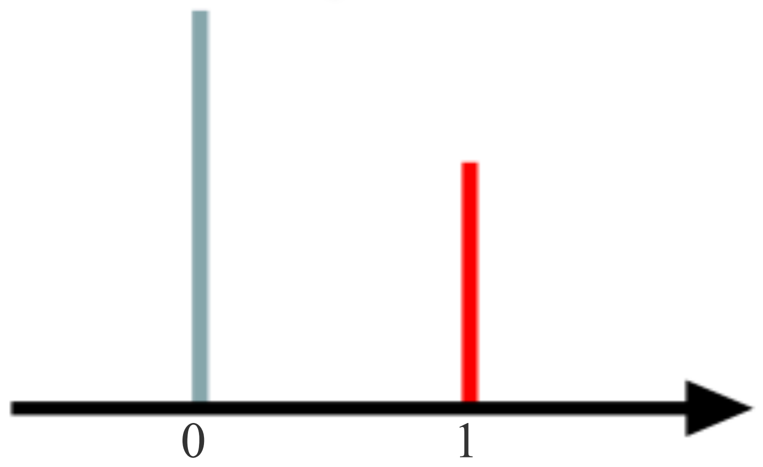
$\Delta L \neq 0$

Geant4 MC Simulation



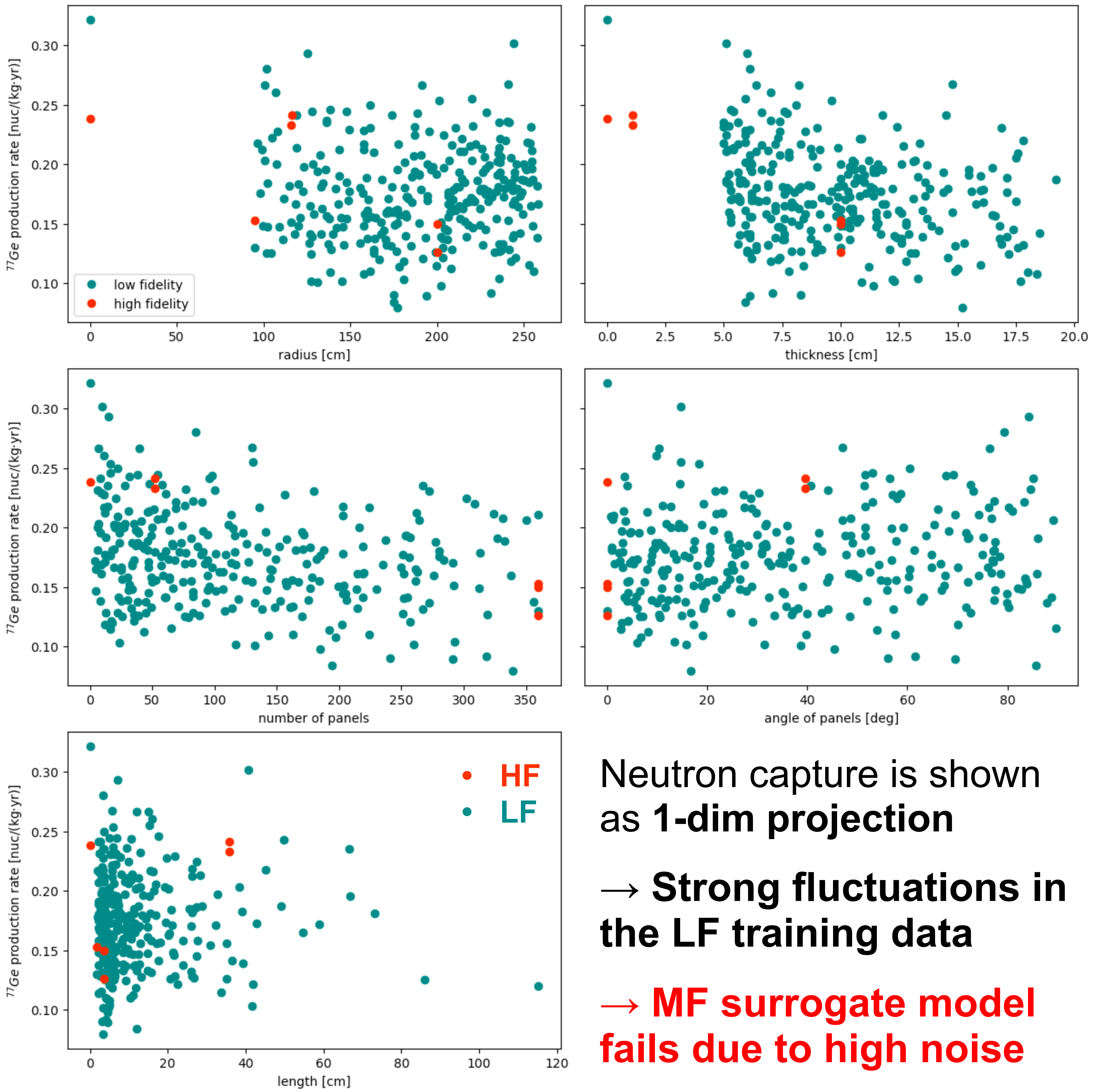
Run Geant4 LF simulations for different moderator configurations

Count number of neutrons being captured given the configuration



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

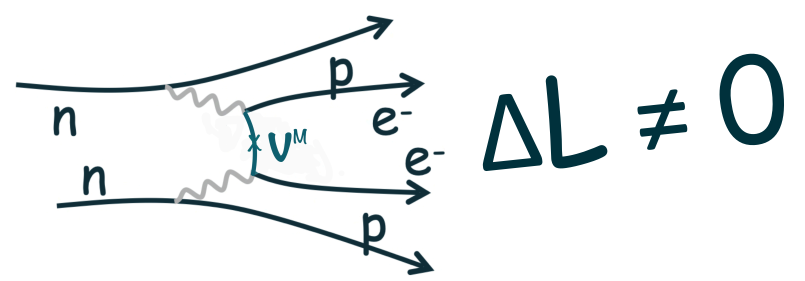
- 300 LF samples, randomly sampled while adhering to parameter constraints
- 4 initial HF samples
- Count number of neutron captures on ^{76}Ge



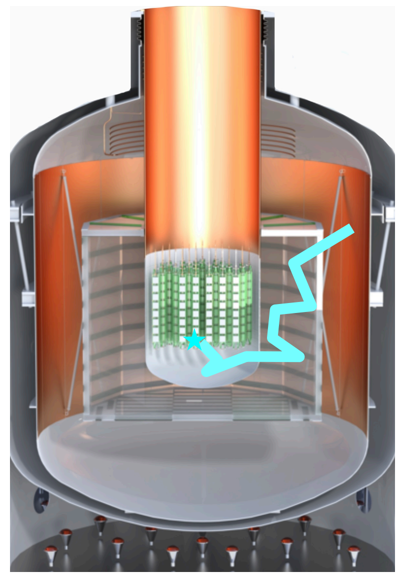
Neutron capture is shown as **1-dim projection**

→ **Strong fluctuations in the LF training data**

→ MF surrogate model fails due to high noise



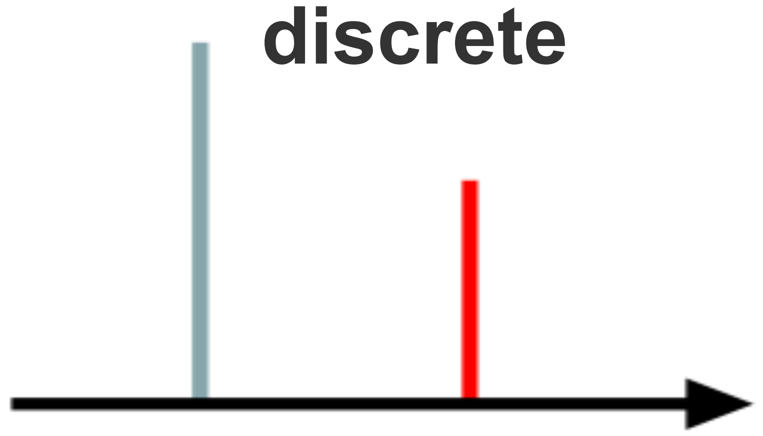
Neutron capture probability



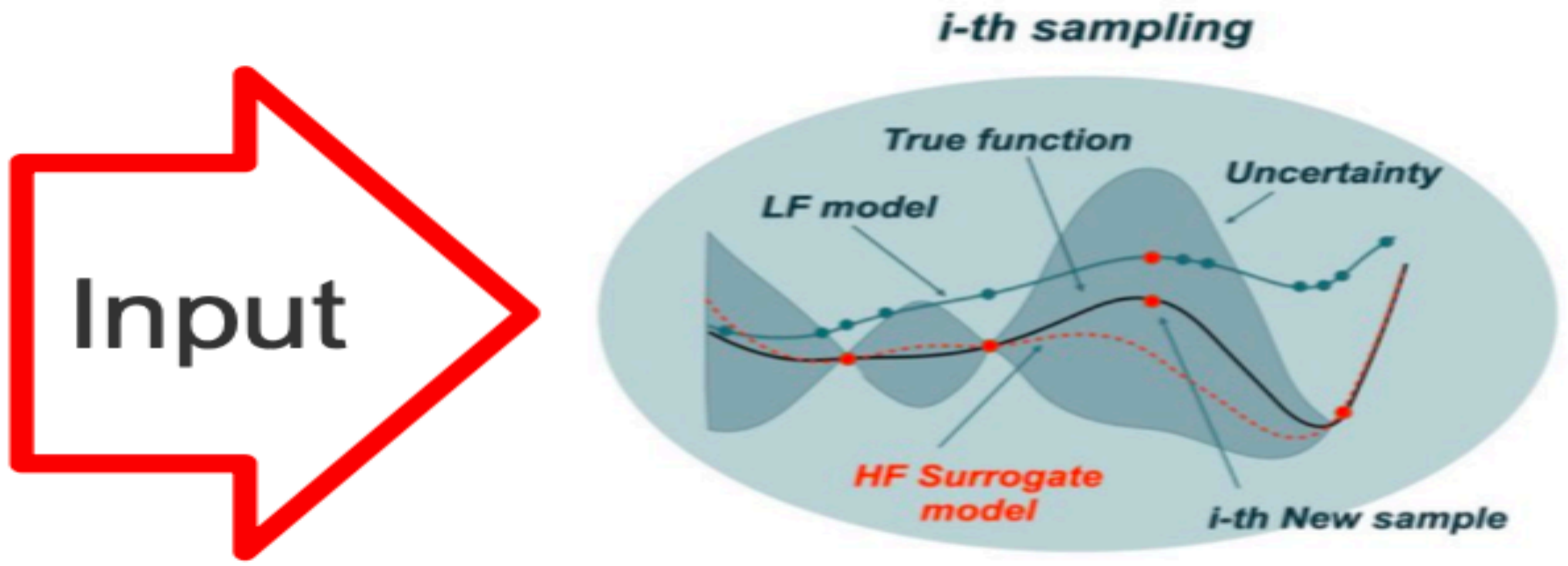
Run Geant4 LF simulations for different moderator configurations

count number of neutrons being captured given the configuration

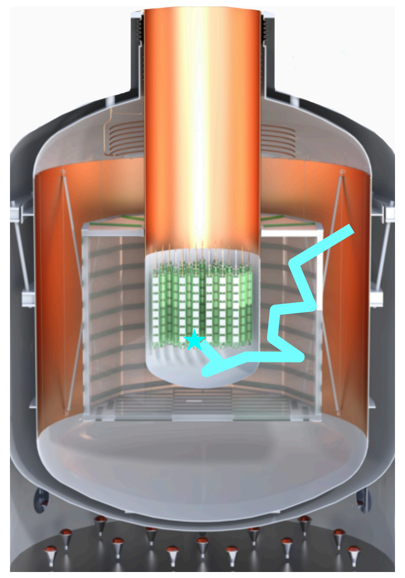
discrete



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



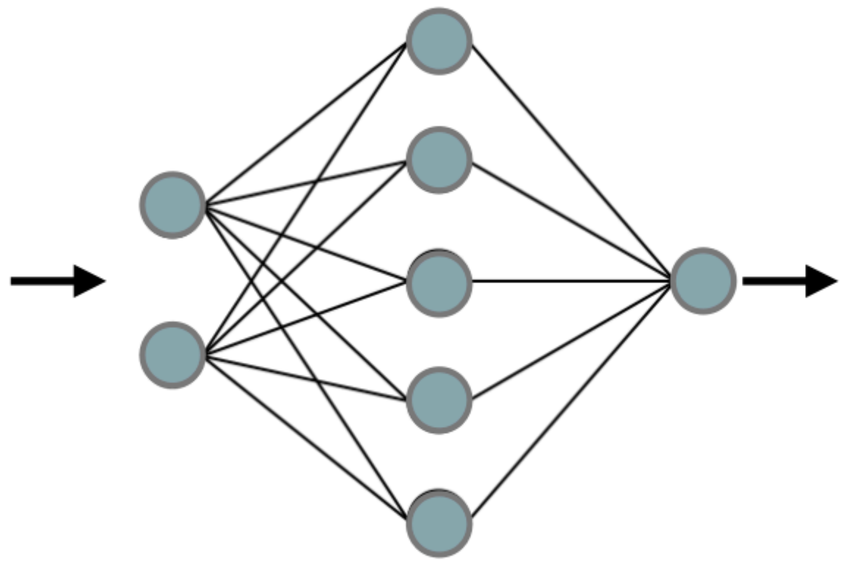
<u>Question</u>: How likely is a neutron being captured with certain physics parameters given a certain moderator configuration?



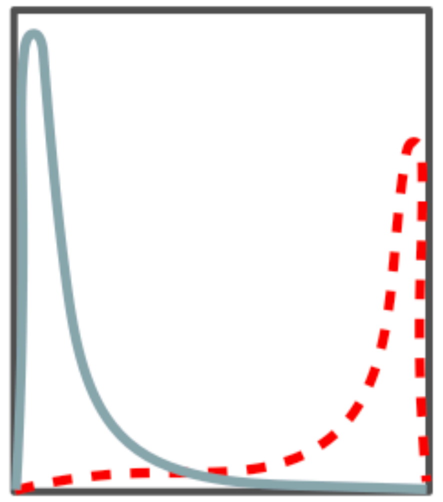
Run Geant4 LF simulations for different moderator configs

physics parameter of each primary neutron in simulation

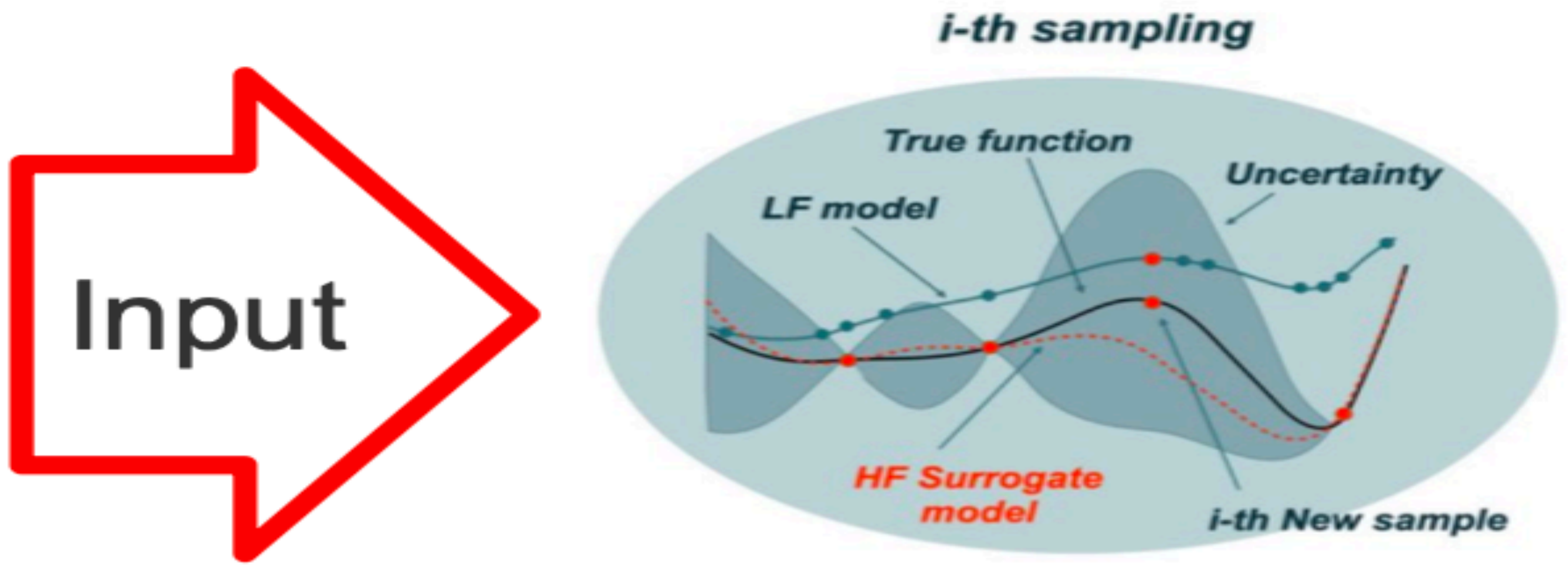
Add Network



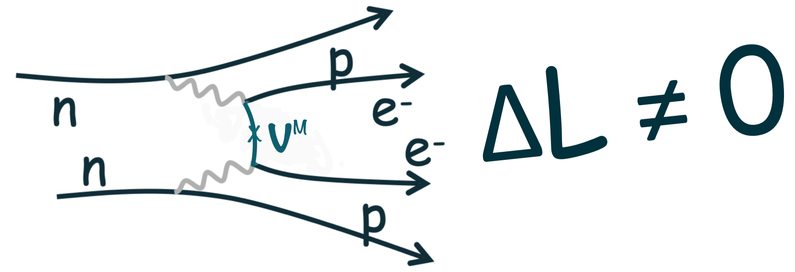
continuous



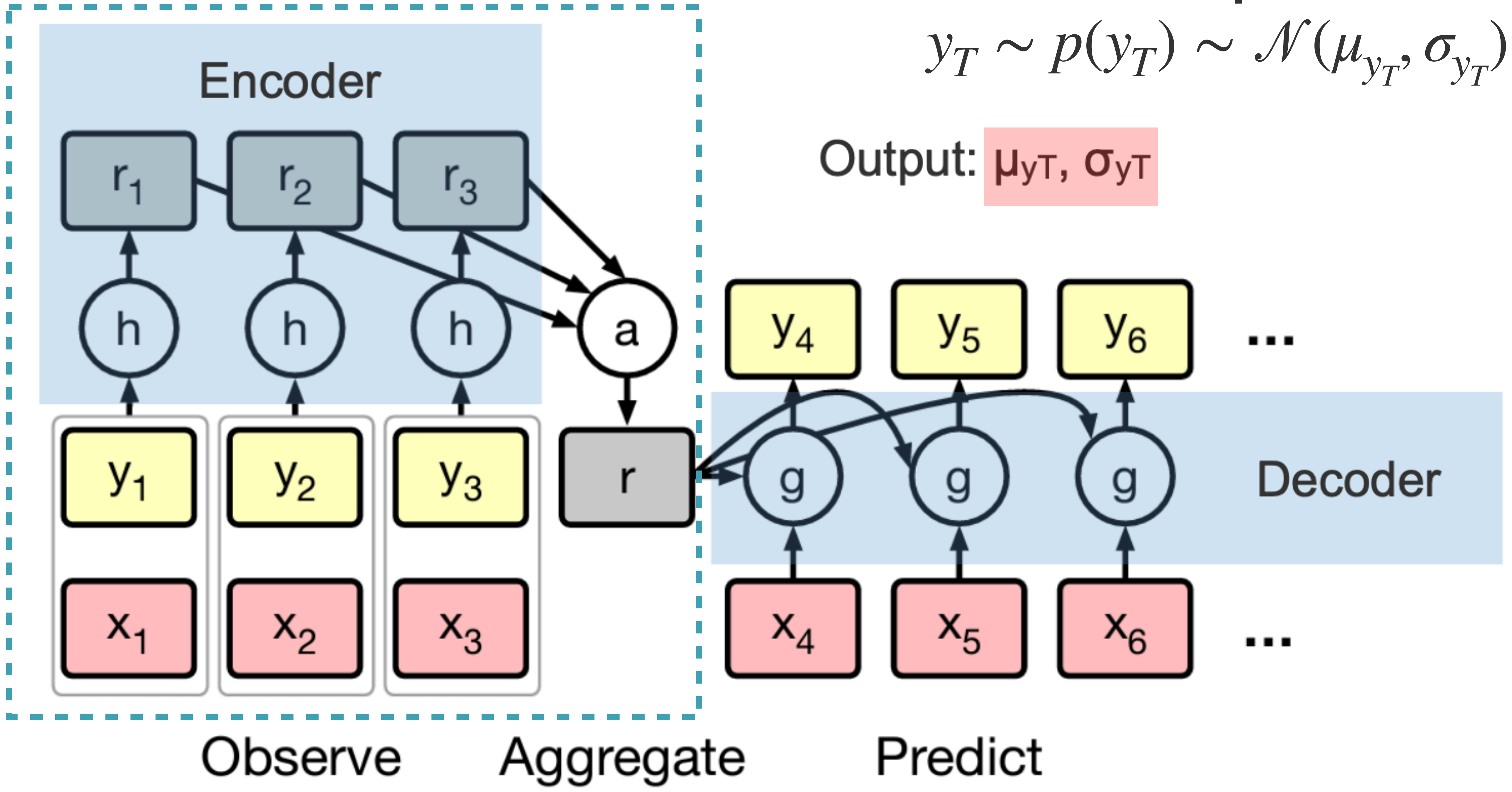
$f(x) \in [0,1]$



We use a conditional neural process (CNP)



Conditional Neural Process (CNP)



Assumption:

$$y_T \sim p(y_T) \sim \mathcal{N}(\mu_{y_T}, \sigma_{y_T})$$

Output: μ_{yT}, σ_{yT}

Context: $(\vec{x}_i, \vec{y}_i)$ Target: $(\vec{x}_j)$

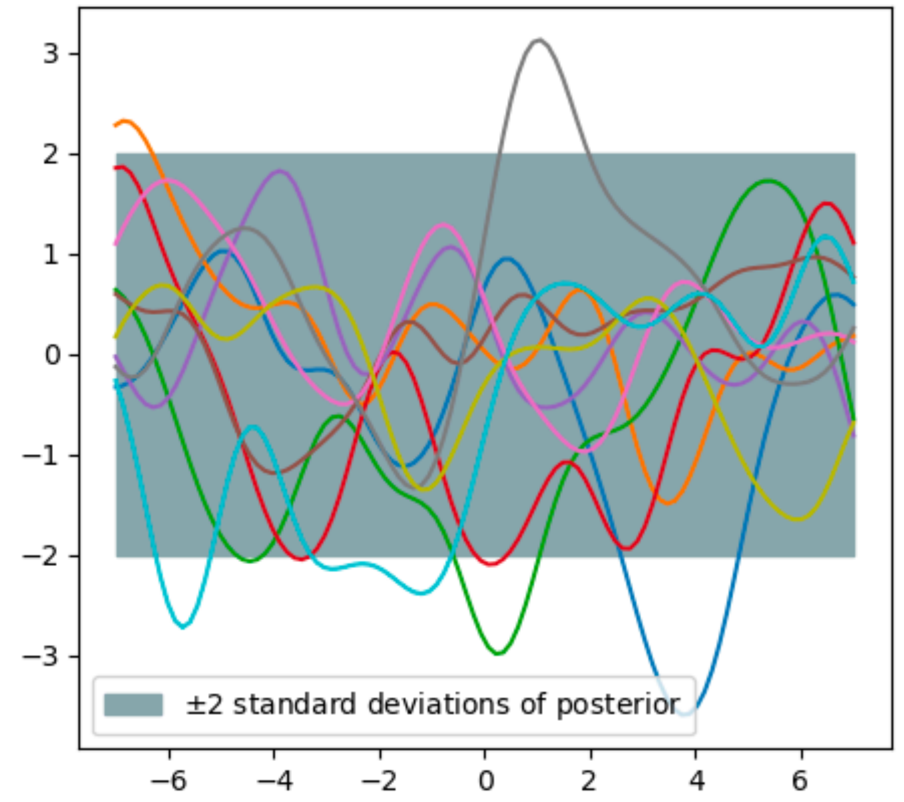
- Learn Contextual Features
- Maximize the Posterior Likelihood to Train
- Uncertainty prediction
- Small dataset size (where avoiding overfitting important)

Analogous to

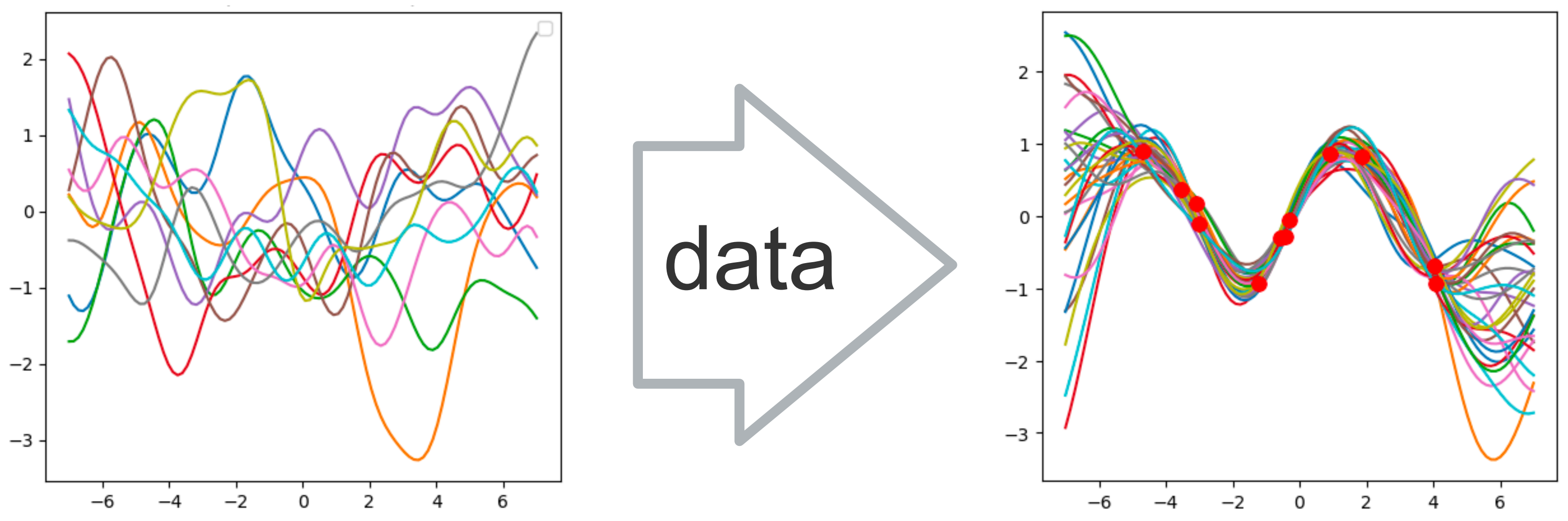
Gaussian Process

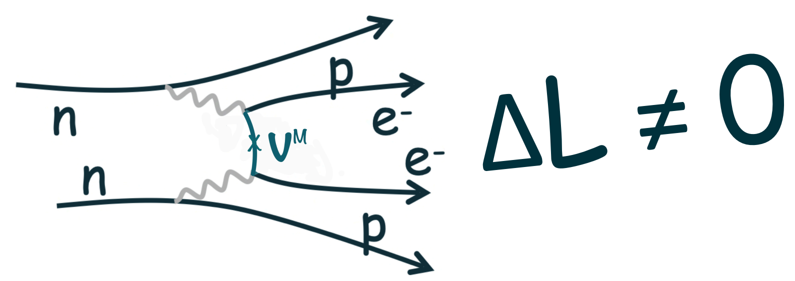
$$f(x) \sim GP(m(x), k(x, x'))$$

mean of posterior



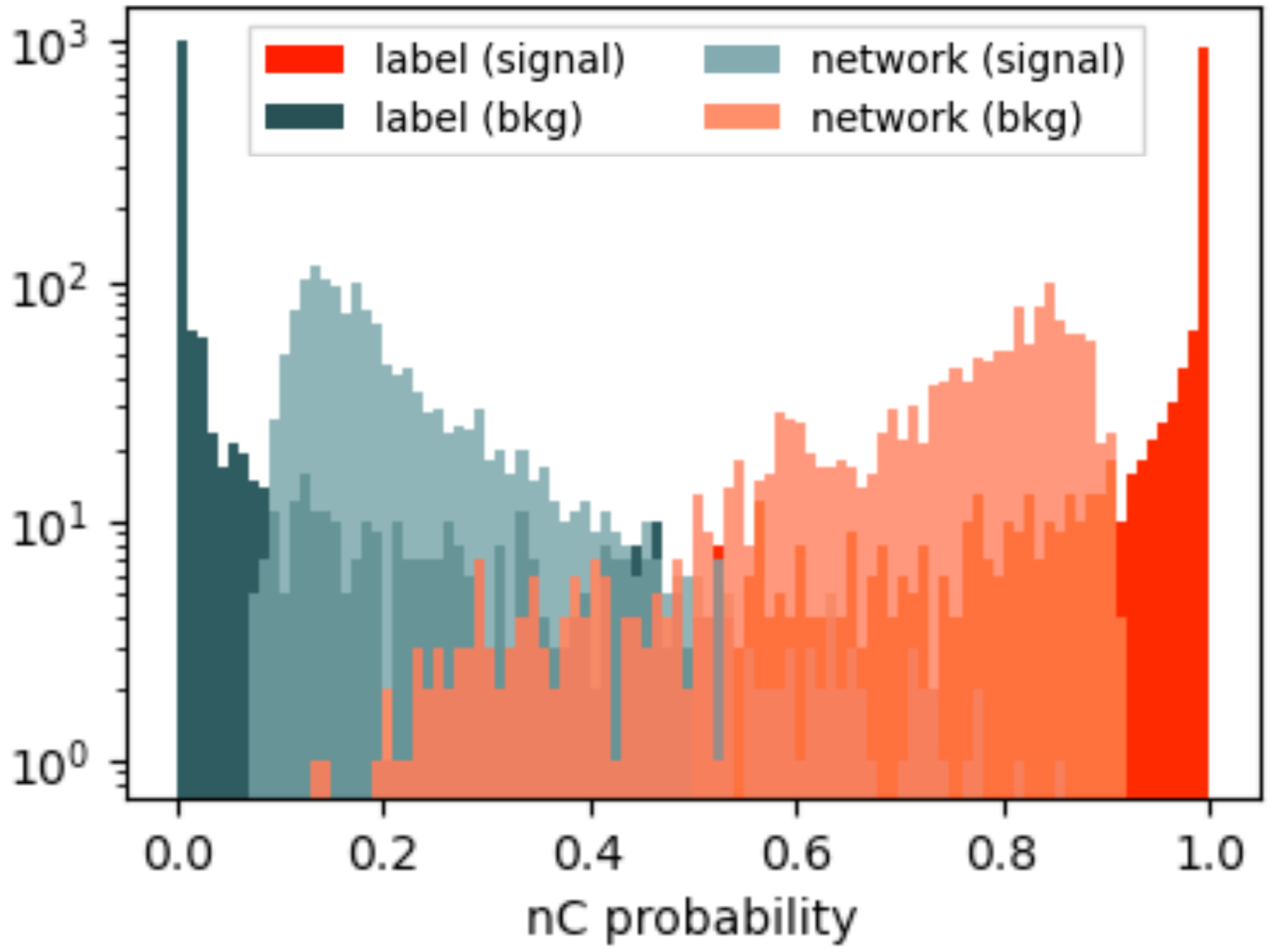
GP prior **GP posterior**

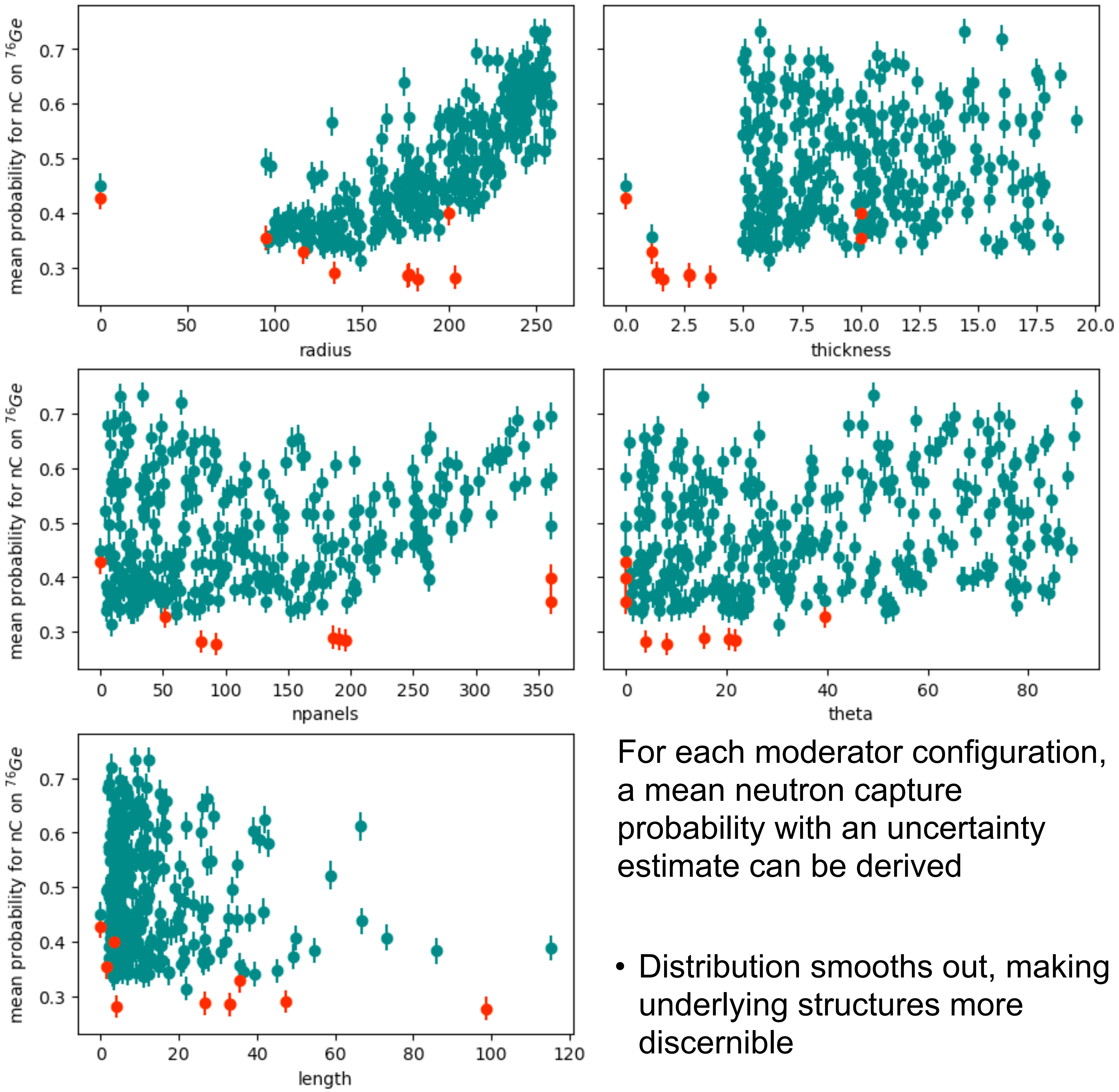




Conditional Neutral Process - Result

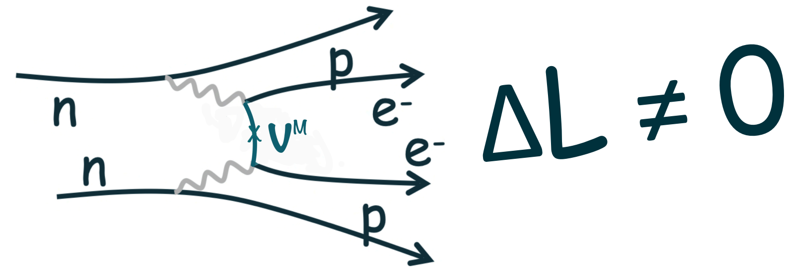
- Signal (red) vs background (blue) **Classification**
- **Mixed-up data augmentation** method used for dealing with the imbalanced training data set
- CNP effectively **learns from neutron physics parameters**
- Separation between signal and background



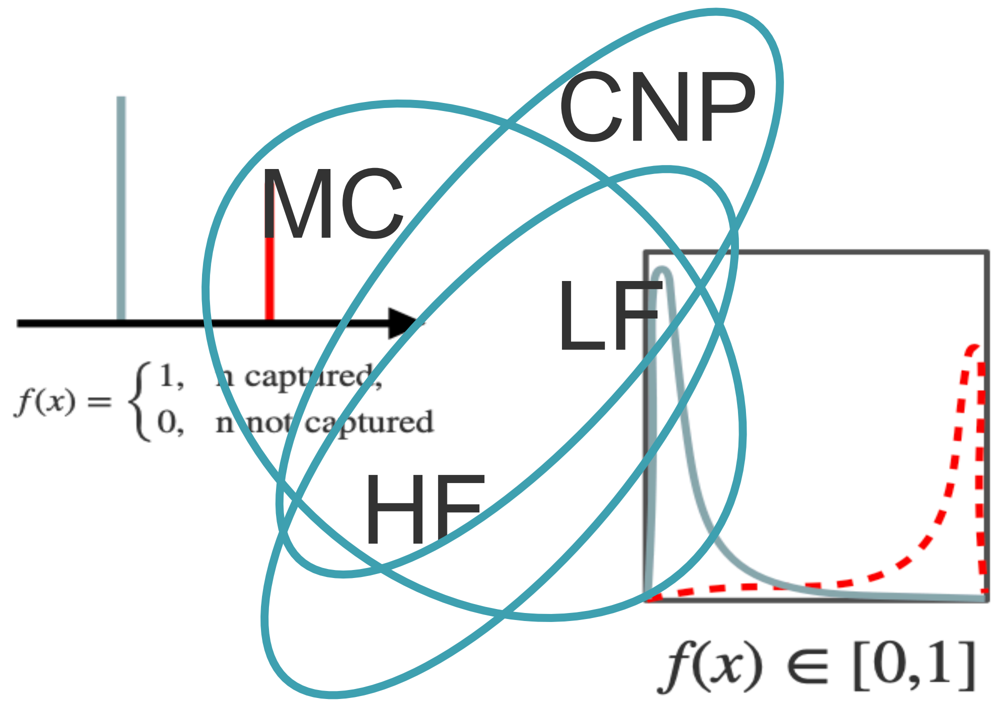


For each moderator configuration, a mean neutron capture probability with an uncertainty estimate can be derived

- Distribution smooths out, making underlying structures more discernible



Combine CNP with Multi-Fidelity Gaussian Processes



- Minimize **noisy black-box** function:

$$\min_{x \in X} \eta(x) \text{ with } \eta(x) = f(x) + \varepsilon, \text{ where } \varepsilon \sim \mathcal{N}(0,\sigma)$$

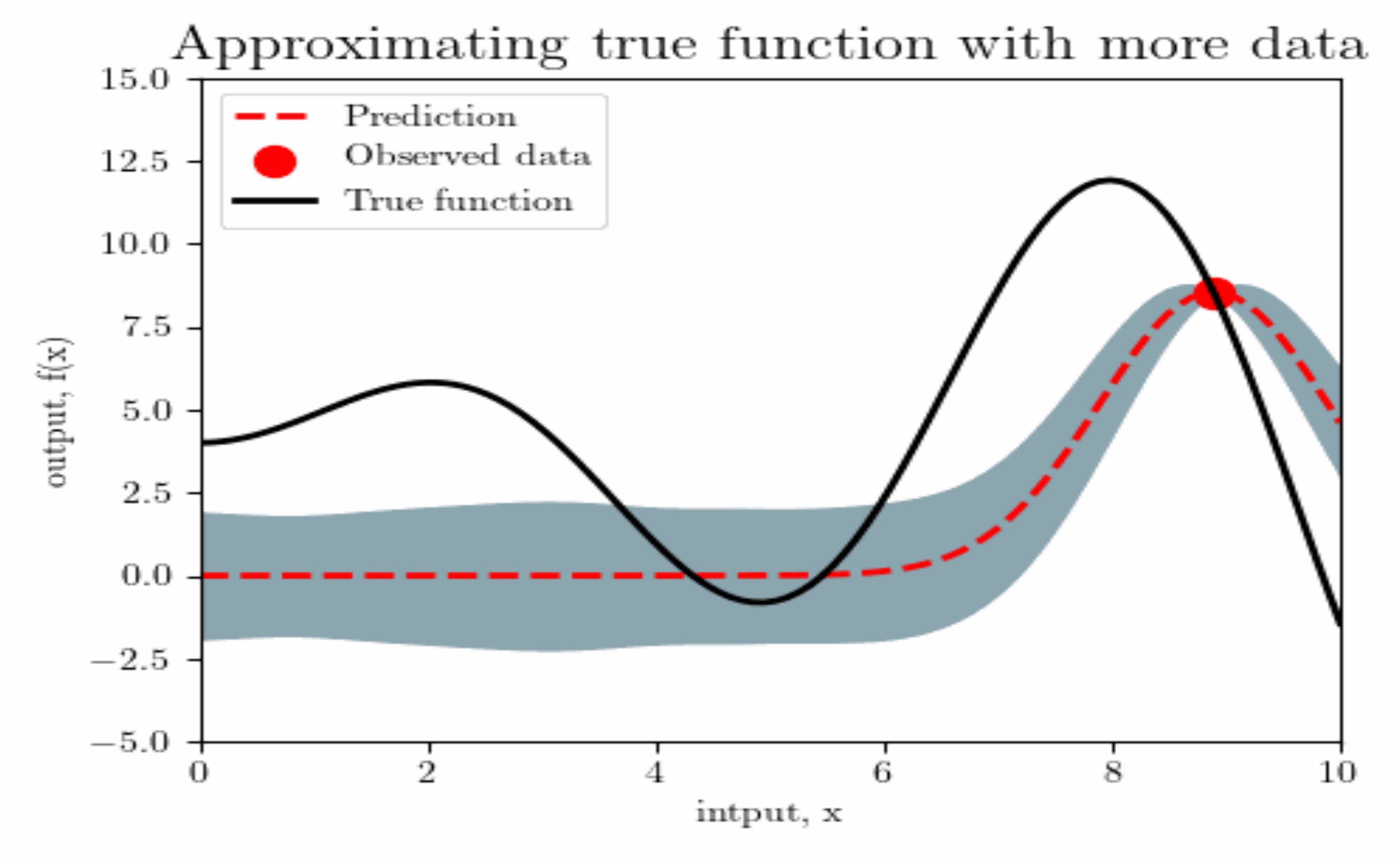
- Multi-Fidelities (MF) ranked hierarchically by accuracy (h=0,…,m)
- Use "co-kriging" model with **GP**:

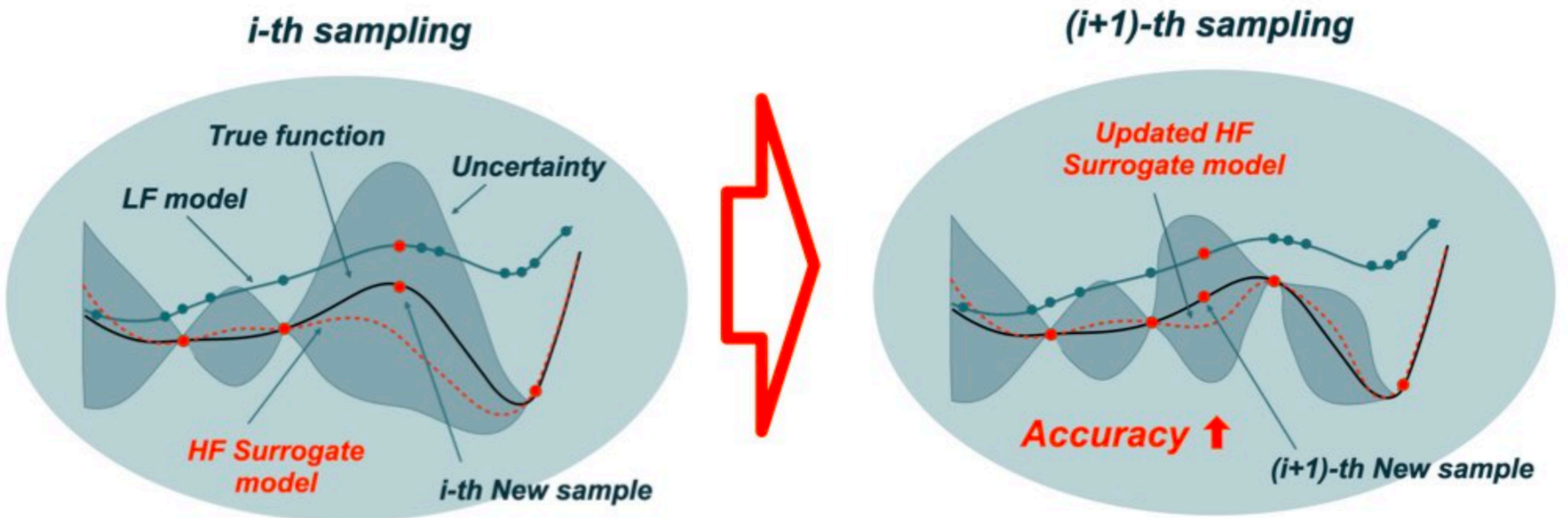
$$\eta_h(x) = \rho_{h-1}\eta_{h-1}(x) + \delta_h(x)$$

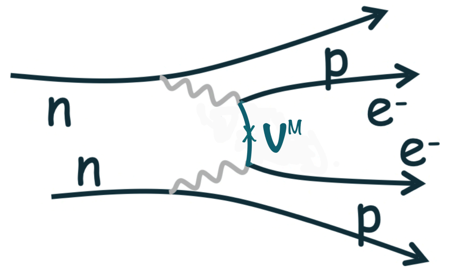
discrepancy term modeled by ***GP***

*correlation to lower fidelity (**GP**)*

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

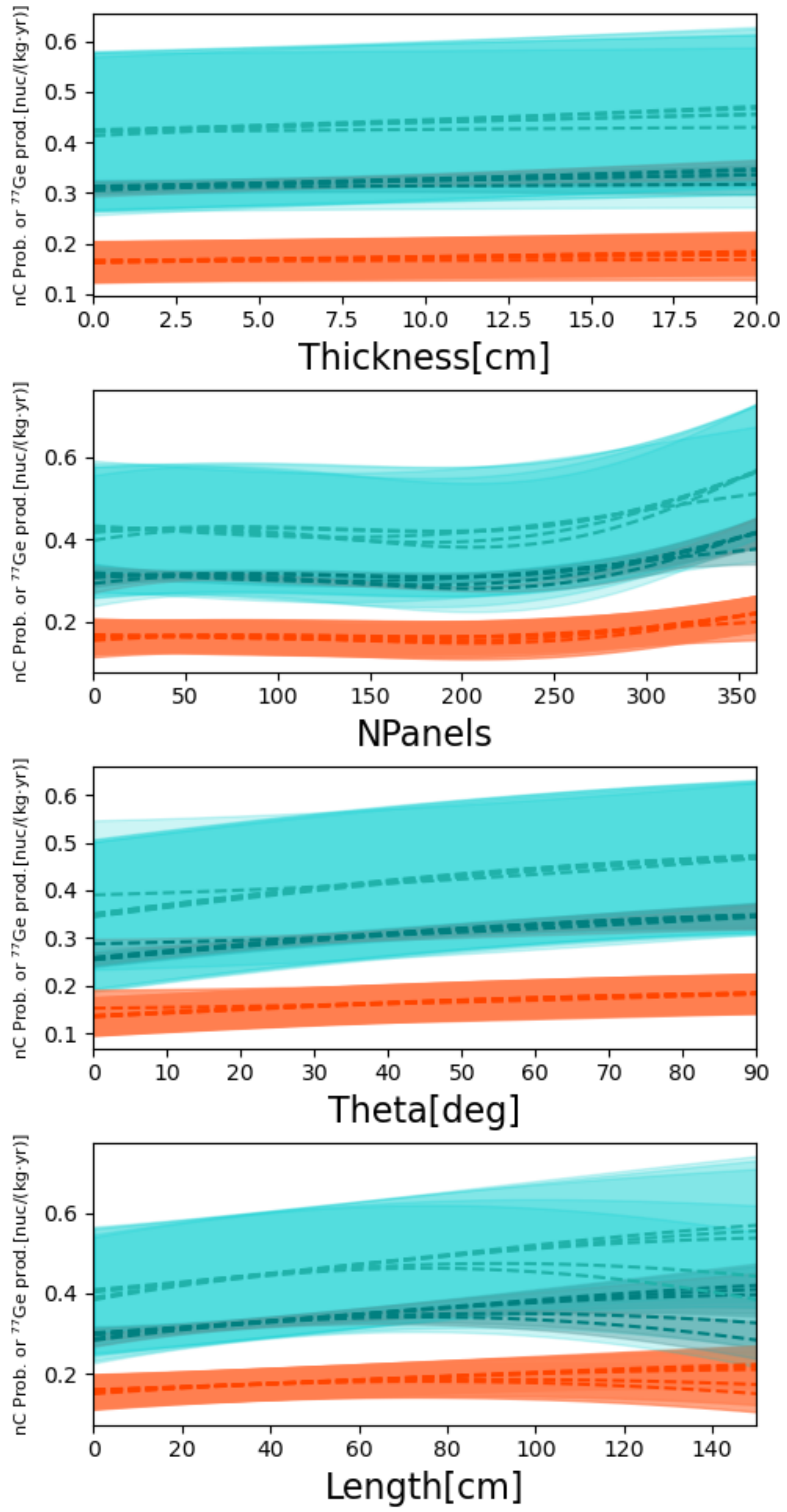




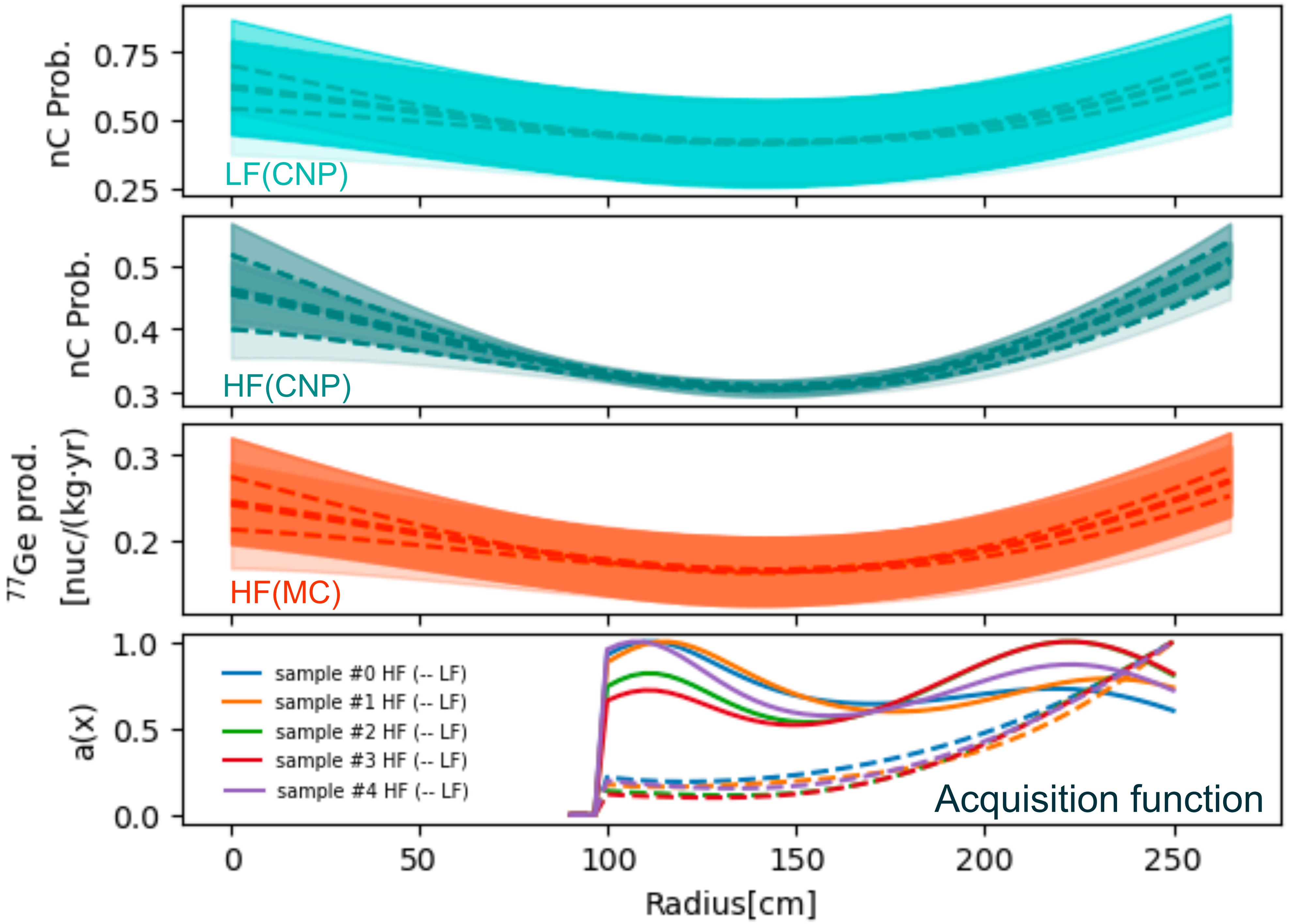


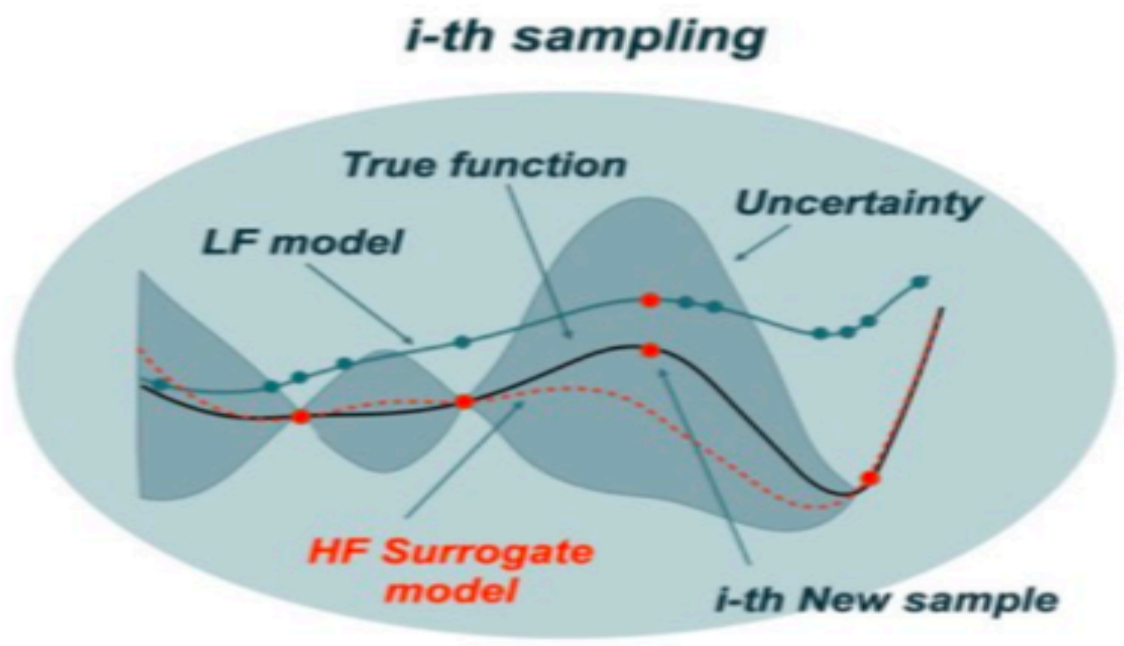
$\Delta L \neq 0$

Multi-fidelity Model - Results

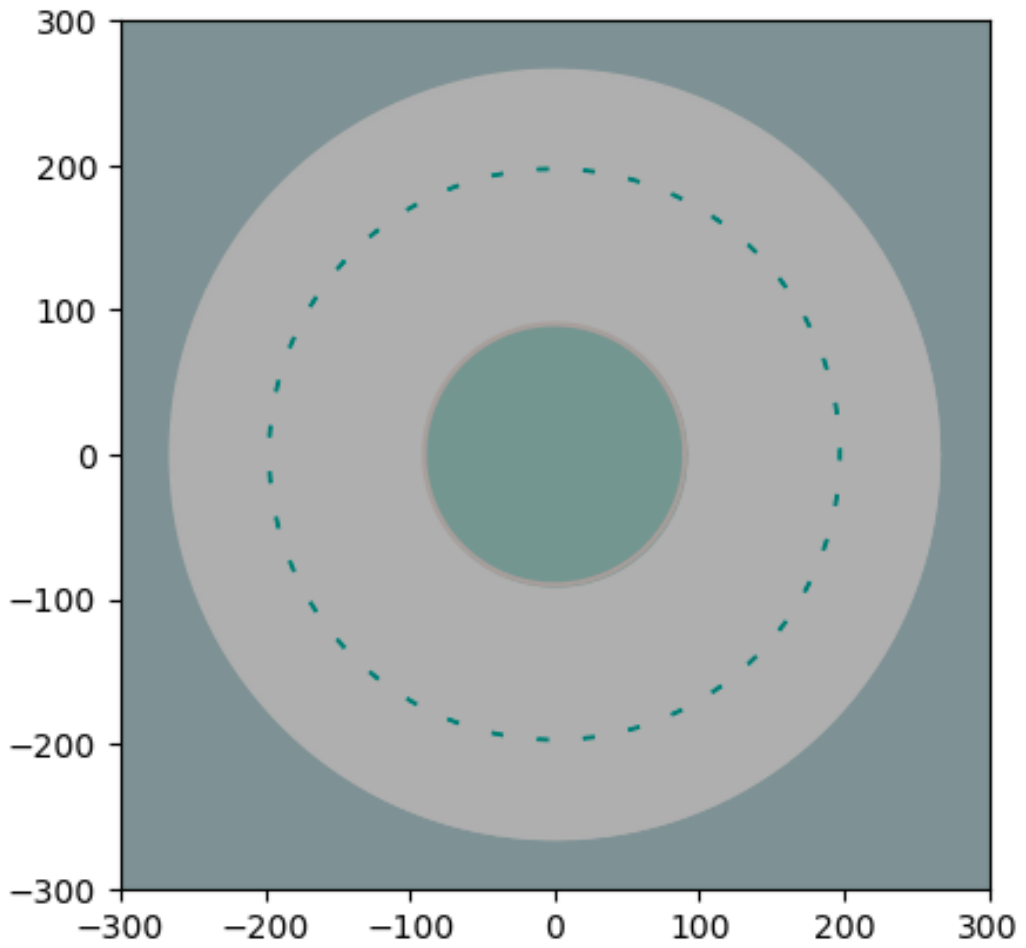


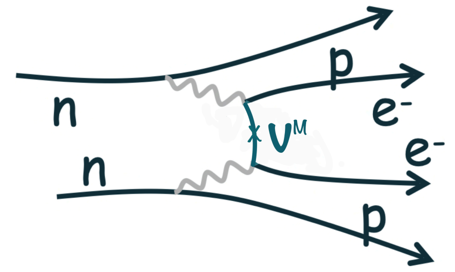
- Modeling of 5 dim space (r, t, θ, n, L) with 3 fidelities (HF(MC), HF(CNP) and LF(CNP))
- model evolution shown as projection on r, t, n, θ and L at a random point in space
- Acquisition function: Integrated variance reduction with parameter constraints





Optimal design found with reduction by a factor of 2.1 and a ^{77}Ge production rate of 0.13 nuc/(kg·yr)





$\Delta L \neq 0$

In a boarder context: Rare Event Trigger Rate Problem

Design Parameters $\theta \in \Theta$ → **Event Simulation** N events, m = trigger w/ signal →

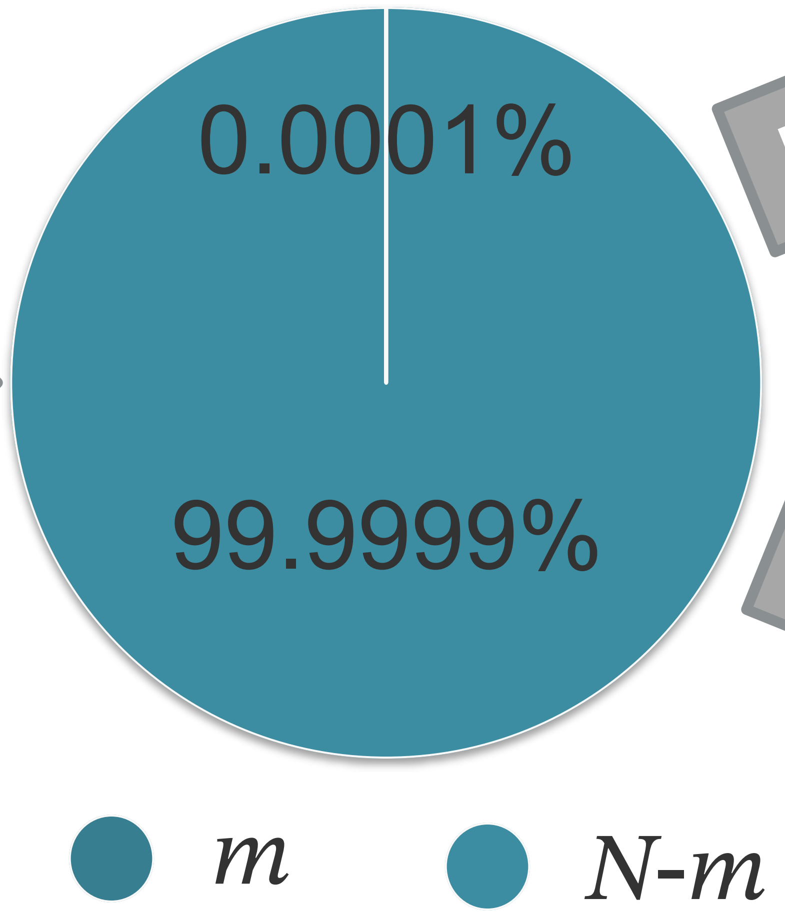
Trigger Probability $p_i(\theta, \phi_i)$ **low**

Rare Event Assumption:

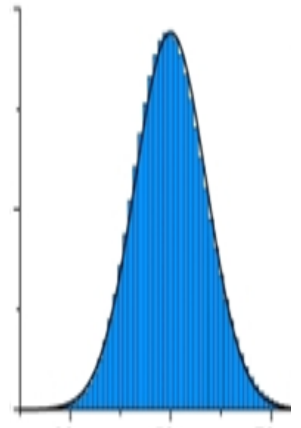
$m \sim$ Poisson$(\lambda(\theta))$, where

$\lambda(\theta) = \bar{p}(\theta) = \sum_{i=1}^{N} p_i(\theta, \phi_i)$

Signal trigger rate $y = \frac{m}{N}$



Large N →



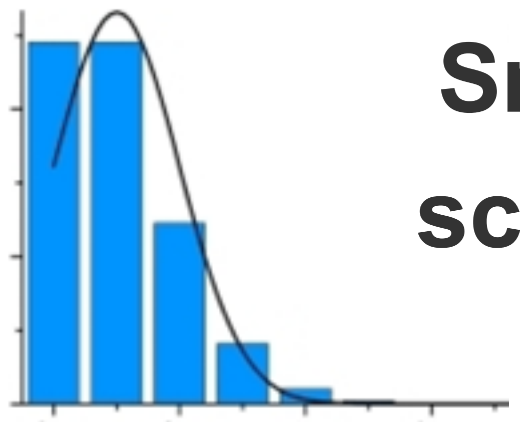
Large N **scenario**

$y \sim \mathcal{N}(\bar{p}(\theta), \frac{\bar{p}(\theta)}{N})$

Low Variance, High Cost.

Key scenarios

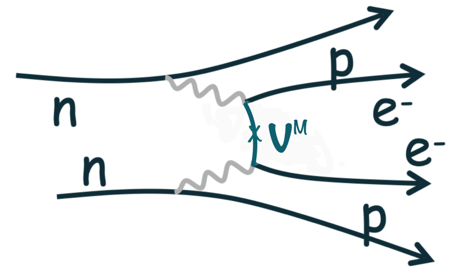
Small N →



Small N **scenario**

$y \in \{0/N, 1/N, \dots\}$ discrete

High Variance, Low Cost.



$\Delta L \neq 0$

Rare Event Surrogate Model

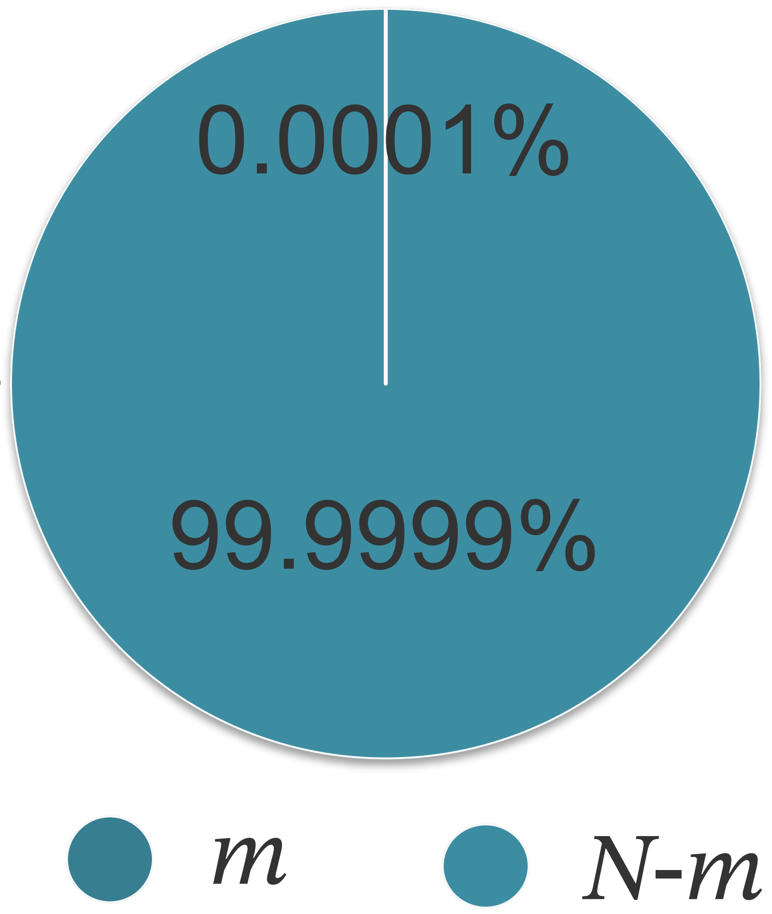
Design Parameters
$\theta \in \Theta$

Trigger Probability
$p_i(\theta, \phi_i)$ **low**

Event Simulation
N events
m = trigger w/ signal

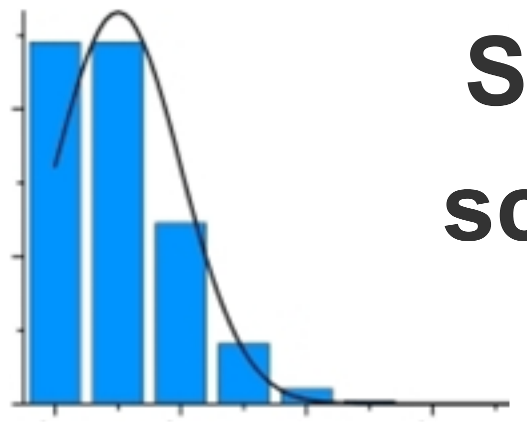
Rare Event Assumption:
$m \sim$ Poisson($\lambda(\theta)$), where
$\lambda(\theta) = \bar{p}(\theta) = \sum_{i=1}^{N} p_i(\theta, \phi_i)$

Signal trigger rate $y = \frac{m}{N}$



Small N

Expensive simulator



Small N scenario

$y \in \{0/N, 1/N, \ldots\}$

High Variance, Low Cost.

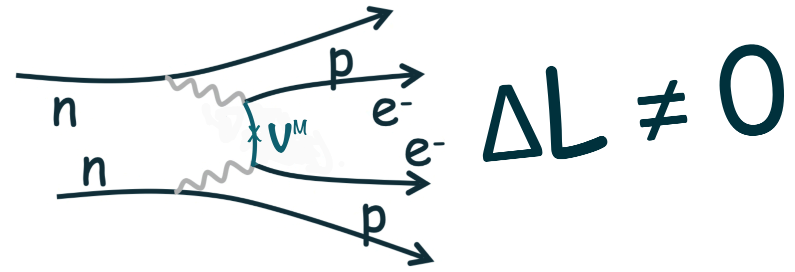
Challenge:

- **Problem**: Large N = accurate but **costly**
- **Solution**: Build a surrogate model combining
  - a predictive model which **approximate** $p_i(\theta \mid \phi_i)$ **with small** N
  - **fidelity splitting**
  - **adaptive sampling**

Approximated by CNP

we calculate: $\bar{p}(\theta) = \sum_{i=1}^{N} p_i(\theta, \phi_i)$

RESuM: A Rare Event Surrogate Model for Nuclear Physics Detector Design



Summary & Conclusion

➡ **Active and passive background reduction is contingent upon LEGEND-1000 selecting a shallower host site where cosmogenic background becomes a primary concern and plays a determining role in achieving its background reduction goals.**

- Various options for moderator designs are currently under active research and are being considered for implementation
- Through **active learning using a Multi-Fidelity Surrogate Model combined with a CNP Network** a solid shield design has been identified - design holds the potential reduction by a **factor of at least 2.1**

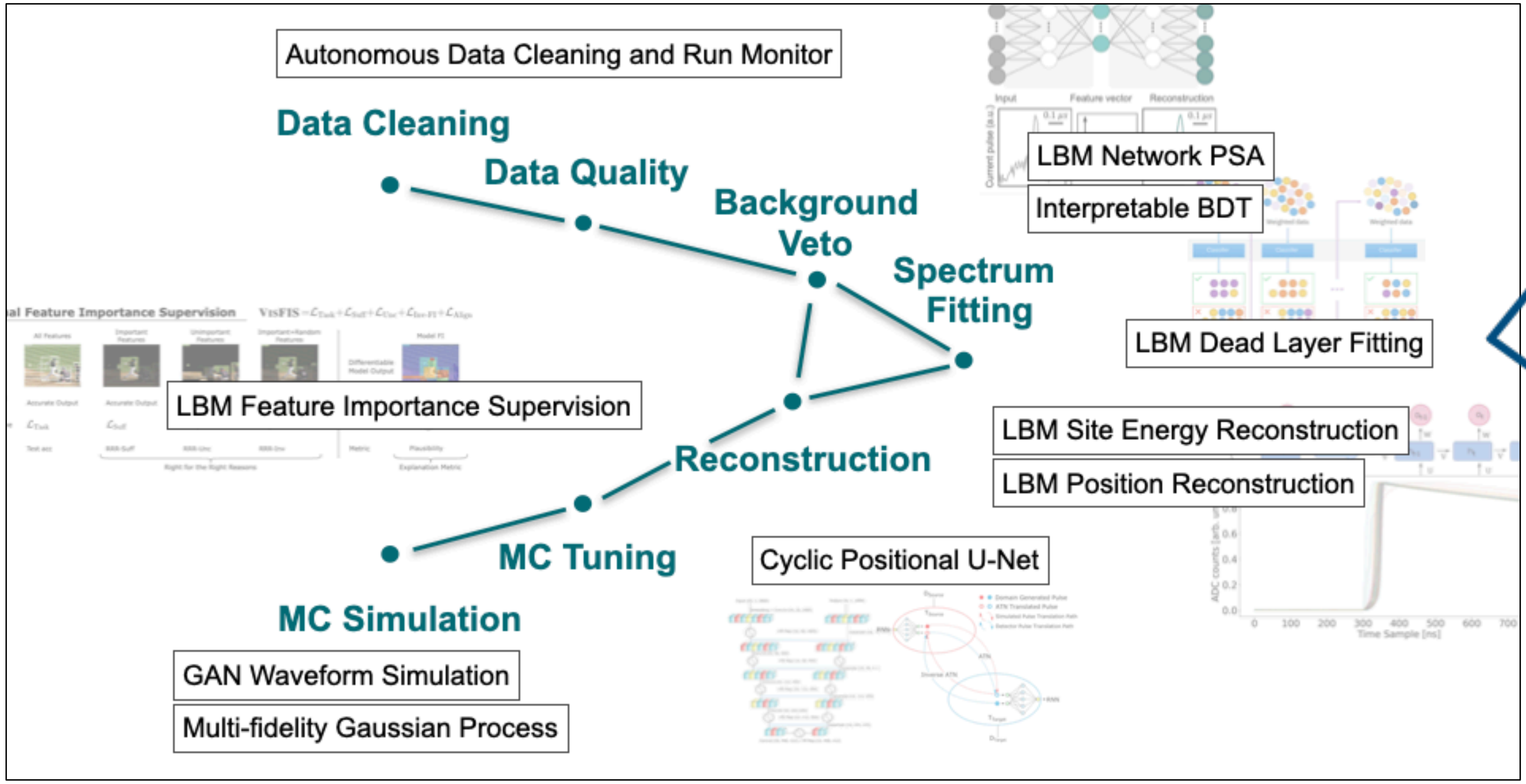
Rare Event Surrogate Model for Nuclear Physics Detector Design

- **Goal:** Find the optimal design parameters θ by minimizing the **event trigger rate** $y=m/N$, but large number of simulations are **costly**, while small simulations lead to **greater uncertainty in** y..
- **Solution**: a surrogate model that approximates the probability distribution p($y|\theta$) based on a limited number of simulations.

➡ **Reduced need for expensive large-scale simulations**

➡ **Efficient exploration of the design space and optimization of the parameters** θ

- **Future Improvements:** Transfer Learning MF-GP model that makes informed decisions by incorporating expected improvements and considering the computational resources associated with each fidelity level
- **Future Improvements:** can we model the CNP prediction and propagate it into the MFGP



Thank you for your attention!
Question?