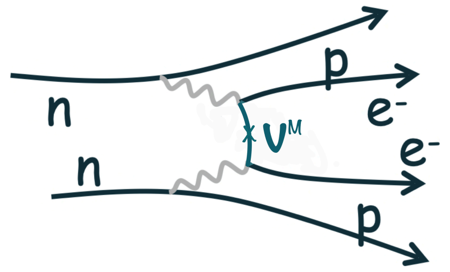
Rare Event Surrogate Model (RESuM) for Physics Detector Design

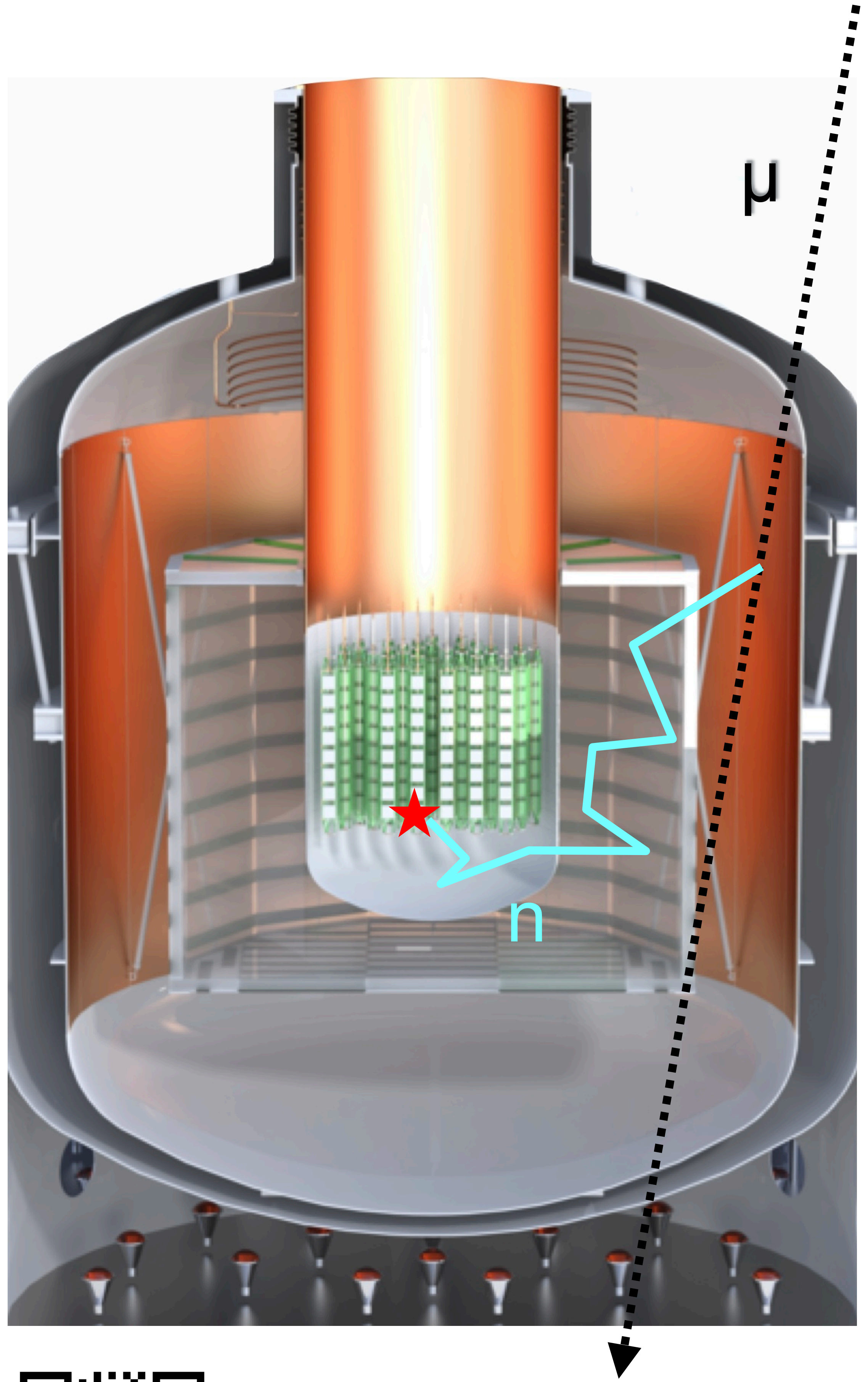
Ann-Kathrin Schuetz

Github

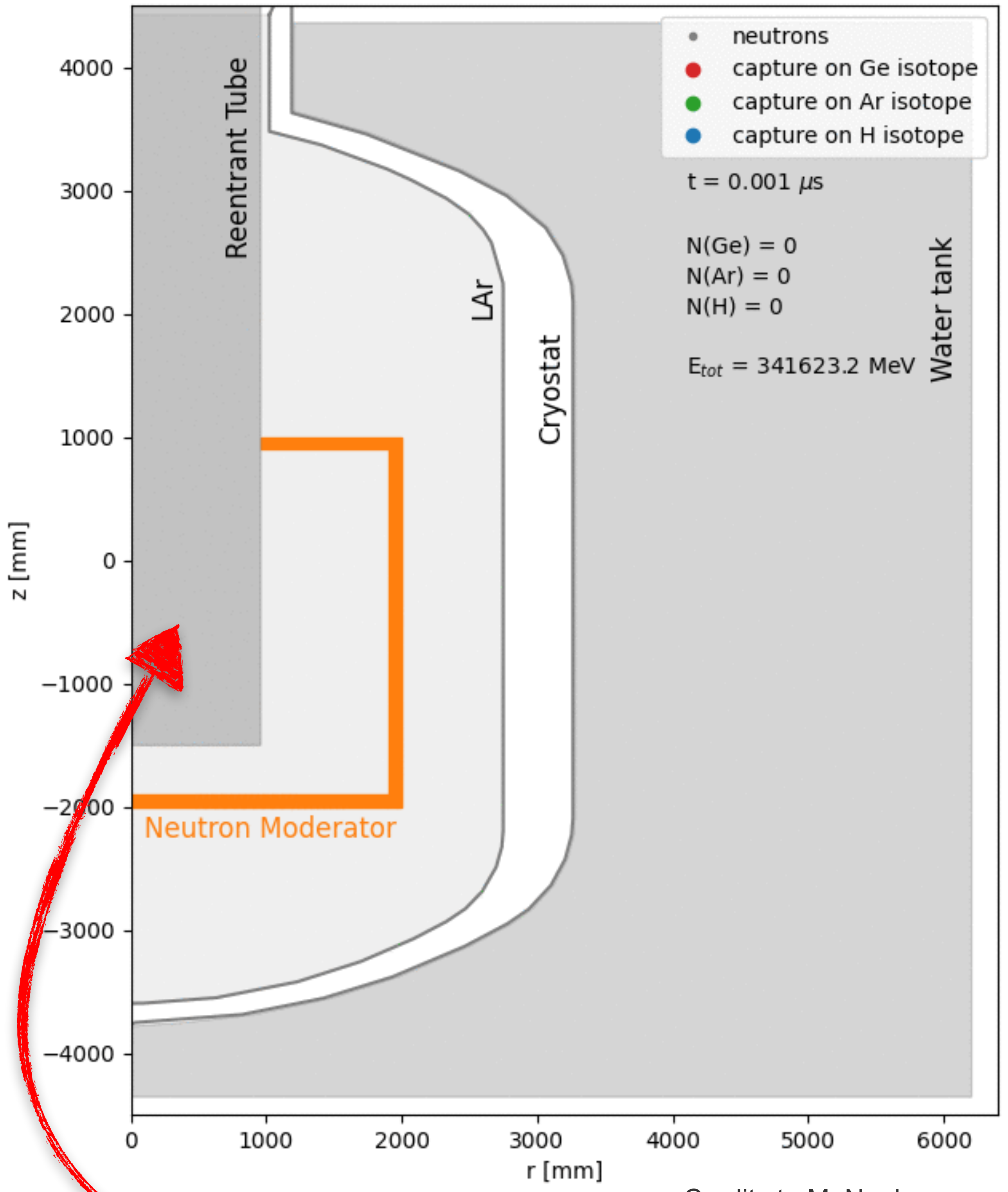


$\Delta L \neq 0$

Motivation - Physics Design Optimization



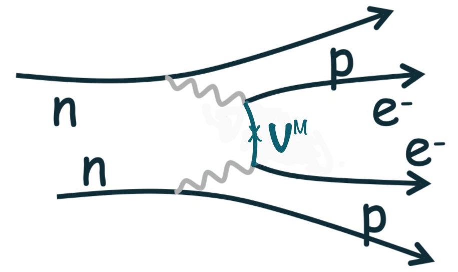
LEGEND



Credits to M. Neuberger

very rare dangerous event

- LEGEND proposed ton-scale experiment searching for ultra-rare neutrinoless double beta decay (a Nobel-prize-level discovery).
- Must suppress **extremely rare backgrounds** from cosmic muon-induced neutrons.
- Simulations are **expensive**, signal is **vanishingly rare.**
- Optimizing designs under such rare-event statistics is intractable.
- Need a rare event surrogate model for efficient, variance-aware optimization.



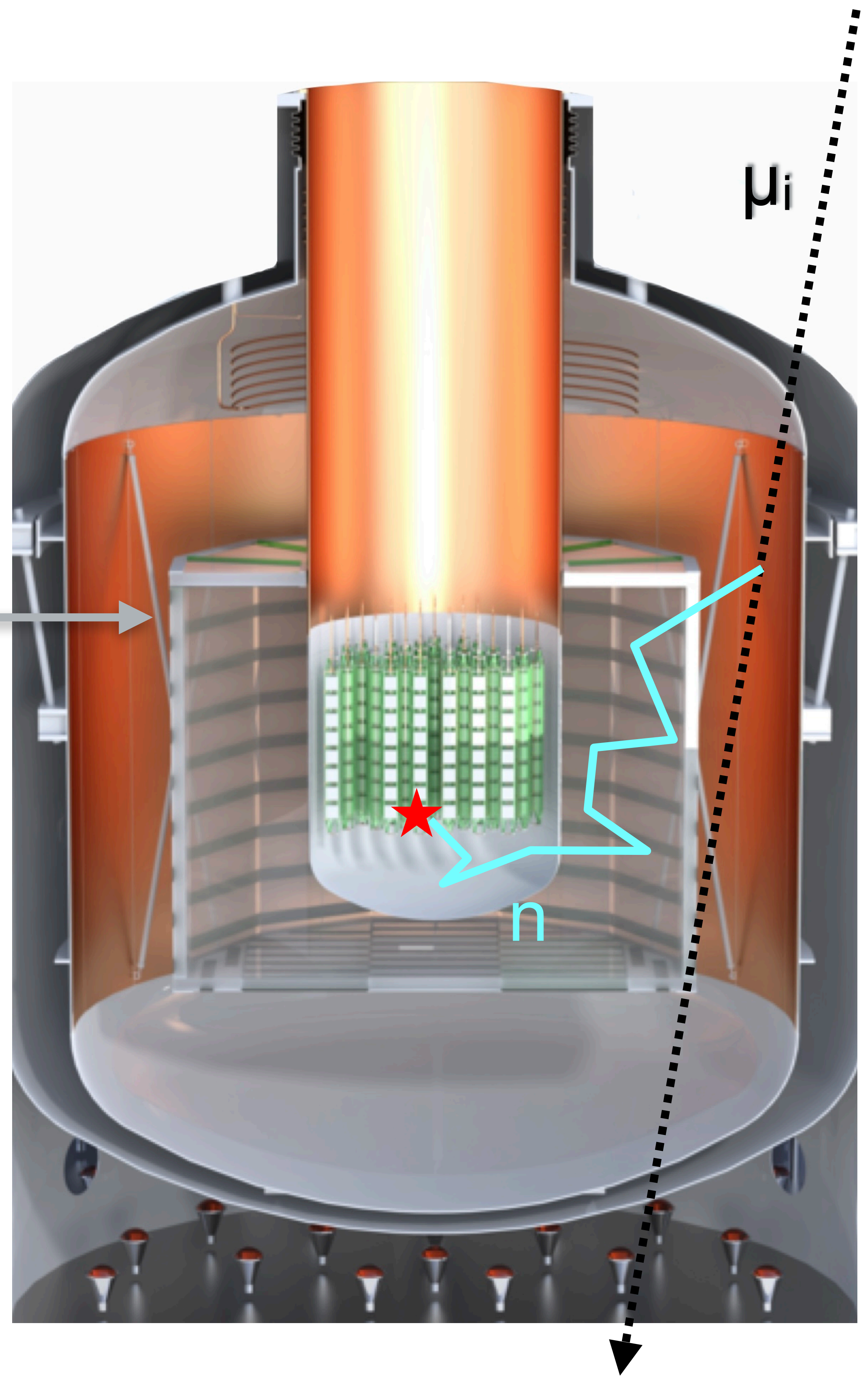
$\Delta L \neq 0$

Let's define a few parameters

Simulation run:
N events with
- design parameter $\boldsymbol{\theta}_k$ and
- event-specific parameter $\boldsymbol{\phi}_{ik}$ (drawn from $g(\boldsymbol{\phi})$)

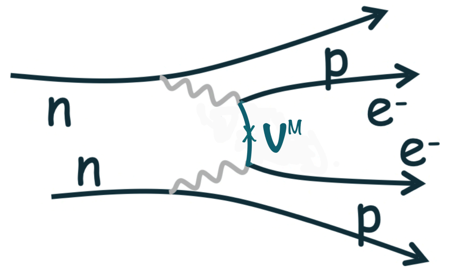
design parameters θ_k
- absorber radius
- absorber thickness
- …

Per simulation run:
θ_k is fixed



event-specific parameters ϕ_{ik}
- muon energy
- muons inital position
- muon momentum
- …

Per simulation run:
N events with randomly drawn ϕ_{ik}



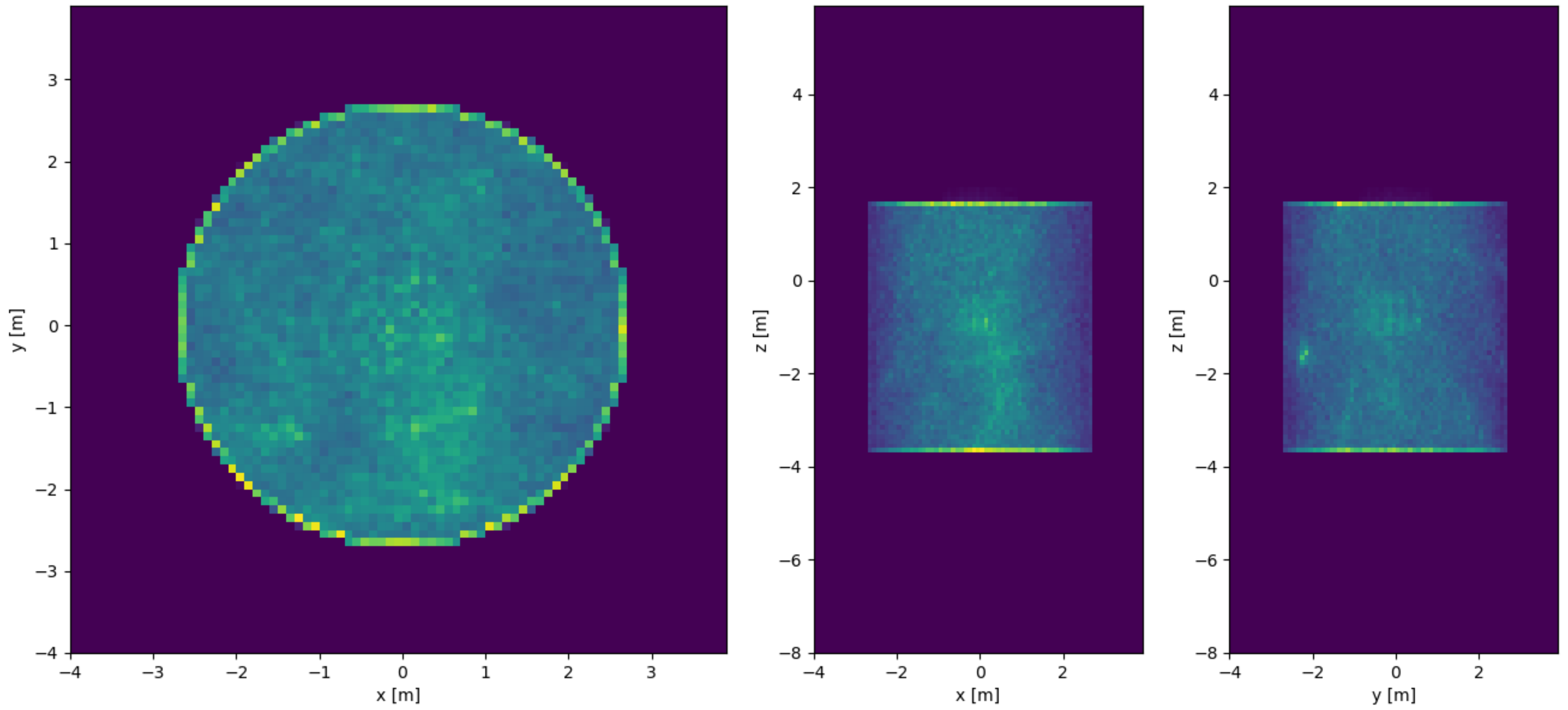
HF & LF simulation

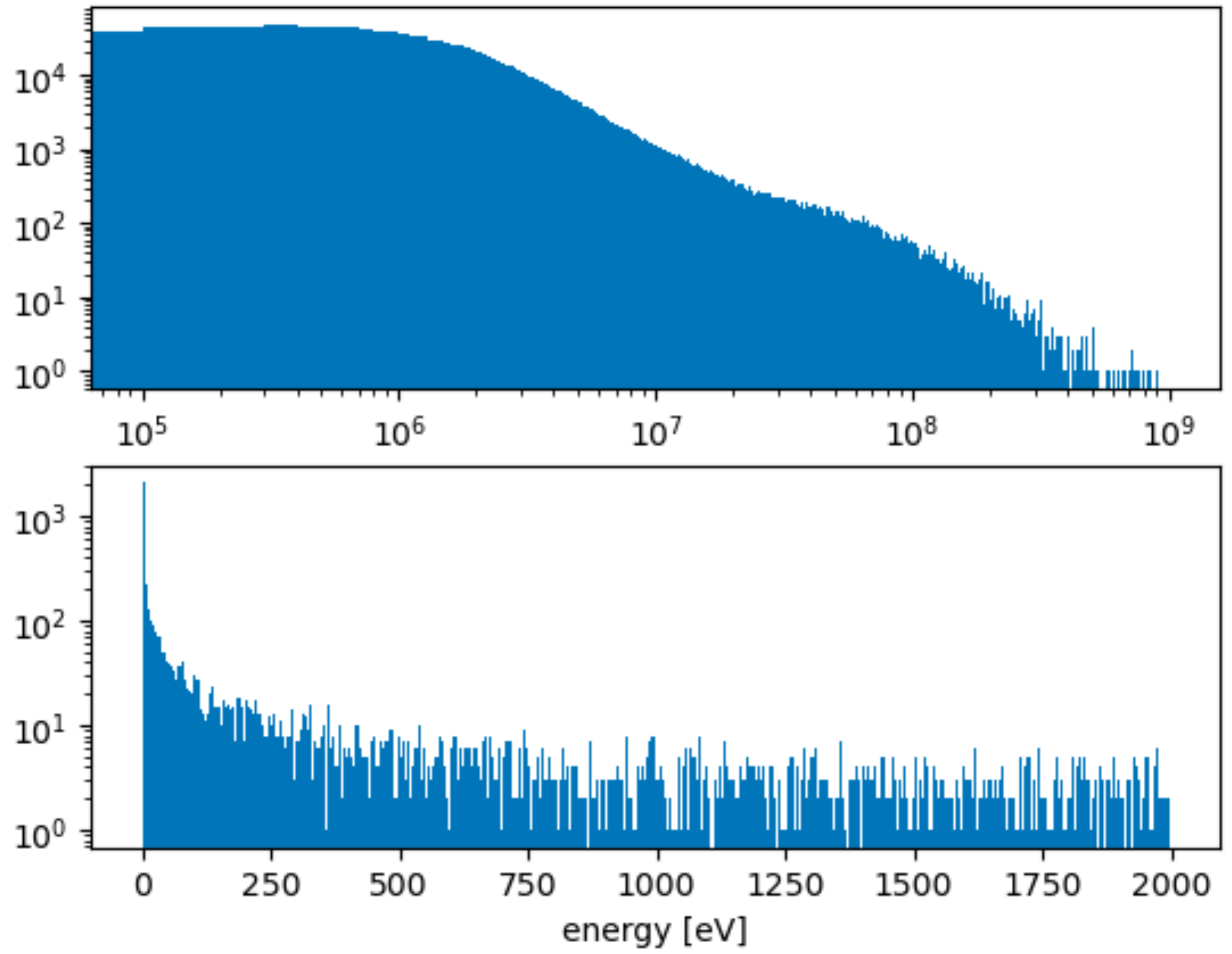
Event specific distribution

$$g(\phi) = \underbrace{g_\mu(\phi_\mu)\, d\phi_\mu}_{\text{muon}} \cdot \boxed{\underbrace{g_n^{\text{ini}}(\phi_n^{\text{ini}} \,|\, \phi_\mu)}_{\text{in}} \cdot \underbrace{g_n^{\text{fin}}(\phi_n^{\text{fin}} \,|\, \phi_n^{\text{ini}})}_{\text{out}}}\ \text{LF}$$

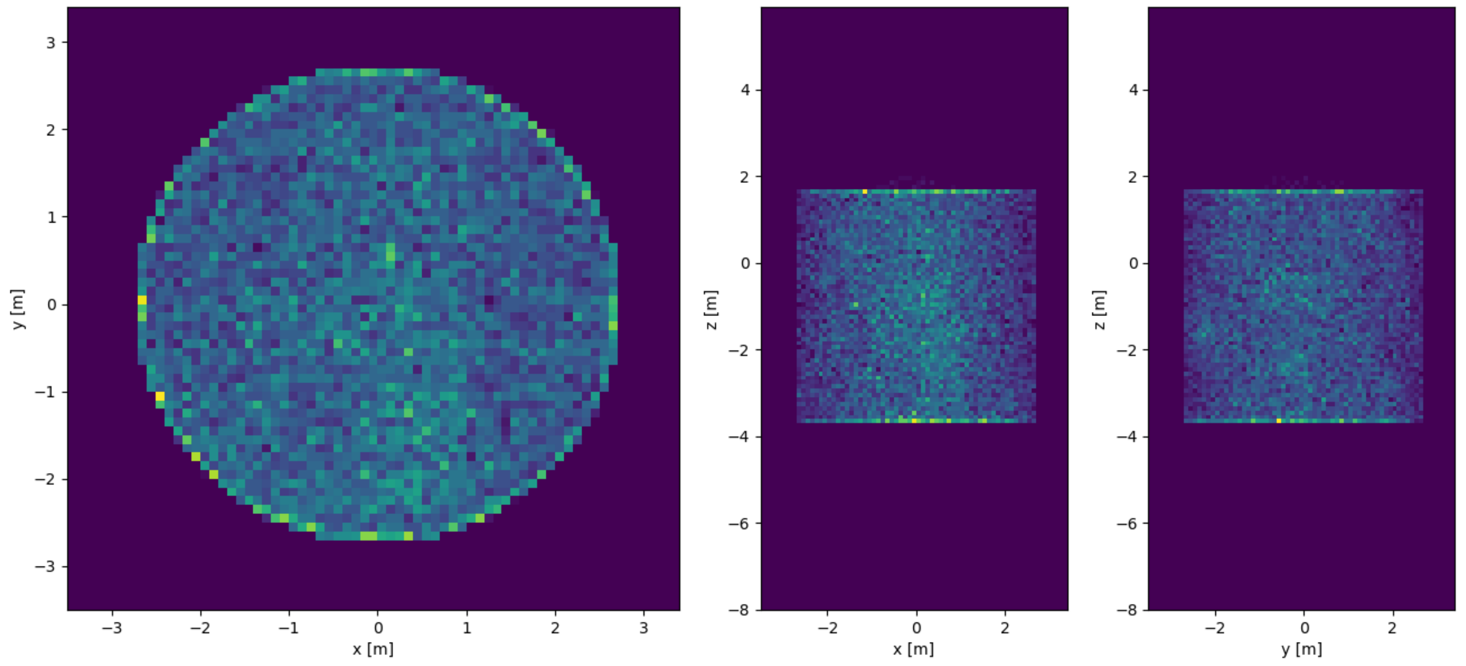
neutron

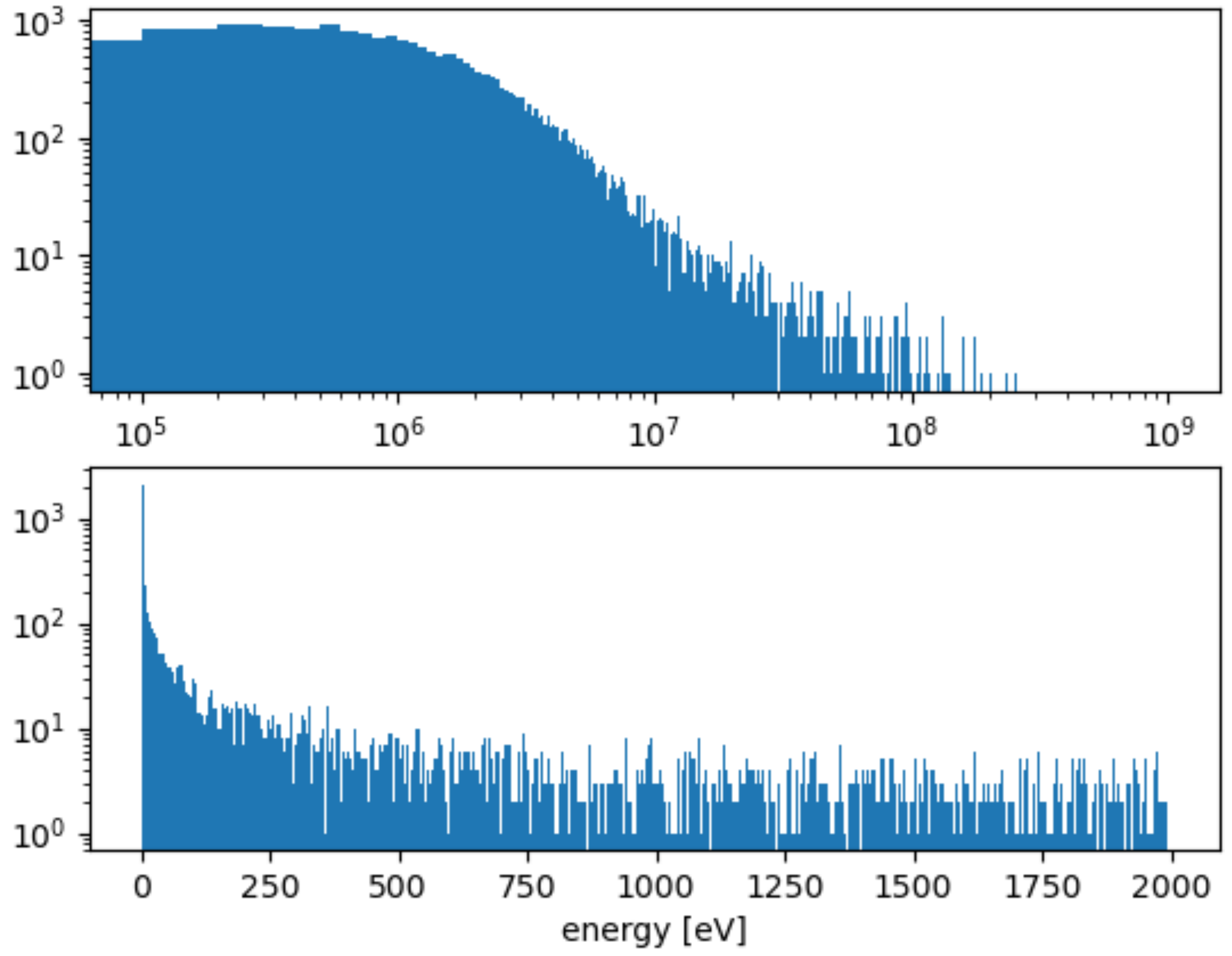
LF input





draw distributions with random neutron starting points from high fidelity simulation



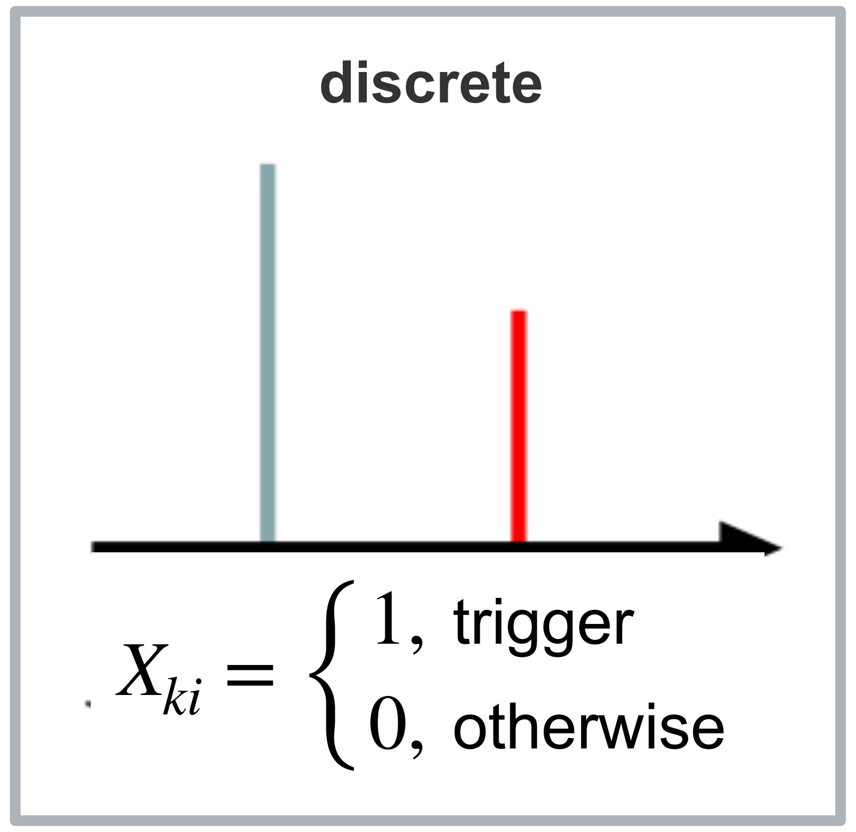


	HF	LF
Primary particle	Muon	Neutron
CPUh per neutron	$1.5\cdot10^{-4}$ ($2\cdot10^{-5}$ per muon)	$3\cdot10^{-6}$
Full detector geometry	✓	✓
Full neutron physics lists	✓	✓
Timing to primary and production info	✓	✗

Rare Event Problem

Simulation run:
N events with
- design parameter $\boldsymbol{\theta}_k$ and
- event-specific parameter $\boldsymbol{\phi}_{ik}$ (drawn from $g(\boldsymbol{\phi})$)

Event Outcome
X_{ik}



Signal trigger rate

$$y = \frac{1}{N} \sum X_{ik}$$

$$\sim \text{Poisson}(N\bar{t})/N$$

$$X_{ik} \sim \text{Bernoulli}(p = t(\boldsymbol{\theta}_k, \boldsymbol{\phi}_{ik}))$$

Trigger Probability
$t(\boldsymbol{\theta}_k, \boldsymbol{\phi}_{i,k})$ **small**

Rare Event Assumption

$$\boxed{y \ll 1}$$

Event Simulation

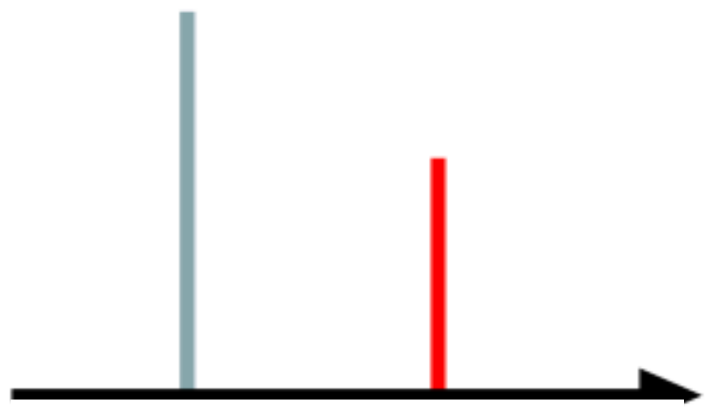
N events with

- design parameter $\boldsymbol{\theta}_k$ and
- event-specific parameter $\boldsymbol{\phi}_{ik}$ (drawn from $g(\boldsymbol{\phi})$)

Event Outcome

X_{ik}

discrete



$$X_{ki} = \begin{cases} 1, & \text{trigger} \\ 0, & \text{otherwise} \end{cases}$$

$X_{ik} \sim \text{Bernoulli}(p = t(\boldsymbol{\theta}_k, \boldsymbol{\phi}_{ik}))$

Trigger Probability

$t(\boldsymbol{\theta}_k, \boldsymbol{\phi}_{i,k})$ **small**

Signal trigger rate

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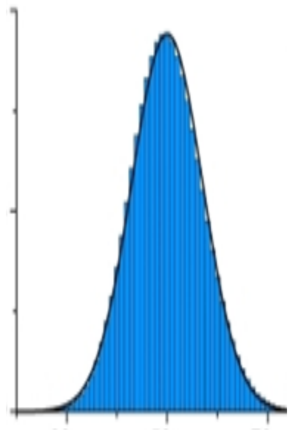
$\boxed{y \ll 1}$

Large N



Large N scenario

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

Low Variance, High Cost.

$N \to \infty$, y will asymptotically approximate the **expected trigger probability**

$$\bar{t}(\boldsymbol{\theta}) = \int t(\boldsymbol{\theta}, \boldsymbol{\phi}) g(\boldsymbol{\phi}) \mathrm{d}\boldsymbol{\phi}$$

Ultimate metric to optimize

$$\boldsymbol{\theta}^\star = \arg\min_{\theta \in \Theta} \bar{t}(\boldsymbol{\theta})$$

Event Simulation

N events with

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Event Outcome

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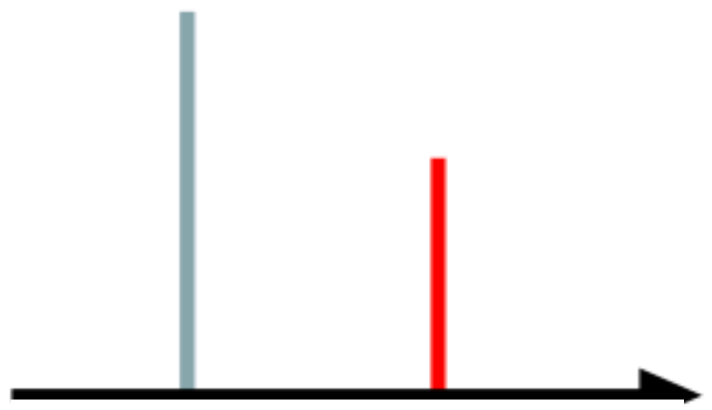
discrete



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Trigger Probability

$t(\boldsymbol{\theta}_k, \boldsymbol{\phi}_{i,k})$ **small**

Signal trigger rate

$$y = \frac{1}{N} \sum X_{ik}$$

$$\sim \text{Poisson}(N\bar{t})/N$$

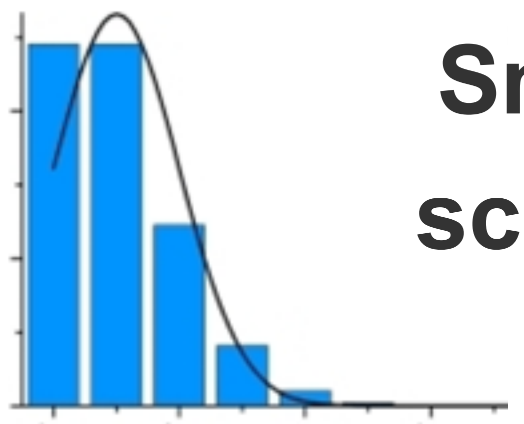
$$\boxed{y \ll 1}$$

Expensive simulator

Small N Scenario as simulation is costly:

- y very sensitive to statistical fluctuations.
- y takes **discrete values** and cannot be approximated by a normal distribution.

Small N

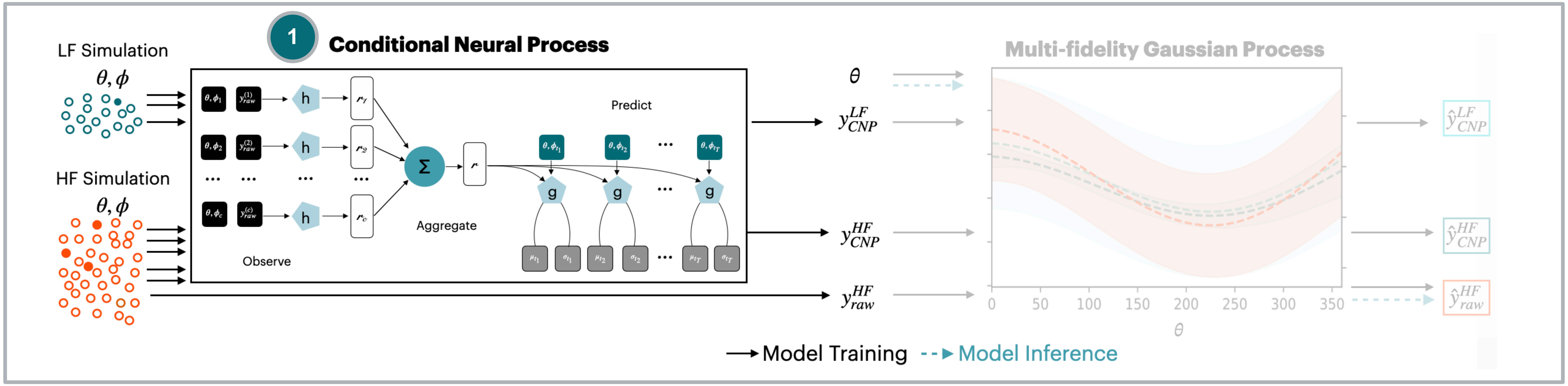


Small N scenario

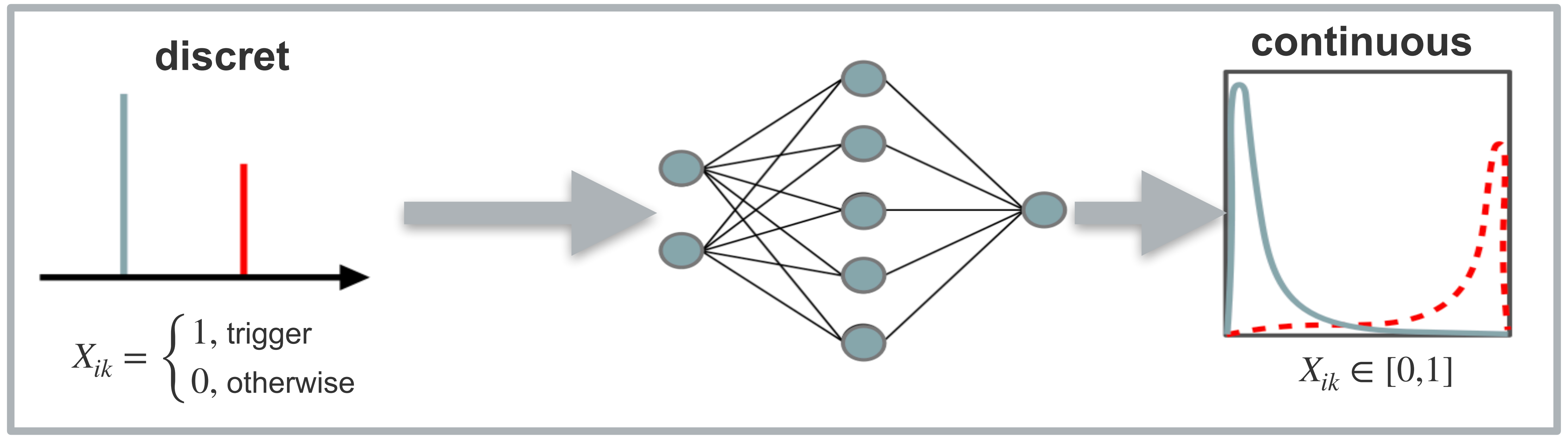
$y \in \{0/N, 1/N, \ldots\}$ discrete

High Variance, Low Cost.

Rare Event Surrogate Model (ReSUM)



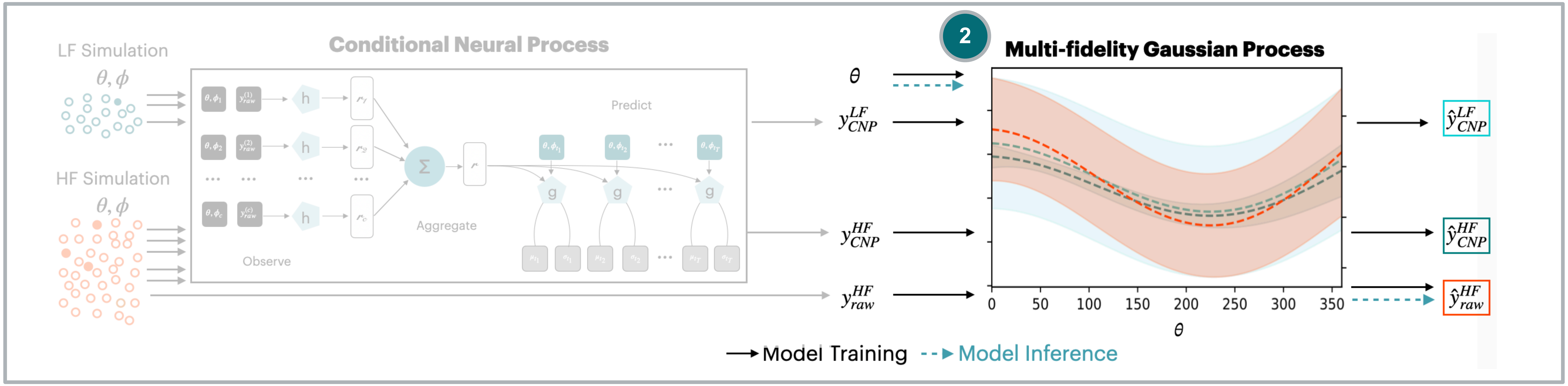
1. Conditional Neutral Process



Mitigate statistical noise

- Converts each discrete event outcome into a continuous score
- Propagates uncertainty awareness into final mapping

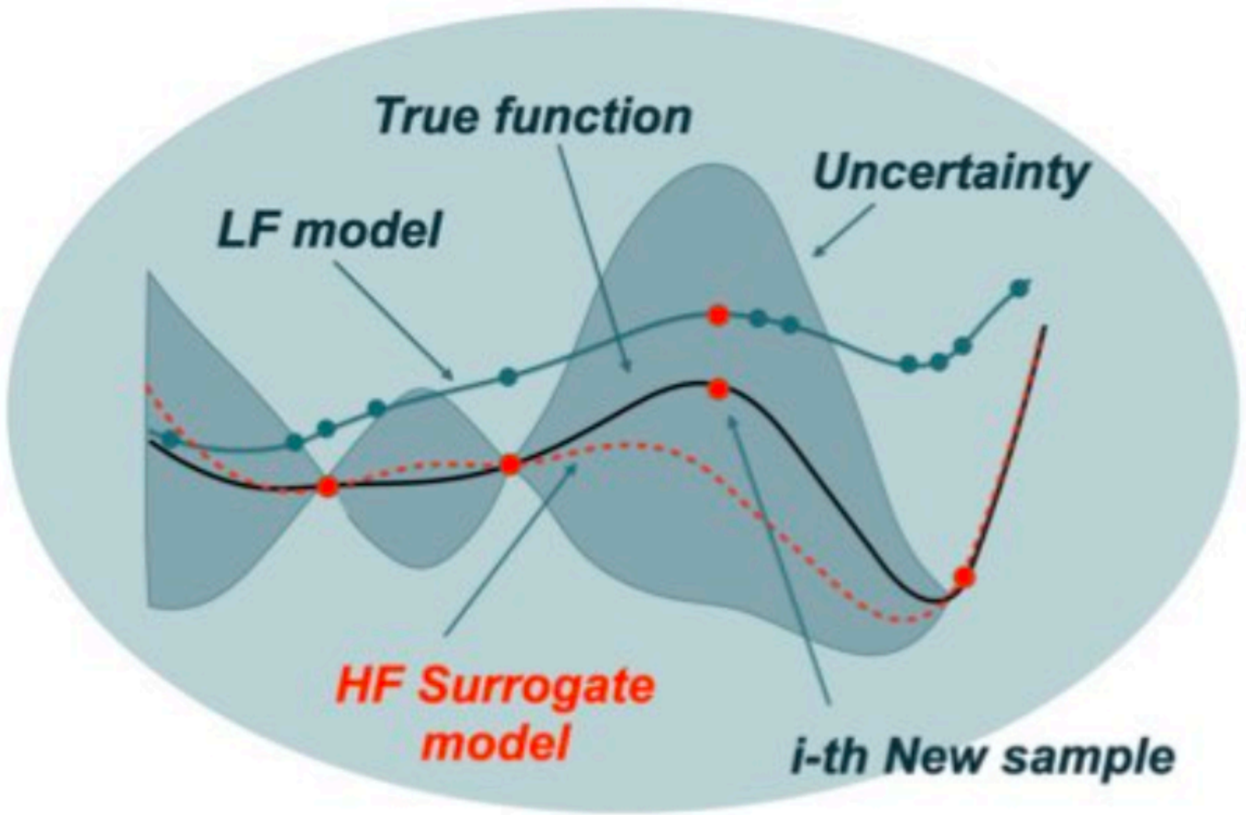
Rare Event Surrogate Model (ReSUM)



2. Multi-fidelity Gaussian Process

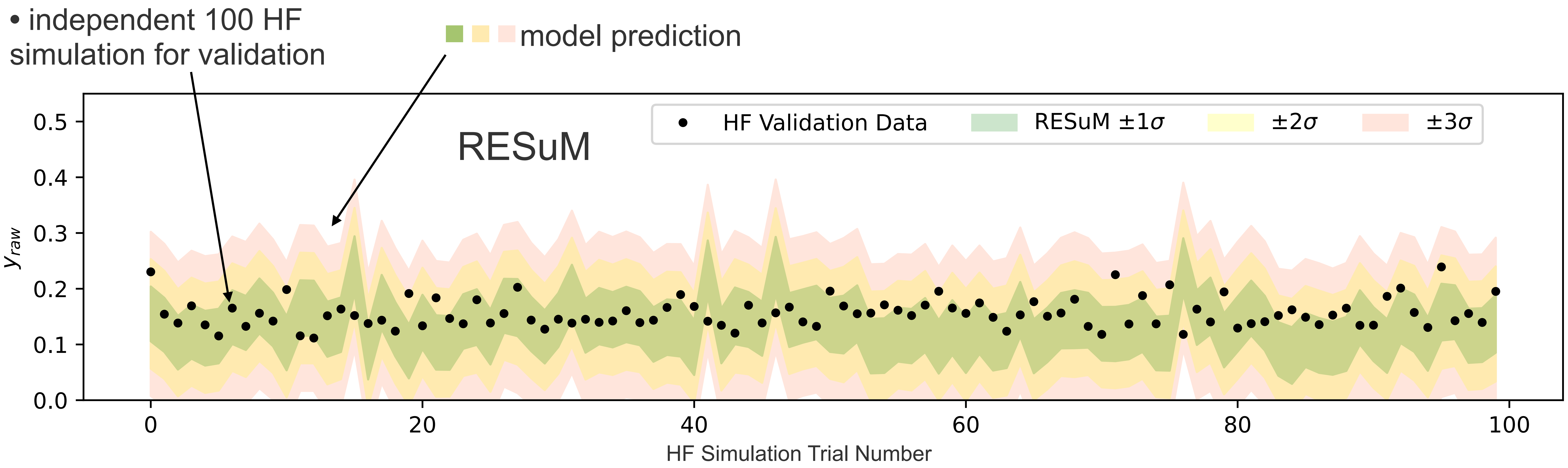
Reduce computational cost

- Multi-Fidelities approach where low-fidelity (LF) helps with space exploration



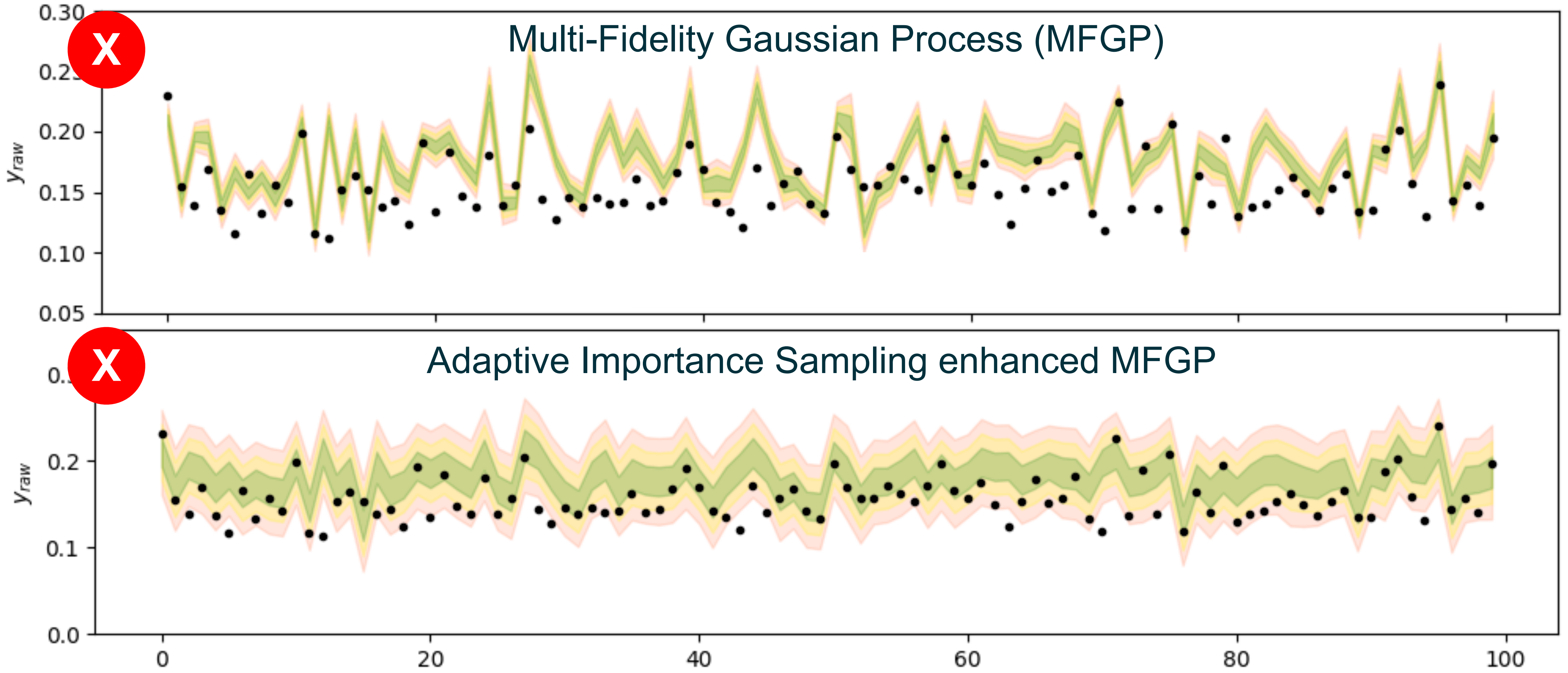
Model Benchmarking

- **96.7% reduction in compute cost**
- **Accurate and calibrated predictions**



Benchmarking Result of RESuM model with respect to different baseline models.

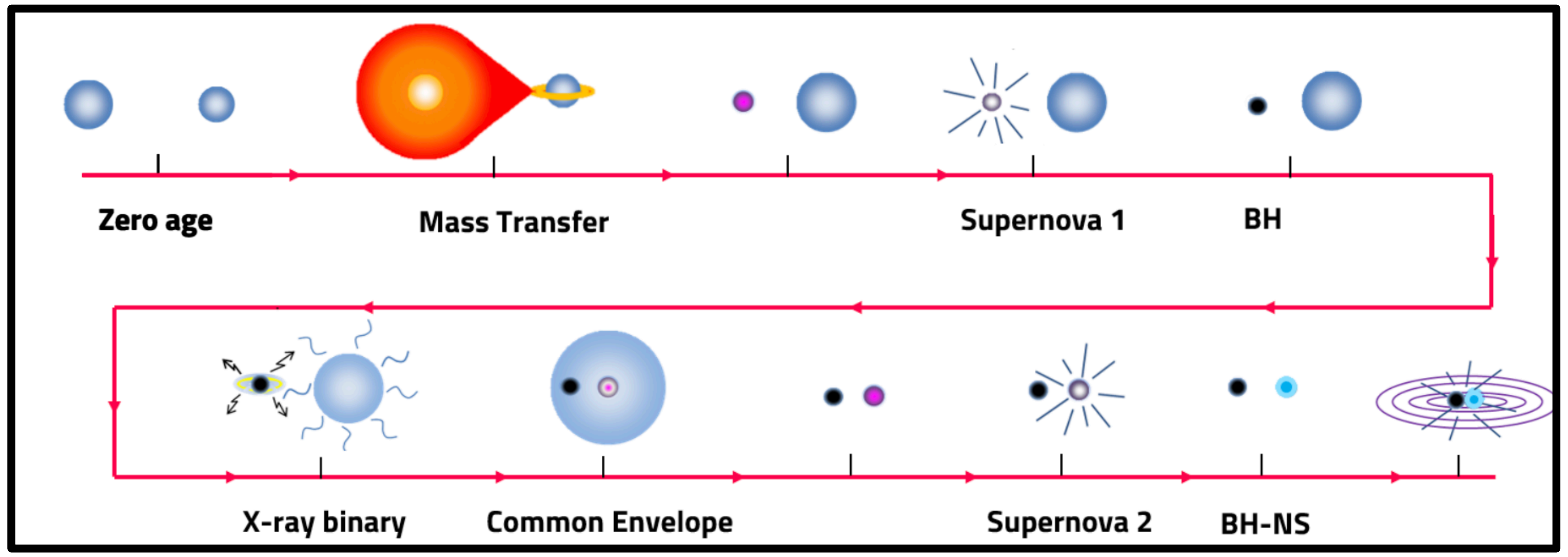
- Overly narrow prediction bands
- Poor alignment
- Predictions lack physical relevance



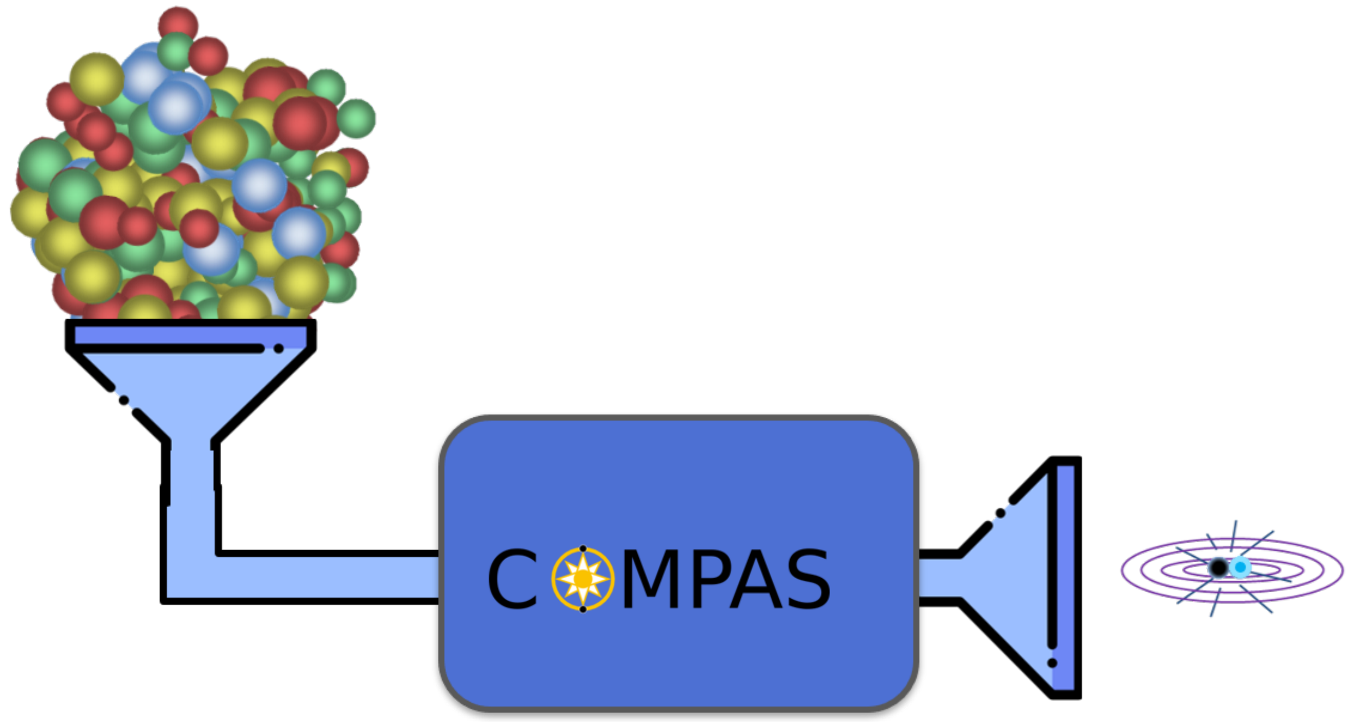
Binary Black Hole Population Synthesis

In Collaboration with **Prof. Floor Broeckgarden (UCSD)**

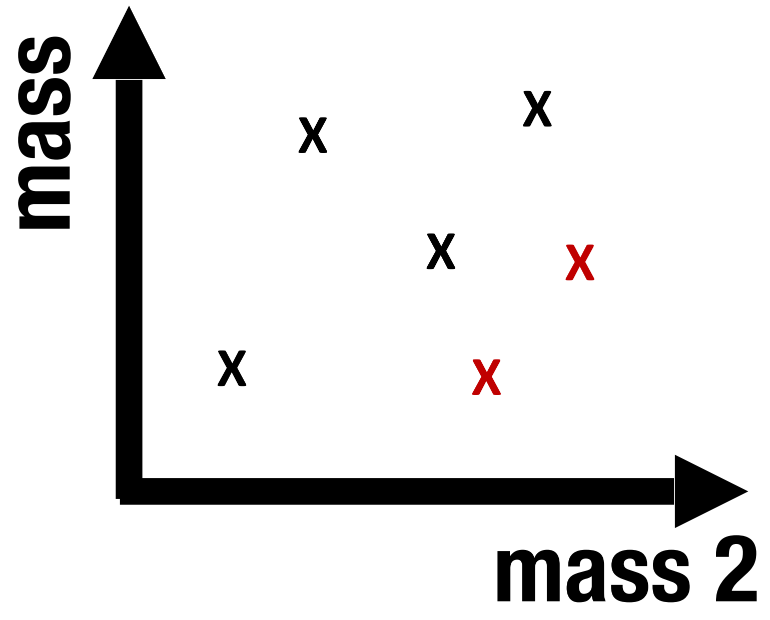
Binary Black Hole Merger Simulation



1 000 000 binaries



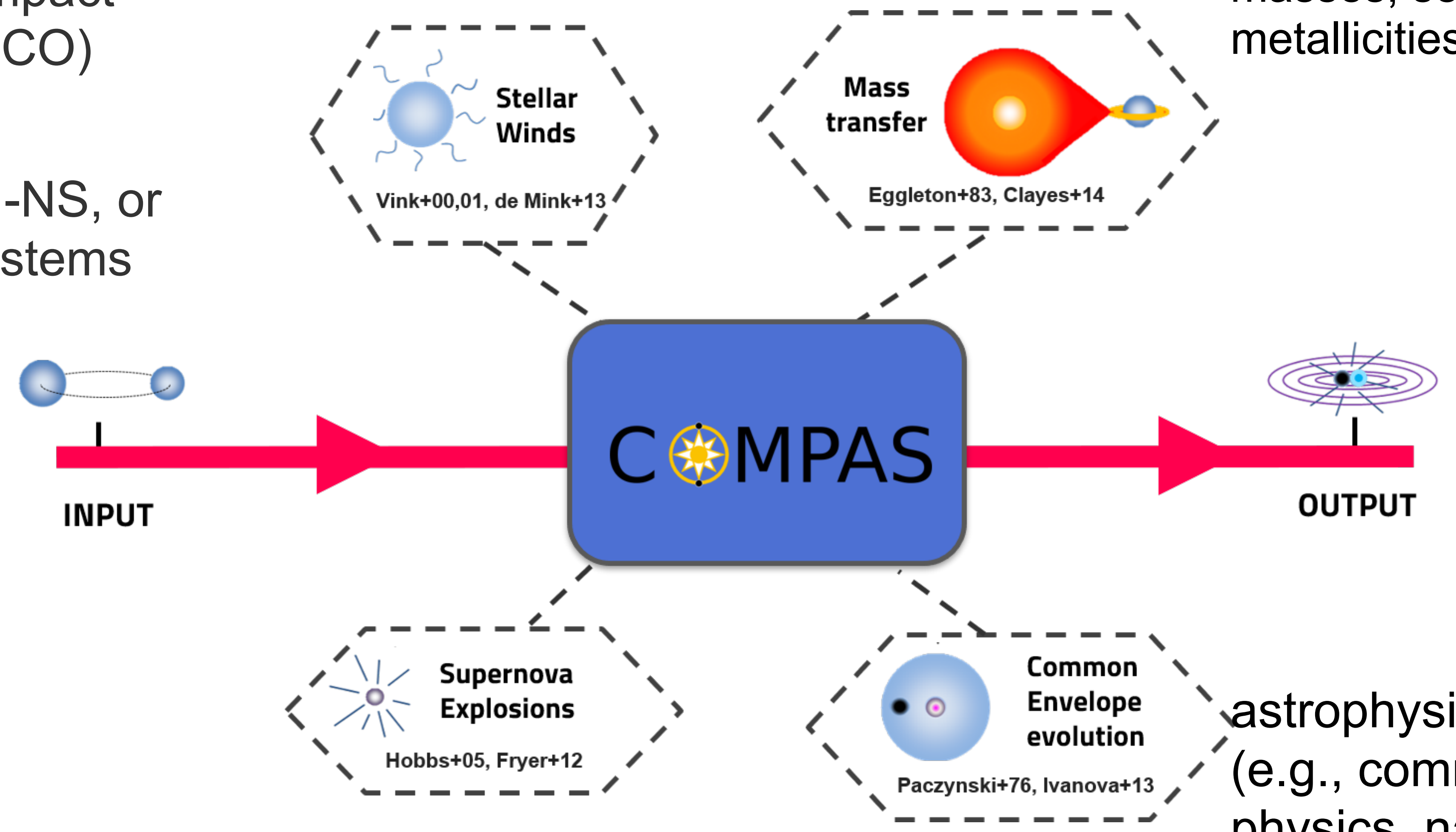
only ~1 merger!



Double Compact Objects (DCO)

BH-BH, BH-NS, or NS-NS systems

initial conditions (e.g., masses, separations, metallicities)



astrophysical models (e.g., common-envelope physics, natal kicks, metallicity effects)

Leads to large Poisson (sampling) noise

- signal to background ratio $1{:}10^6$
- convergency only for $N > 3 \cdot 10^8$
- 180 CPUh
- high statistical uncertainties due to limited sample size
- most interesting gravitational wave sources occur in extreme tails of distr.

[Pictures from F. Broeckgarden]

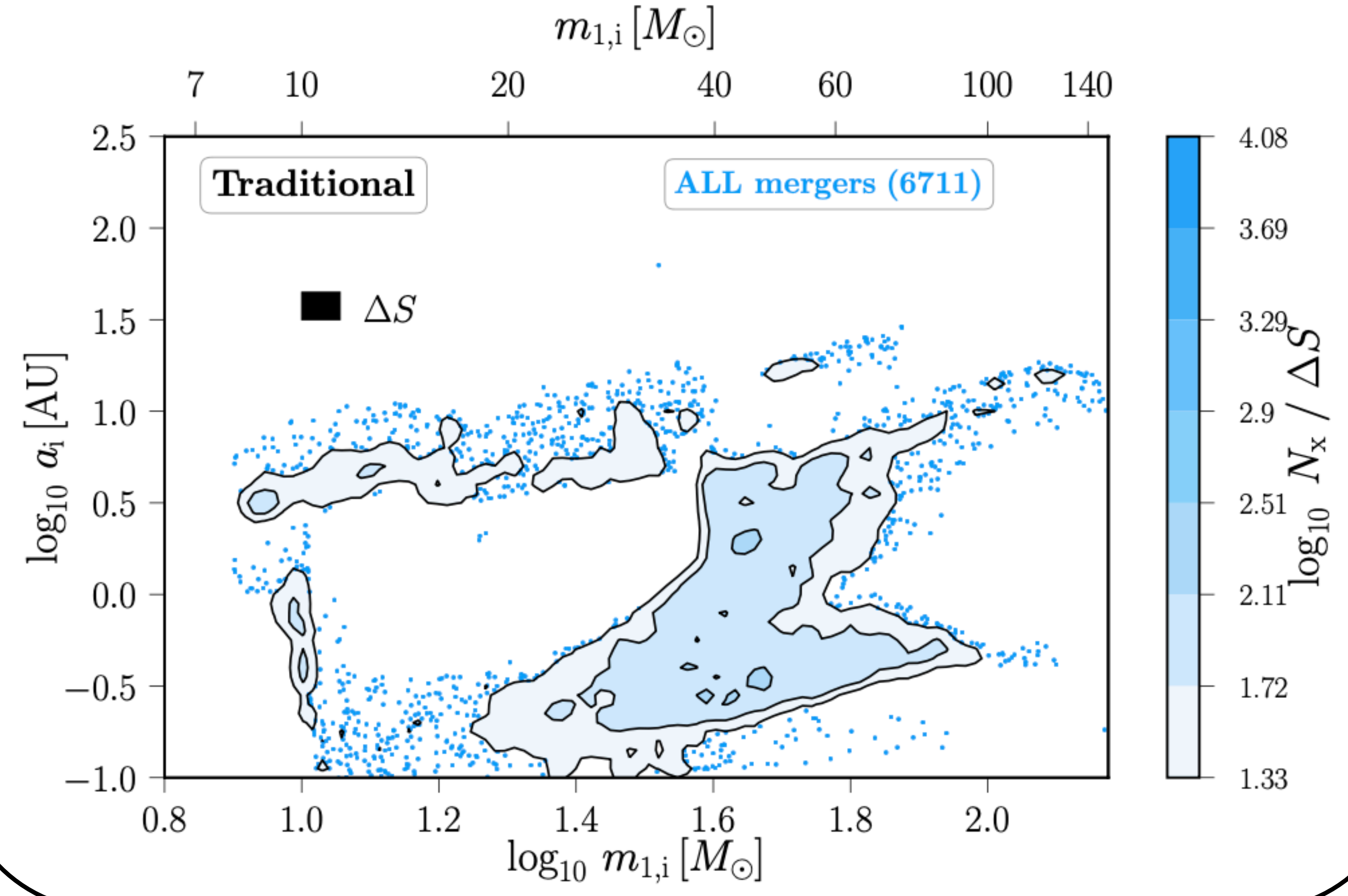
Binary Black Hole Population Synthesis

In Collaboration with **Prof. Floor Broeckgarden (UCSD)**

Goal: Higher resolution mapping of initial conditions leading to mergers

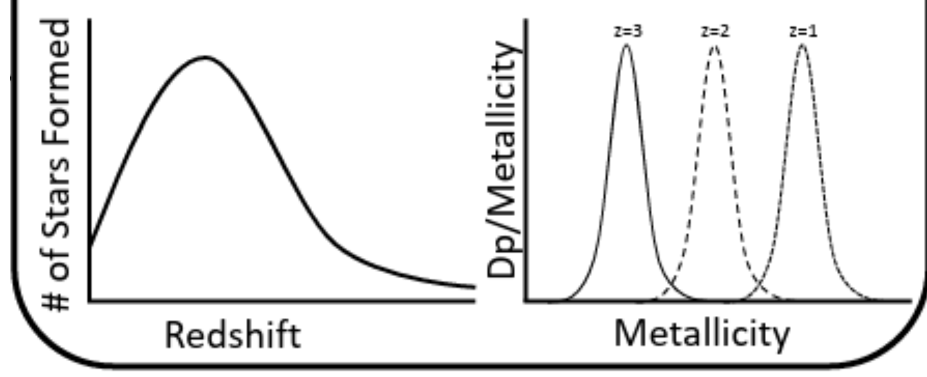
Step 1:
Binary Evolution

Step 2:
High resolution mapping via RESuM

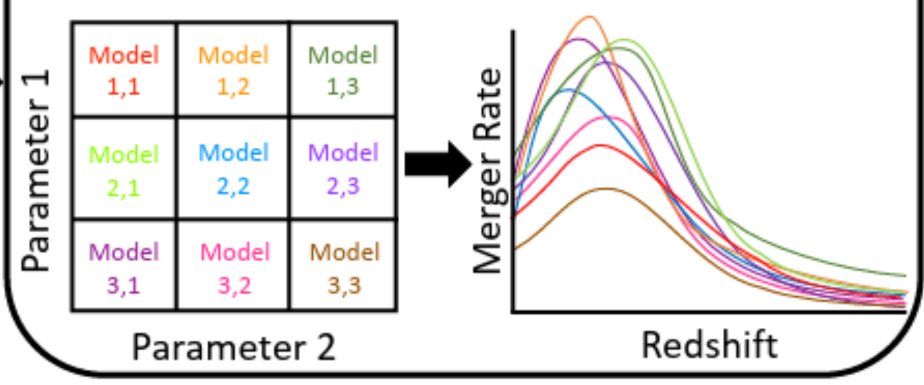


RESuM
+ improved Regression with PCA combined with MCMC sampling
+ Improved adaptive learning via Expected Improvement (EI)

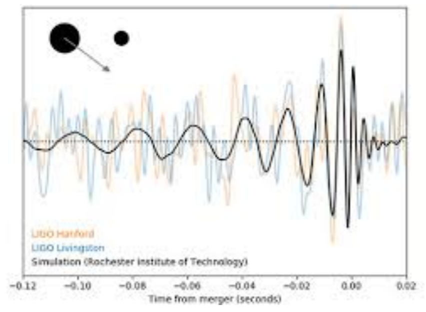
Step 3:
Model MSSFR



Step 4:
Find Each Model's $R(z)$



Step 5:
Bayesian inference



[Pictures from F. Broeckgarden]

1 BERKELEY LAB 2 UNIVERSITY OF CALIFORNIA SAN DIEGO U.S. DEPARTMENT OF ENERGY Office of Science

Rare Event Surrogate Model (RESuM) for Physics Detector Design

Ann-Kathrin Schuetz[1] Alan Poon[1] Aobo Li[2]

For more details see our paper

ICLR
International Conference On Learning Representations

Spotlight