





# Simulation-based Inference for Precision Neutrino Physics through Neural Monte Carlo Tuning

Arsenii Gavrikov, **Andrea Serafini**, Dmitry Dolzhikov on behalf of the JUNO Collaboration

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# Simulation-based Inference for Precision Neutrino Physics through **Neural Monte Carlo Tuning**

Our ML guru -

ML guru JUNO analysis fit/statistics enthusiasts
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### The JUNO experiment

#### What is JUNO (Jiangmen Underground Neutrino Observatory)? [1]

- Large-scale, next-generation liquid scintillator (LS) detector
- It features a massive 20-kiloton LS target
- Monitored by over 43,000 Photomultiplier Tubes (PMTs) to detect light

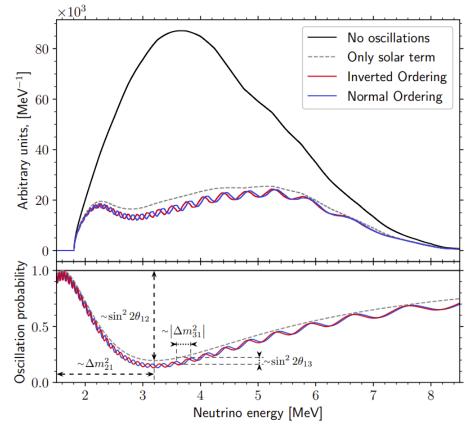
#### **Primary Physics Goals** [2, 3]

- Determine the **Neutrino Mass Ordering** (NMO).
- Measure three neutrino oscillation parameters ( $\Delta m^2_{21}$ ,  $\Delta m^2_{31}$ ,  $\sin^2\theta_{12}$ ) with sub-percent precision
- Broad physics program including geoneutrinos, supernovae, and more

#### The Core Challenge

- Unprecedented <3% @ 1 MeV energy resolution and</li>
   <1% control over energy-scale systematic uncertainties</li>
- → need for on highly accurate and well-tuned Monte Carlo (MC) simulations!



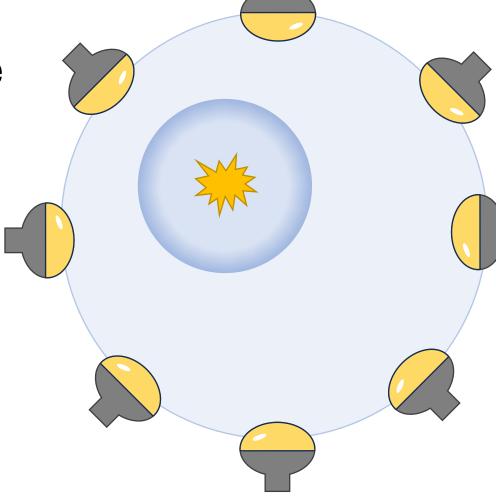


[3] JUNO Collaboration 2025 Chinese Phys. C 49 3, 033104

The Energy Response Challenge

#### **How JUNO Detects Events**

- JUNO is a **calorimeter**: a particle deposits energy in the scintillator.
- The scintillator emits light collected by PMTs and measured as a total number of photo-electrons (NPE) → our proxy for the visible energy



## The Energy Response Challenge

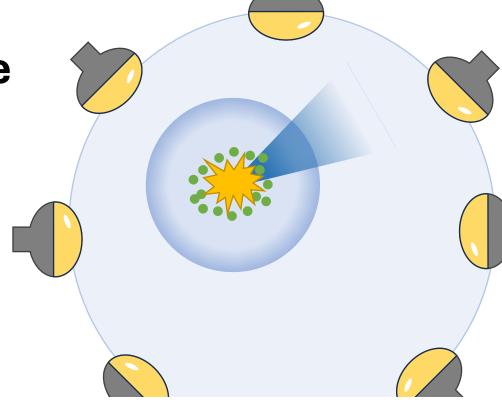
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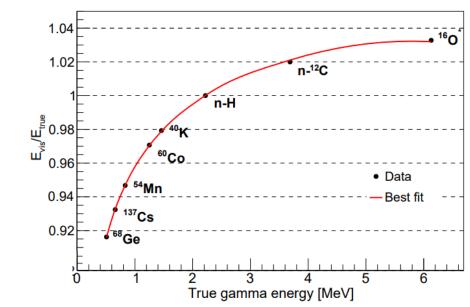
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#### The Problem: A Non-Linear Response

- The relationship between true deposited energy and NPE is **not linear**.
- Non-linearity in the MC modeled by three key physical parameters:
  - Birks' Coefficient  $(k_B)$   $\downarrow$ : models quenching (energy lost as heat instead of light at high ionization) reducing the signal.
  - Cherenkov Factor  $(f_C) \uparrow$ : models the fraction of Cherenkov light produced by secondary particles absorbed and re-emitted.
  - Light Yield (Y) ↑: models the overall scaling factor for the number of scintillation photons emitted per unit energy (after quenching).





## The Energy Response Challenge

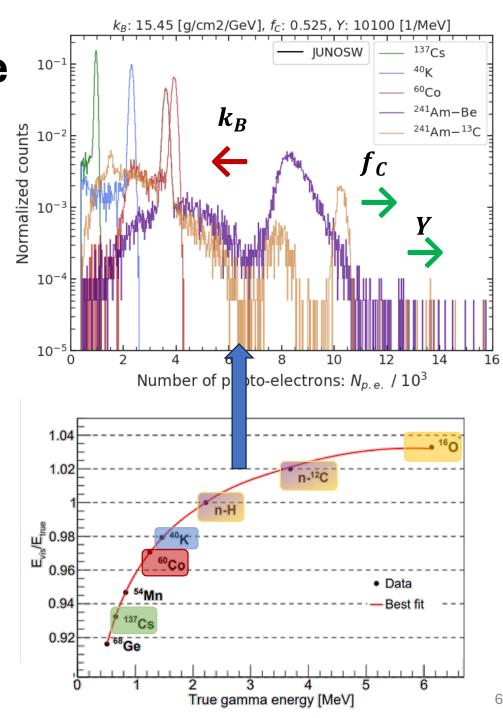
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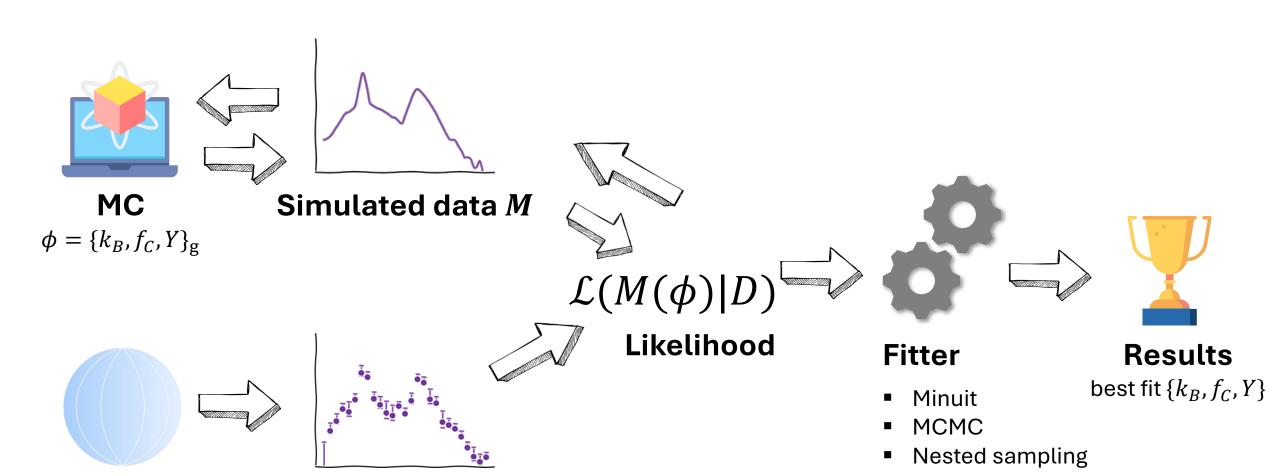
Our Task: tune  $(k_B, f_C, Y)$  so that our MC matches real calibration data.



Calibration data D

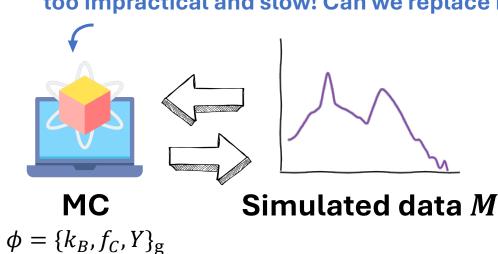
The **most straightforward approach** would be...

**JUNO** 

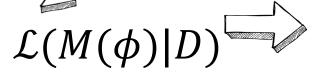


The **most straightforward approach** would be...

too impractical and slow! Can we replace it with a surrogate model?



At each step of the fit, we generate a lot of events with full MC to build spectra of the sources with the corresponding kBg fCg LYg



Likelihood



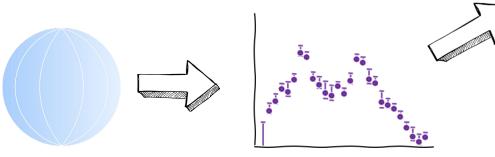
**Fitter** 

**Results** best fit  $\{k_B, f_C, Y\}$ 

- **Analytically intractable**
- MCMC

Minuit

Nested sampling



**JUNO** 

Calibration data D

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**Neural Likelihood Estimation (NLE)** 

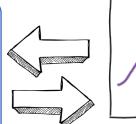


 $\phi = \{k_B, f_C, Y\}_{g}$ 

**Training** 

Fast ML model to get spectra for  $\phi$  $p(x|\phi)$ 

(able to interpolate in param space)





ML generated data M



Likelihood

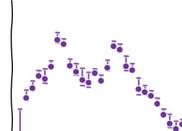




Results

best fit  $\{k_B, f_C, Y\}$ 





**Approximated with SBI** 

Minuit

MCMC

**Fitter** 

Nested sampling





Calibration data D

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**Training** 



MC

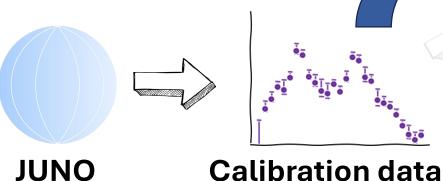
$$\phi = \{k_B, f_C, Y\}_{g}$$

**Neural Posterior Estimation (NPE)** directly outputting the posterior for  $\phi$ ,  $q(\phi|D)$ 

WHY NOT?

#### We wanted to:

- 1. keep model under control
- 2. use **std.** inference **techniques**
- 3. eventually use NLE as **spectra** generated data M **generator** (MC surrogate)





### **Two Neural Likelihood Estimators**

- + straight and reliable model
- requires pre-defined binning



**Multi-output regressor** 

Aims to directly learn a mapping from the parameters and a source type to the histogram representing the spectra PDF

We use a **Transformer encoder-based** model [1] as the density estimator (TEDE)

Conditions: **kB**, **fC**, **LY** + source

type S



- + exact probability density function
- + no pre-defined binning
- + opens a possibility of an unbinned fit

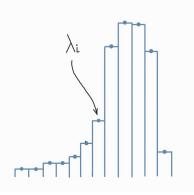
#### Normalizing Flow-based model

Aims to learn the exact conditional **probability** of the energies\* for a given set of parameters and a source type:

We use **Normalizing Flows**-based model [2] to evaluate the exact conditional probability for the events and build the PDF Provides **PDF** estimation by outputting a histogram



### TEDE

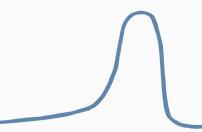


Provides the **exact** conditional PDF for any energy value:

 $P(E \mid k_B, f_C, L_y, S)$ 

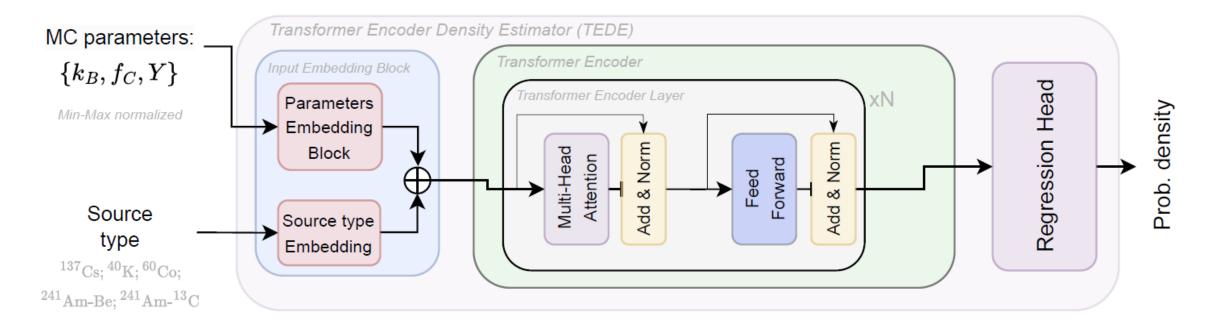


**NFDE** 



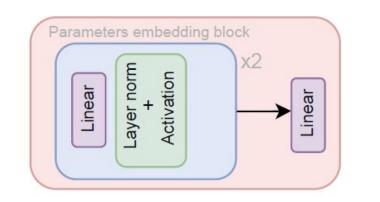
\*represented by amount of light collected

### **Transformer Encoder-based Density Estimator (TEDE)**



#### Multi-output regressor is based on the **Transformer's [1] encoder**:

- A powerful architecture, well known for NLP and CV applications
- Each condition (MC parameter or source type) is treated as a token
- Regressor Head block to convert outputs to the spectra PDF with pre-defined binning (bin size of 20 PEs)

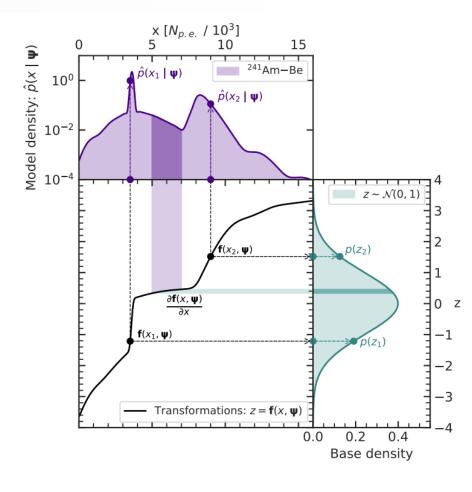


[1] Vaswani A et al, arxiv: 1706.03762

### Normalizing Flows-based Density Estimator (NFDE)

#### Normalizing flows [1]:

- o **generative** ML model aimed to **explicitly model a density estimation**
- o generalizable for modeling **a conditional density estimation** as well
- based on an idea of transforming a simple known distribution
   (e.g. standard Gaussian) to the complex, desired distribution by applying
   multiple learnable (using data) and invertible transformations called flows.

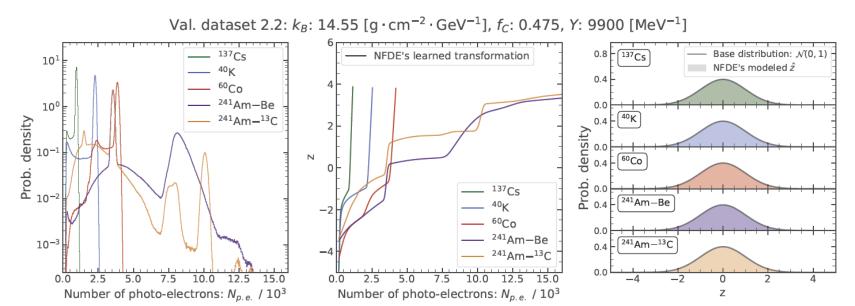


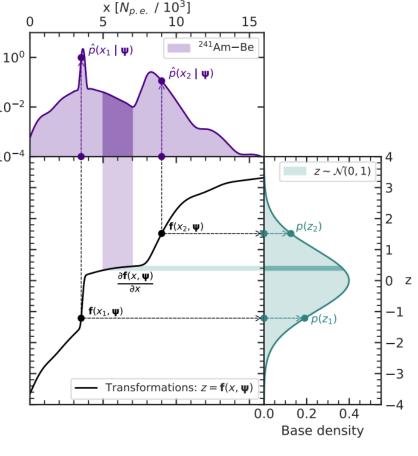
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Model density:  $\hat{\rho}(x \mid \Psi)$ 

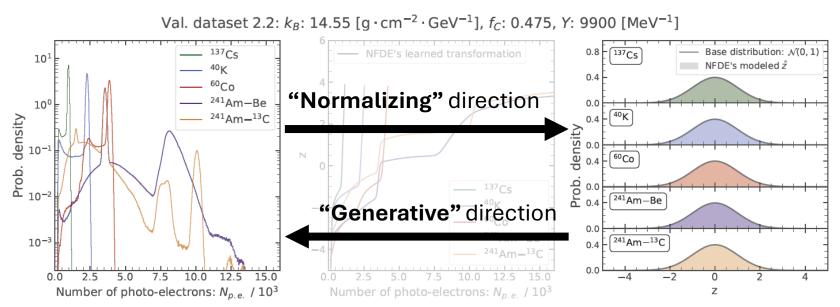
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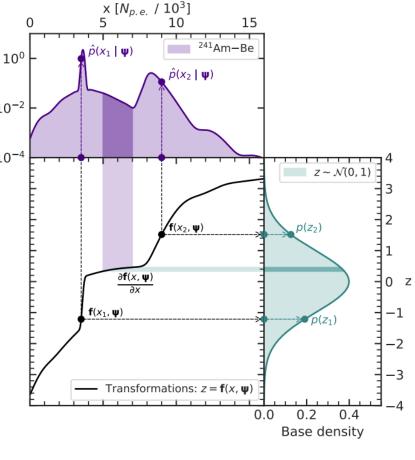
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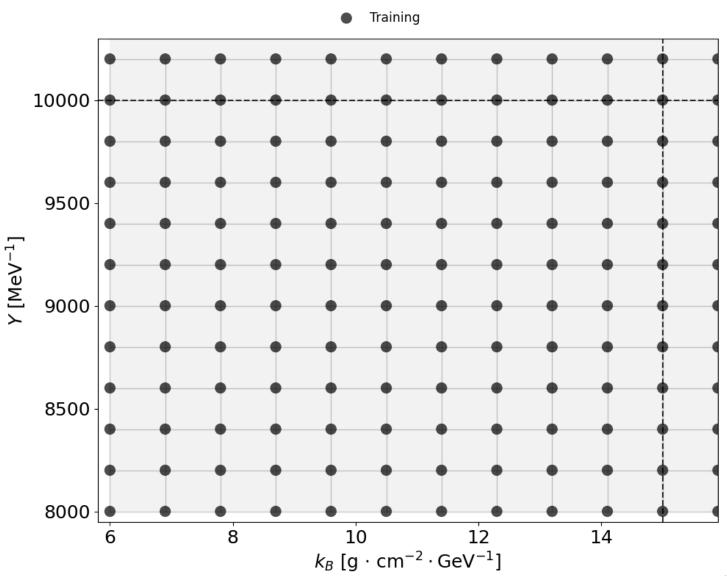
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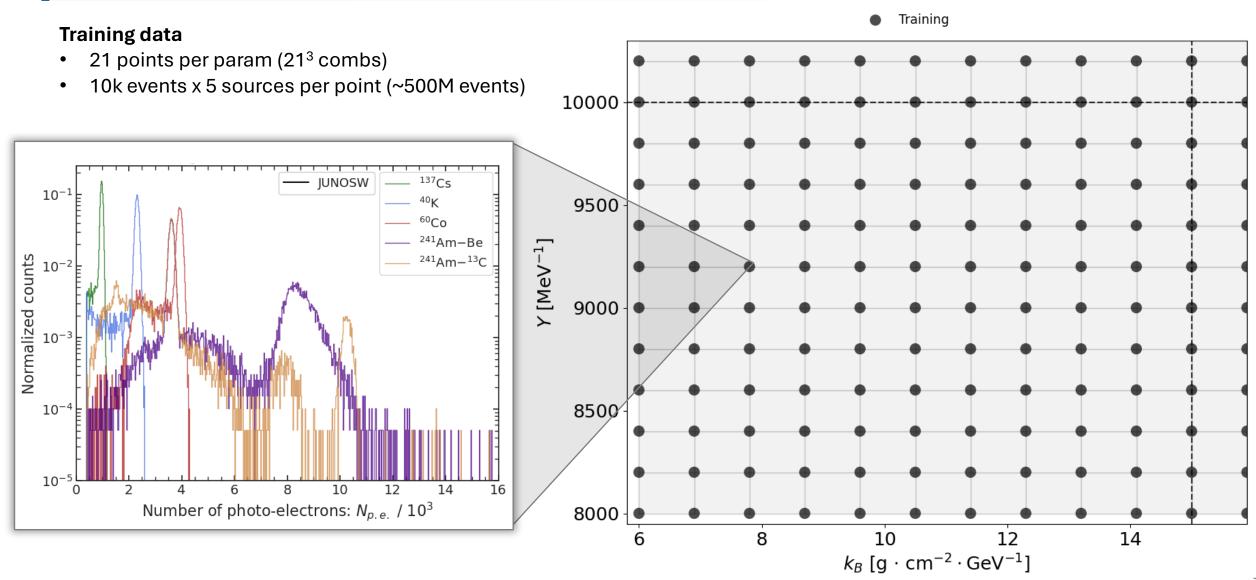
Y and k<sub>B</sub> example

#### **Training data**

- 21 points per param (21<sup>3</sup> combs)
- 10k events x 5 sources per point (~500M events)



Y and k<sub>B</sub> example



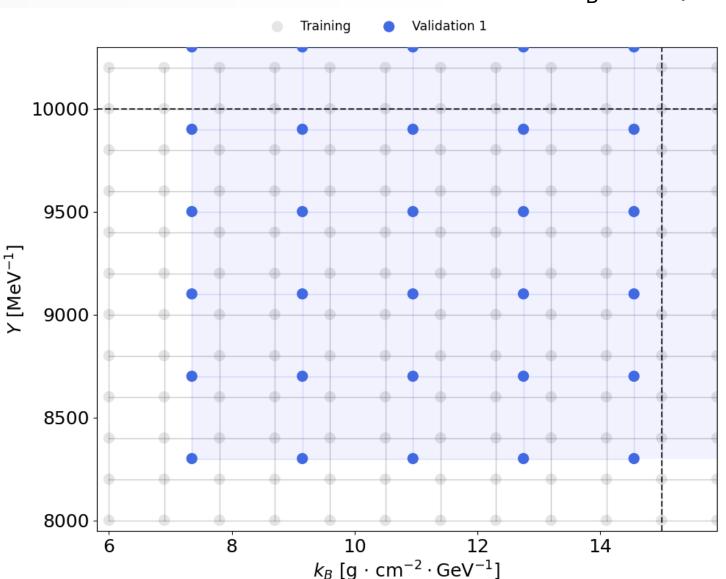
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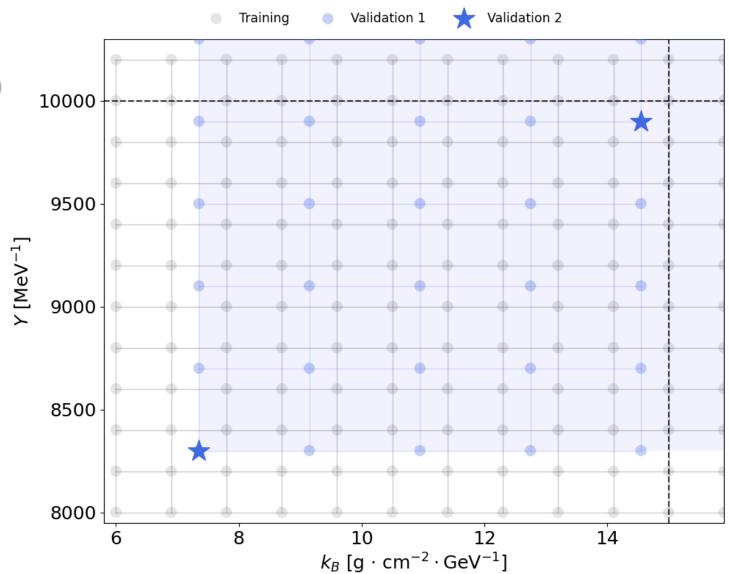
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- 3 points in total
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- → anchor PDF to high-stat spectra



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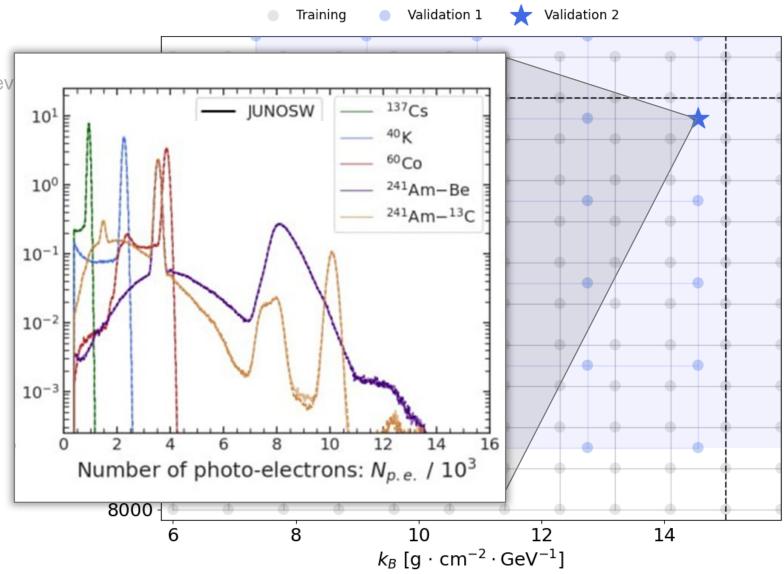
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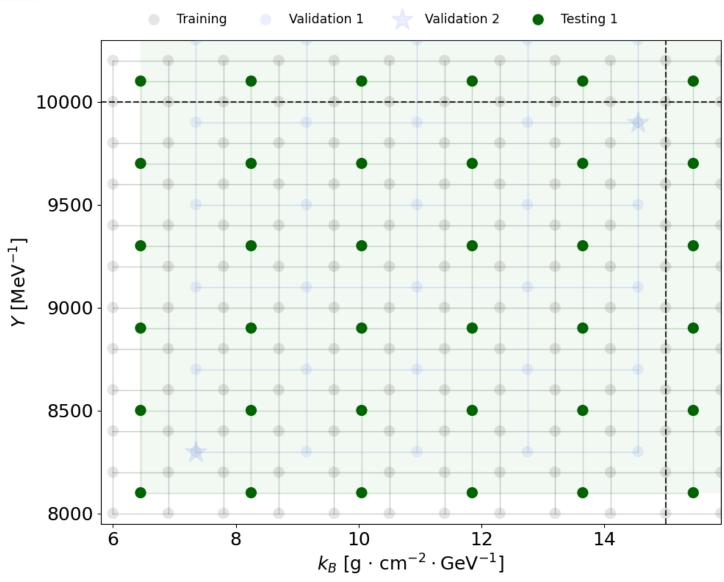
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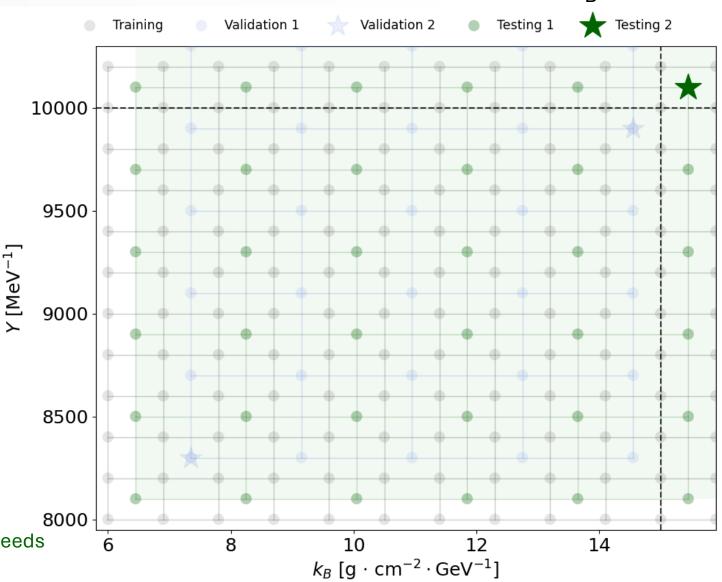
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- 1 point
- 1000 x [1k; 2k; 5k; 10k; 25k] events x 5 with diff. seeds
- → Analysis of **systematic uncertainty** of the model



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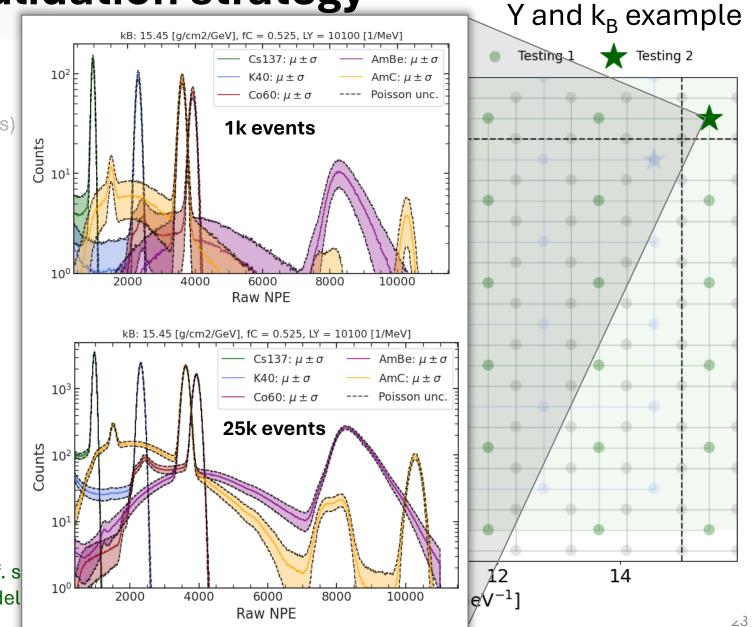
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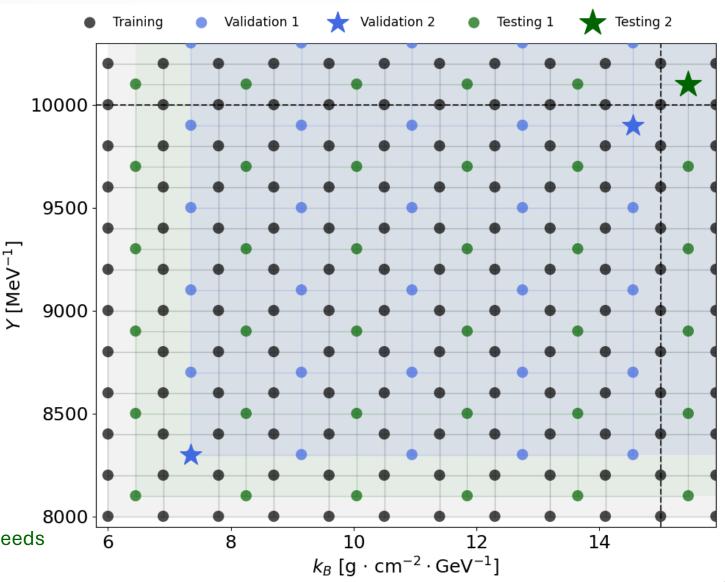
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### Training and validation of the models

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- As validation metrics we use p-norm distances between distributions' CDFs:

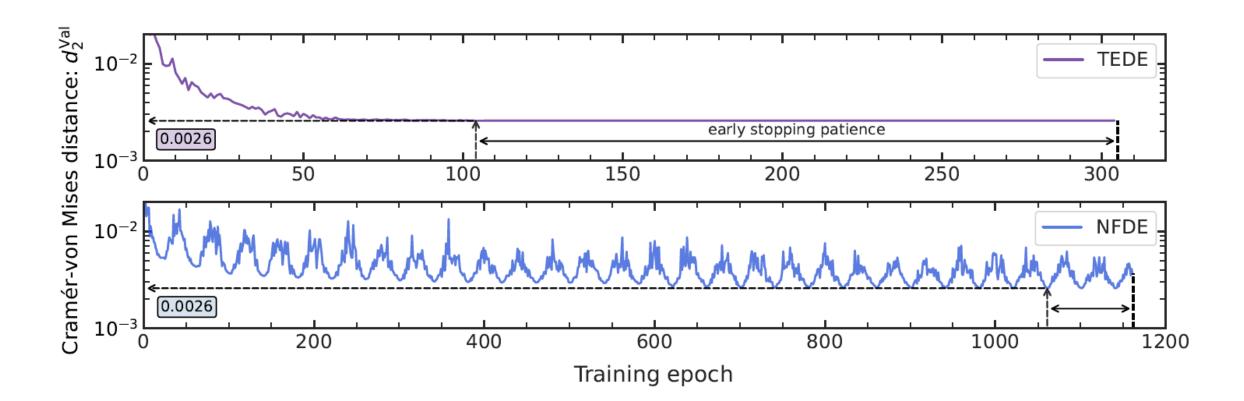
$$d_p(F_u,F_v) = \left(\int_{-\infty}^{+\infty} \left|F_u(x) - F_v(x)
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as it is applicable for both TEDE and NFDE cases

p = 1: Wasserstein distance

p = 2: Cramer-von Mises distance

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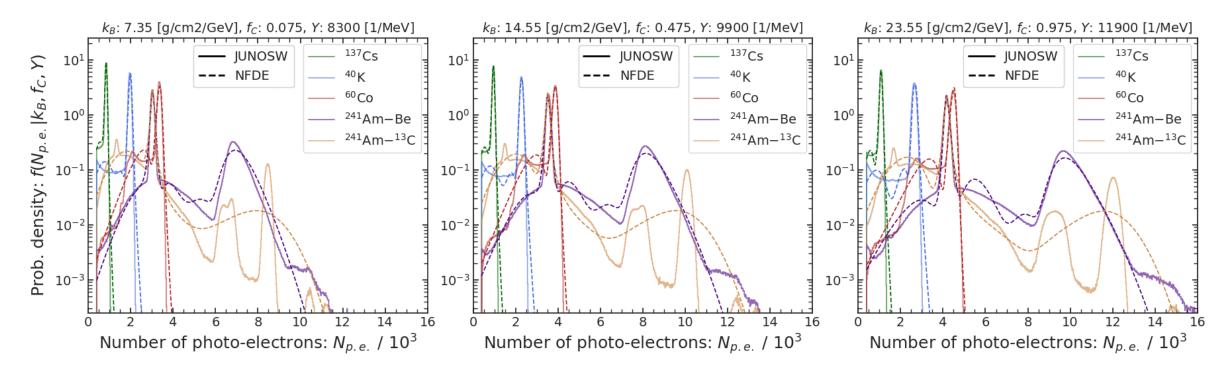
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Validation dataset №2. Epoch: 0, Iteration: 927,  $d_1^{V_2} = 0.0544$ ;  $d_2^{V_2} = 0.0323$ ;  $d_{\infty}^{V_2} = 0.0598$ 



### **Parameter estimation**

#### **Example with NFDE:**

- Combined fit on all sources together
- Cost function: Extended unbinned likelihood
- Optimizer: Nested Sampling (ultranest)\*
- → Estimate the kB, fC, LY best parameters
- → Explores full phase space, **provides full posterior**
- → Shows correlations between the parameters

#### training points



the testing dataset  $N^{o}1$  point is between the points from the training dataset: **interpolation** 

### Parameter estimation

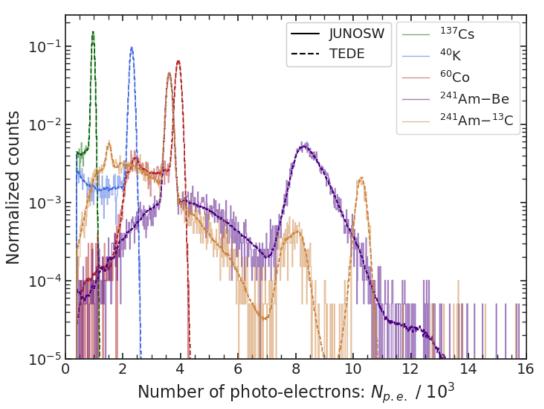
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Model provides spctra estimates for *any* continuous values of the parameters

Model interpolation smooth and denoised





### **Parameter estimation**

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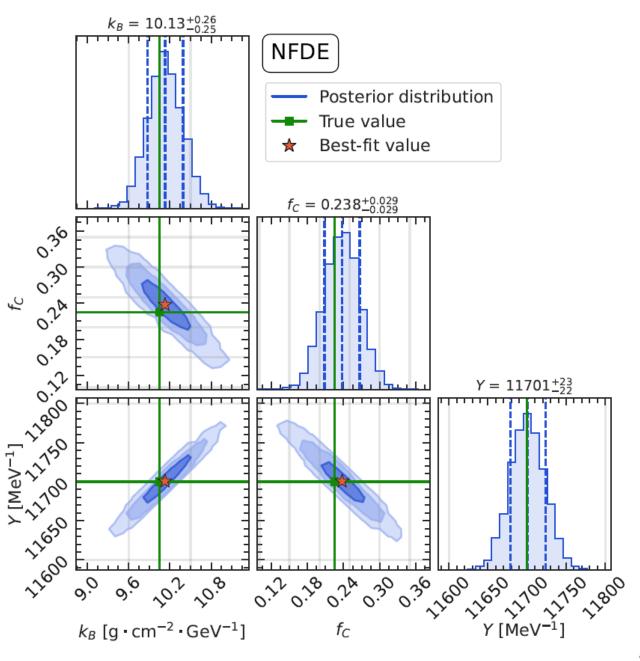
#### Parameters estimation combined:

o kB: **10.13 +- 0.26** | 10.05 [g/cm<sup>2</sup>/GeV]

o fC: **0.238 +- 0.029** 0.225

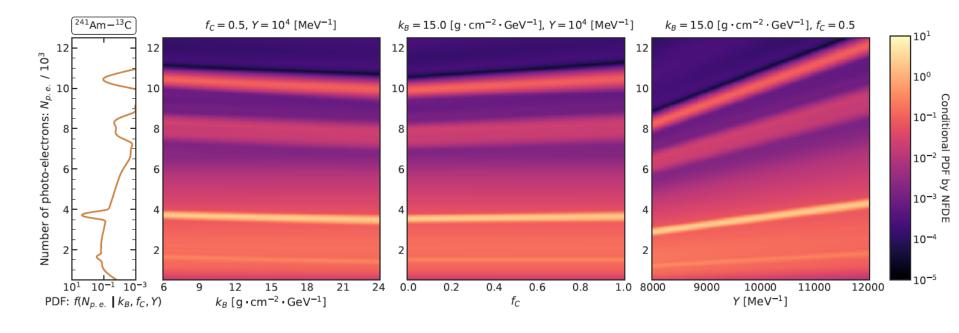
LY: 11701 +- 23 | 11700 [1/MeV]

 $\rightarrow$  well within 1 $\sigma$  (fluctuations expected for 1 fit)

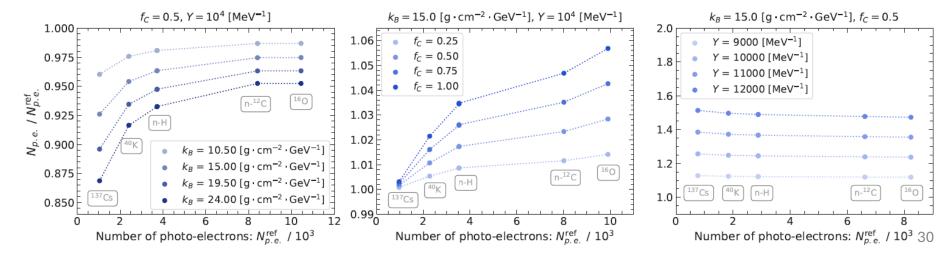


### Learned dependences

 PDF vs. parameter (almost linear)



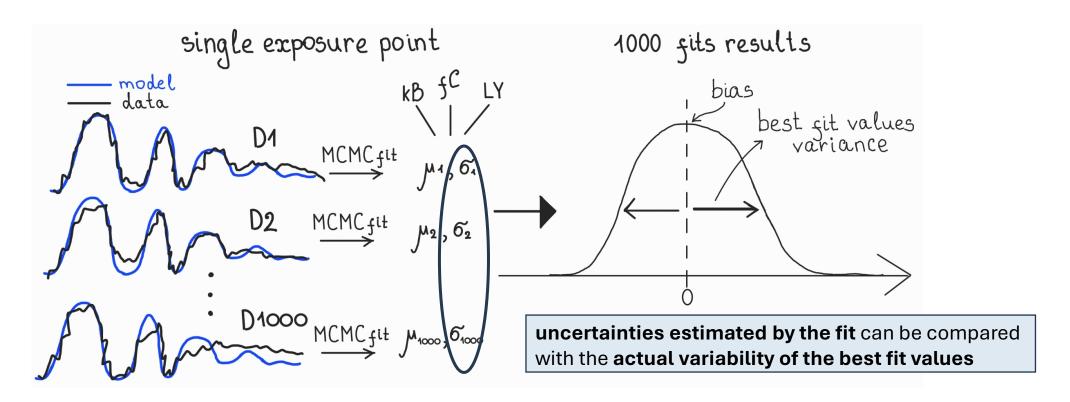
2) PDFs vs. energy (NPE)(energy non-linearity)



## **Evaluate ML-driven systematic uncertainty**

To perform systematic uncertainty estimation analysis, we use the testing dataset 2:

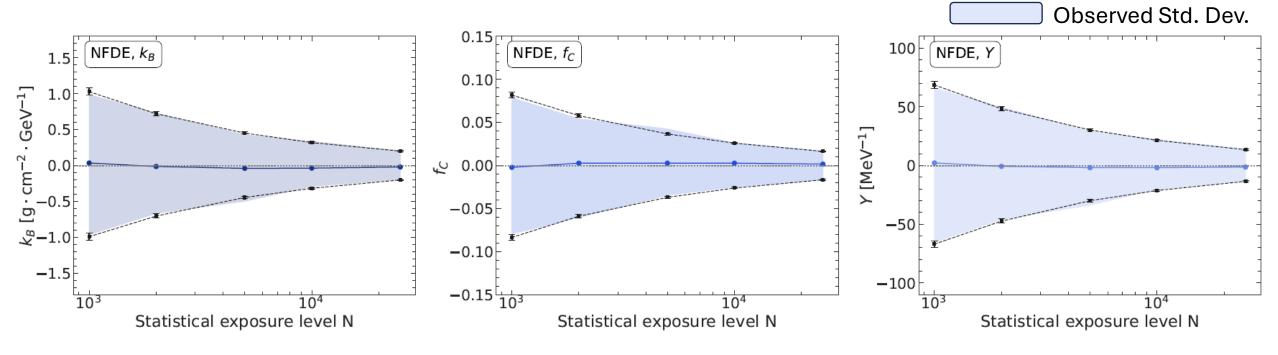
- Unseen during training point in the parameter space: kB, fC, LY = (15.45, 0.525, 10100)
- o **5 different exposures**: 1k, 2k, 5k, 10k, 25k events
- o 1000 datasets with different MC generator seed per each exposure



### Estimation of ML-driven systematic uncertainty

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- o **5 different exposures**: 1k, 2k, 5k, 10k, 25k events
- 1000 datasets with different MC generator seed per each exposure
- → Estimated uncertainty matches observed variability

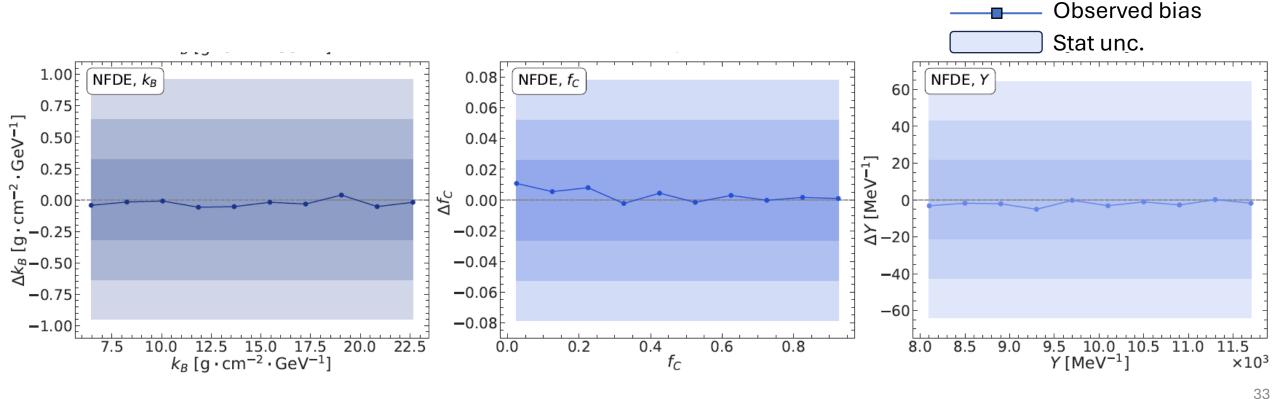


Estimated Stat. Unc.

### **Estimation of ML-driven systematic bias**

Using the testing dataset 1, one can check the bias across different points:

- Run MCMC fits per each testing point of the dataset
- Compare bias with the uncertainty **obtained by the previous analysis** for the 10k exposure point
- → Observed biases are well within the uncertainty



## Summary

Challenge: systematics investigation for precision neutrino physics with JUNO and accurate energy calibration

→ requires an extremely **well tuned MC**, but the **traditional MC tuning** process is **computationally prohibitive**.

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**Solution:** we developed a **Simulation-Based Inference framework** using two **neural likelihood estimators** (TEDE and NFDE) that replace the slow MC simulation with a **fast, accurate surrogate** models.

#### **Key Achievements:**

- our models successfully learn the complex, non-linear energy response of the JUNO detector MC, including the strong correlations between  $k_B$ ,  $f_C$  and Y parameters in the MC.
- when integrated with **Bayesian inference**, our method recovers all parameters with **near-zero systematic bias**.
- parameter uncertainties are limited purely by statistics and scale correctly as 1/  $\sqrt{N}$ 
  - → possible to achieve <1% systematics

This provides a flexible (binned or unbinned) framework for MC tuning with data! ©

Thanks!

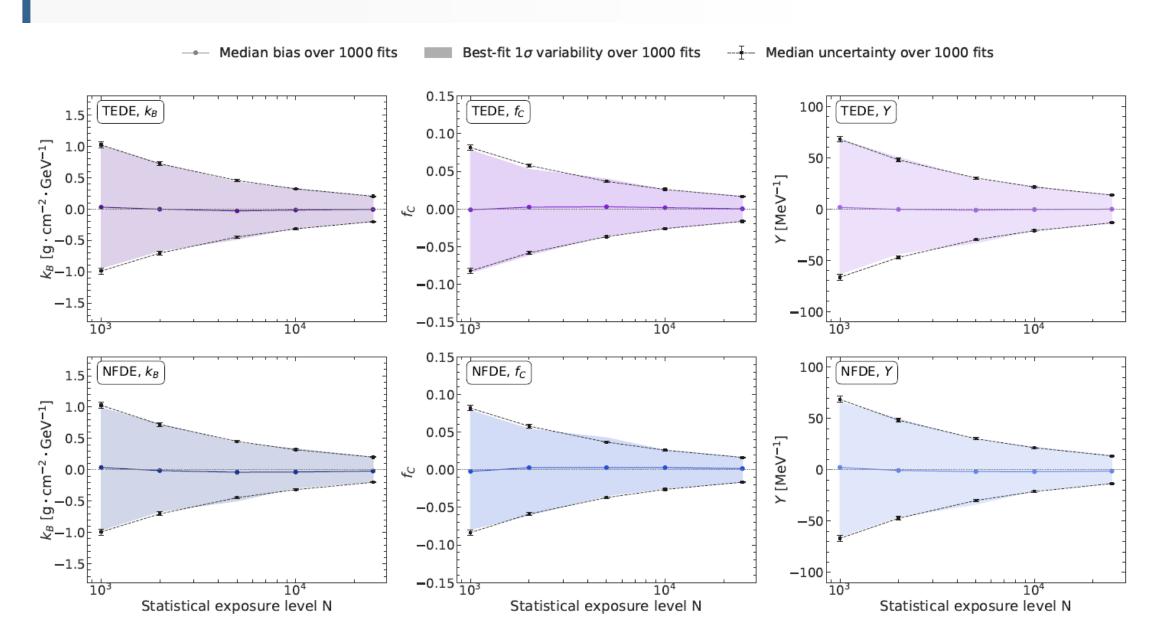
Repo

**Pre-print** 

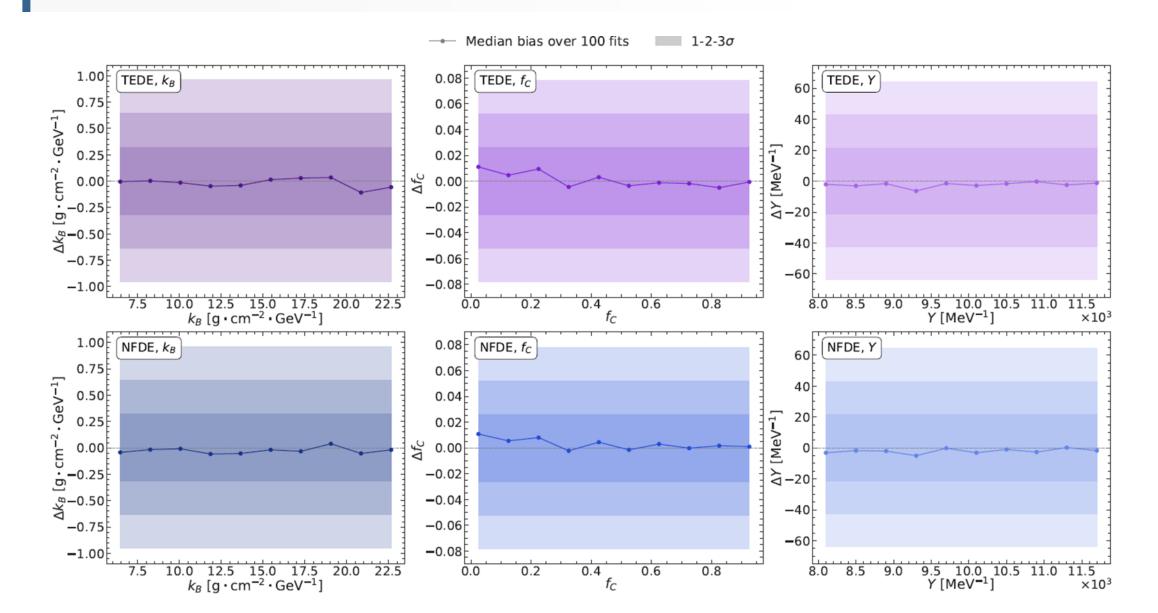




### **TEDE vs. NFDE (uncertainty)**



### TEDE vs. NFDE (bias)



# Hyperparameters optimization

Hyperparameters	TEDE	NFDE			
Model architecture hyperparameter	Model architecture hyperparameters				
$n_{ m tokens}$	$\{k \mid k \in \mathbb{N}, 1 \le k \le 5\} \colon 1$				
$d_{ m model}$	$\{50k \mid k \in \mathbb{N}, 1 \le k \le 10\} \colon 100$				
$n_{ m head}$	$\{5, 10, 25\}$ : 10				
$n_{ m layers}$	$\{k \mid k \in \mathbb{N}, 1 \le k \le 5\} \colon 4$				
$d_{ m ff}$	${32k \mid k \in \mathbb{N}, 1 \le k \le 15}: 384$				
$n_{ m flows}$		$\{100 + 5k \mid k \in \mathbb{Z}, 0 \le k \le 20\}$ : 120			
$n_{ m units}$		$\{10 + 5k \mid k \in \mathbb{Z}, 0 \le k \le 8\} \colon 30$			
Flow type		Planar (fixed)			
Dropout rate	$\{p_{\text{drop}} \mid 0.0 \le p_{\text{drop}} \le 0.5\} \colon 0.0$				
Activation function [90]	Relu, <b>Gelu</b>	ReLU, <b>GeLU</b> , Tanh, SiLU			
Softmax temperature	$\{T \mid 0.25 \le T \le 3.0\} \colon 2.03$				
General training hyperparameters					
Optimizer [94, 95]	AdamW, RMSprop	AdamW (fixed)			
Learning rate	$\{\eta \mid 10^{-5} \le \eta \le 10^{-2}\} \colon 1.9 \times 10^{-3}$	$10^{-4}$ (fixed)			
Scheduler type [96, 97]	Exponential, ReduceOnPlateau, CosineAnnealing, None	ReduceOnPlateau, CosineAnnealing			
Weight decay	$\{\lambda \mid 10^{-6} \le \lambda \le 10^{-1}\} \colon 8 \times 10^{-5}$	$10^{-4}$ (fixed)			
Batch size	$\{2^k \mid k \in \mathbb{N}, 4 \le k \le 9\} \colon 64$	50 (fixed, 1 per a CPU unit)			
Optimizer-specific hyperparameters					
Adam $\emptyset$ decay rate $eta_1$	$\{\beta_1 \mid 0.5 \le \beta_1 \le 0.95\} \colon 0.930$	$\{\beta_1 \mid 0.5 \le \beta_1 \le 0.95\} \colon 0.87$			
Adam $\emptyset$ decay rate $eta_2$	$\{\beta_2 \mid 0.9 \le \beta_2 \le 0.999\} \colon 0.929$	$\{\beta_2 \mid 0.9 \le \beta_2 \le 0.999\} \colon 0.901$			
RMSprop parameter $lpha$	$\{\alpha \mid 0.9 \le \alpha \le 0.999\}$ : -				
Scheduler-specific hyperparameters					
Cosine annealing period $T_{ m max}$	$\{T_{\max} \mid 5 \le T_{\max} \le 75\}: -$	$\{T_{\text{max}} \mid 5 \le T_{\text{max}} \le 75\} \colon 50$			
Exponential rate $ au$	$\{\tau \mid 0.8 \le \tau \le 0.99\} \colon 0.92$				
Reduce on plateau factor $\gamma$	$\{\gamma \mid 0.8 \le \gamma \le 0.99\}: -$	$\{\gamma \mid 0.8 \le \gamma \le 0.99\}: -$			
Optimization procedure setting					
Number of trials	250	25			
Accelerator	GPU	50 parallel CPUs			

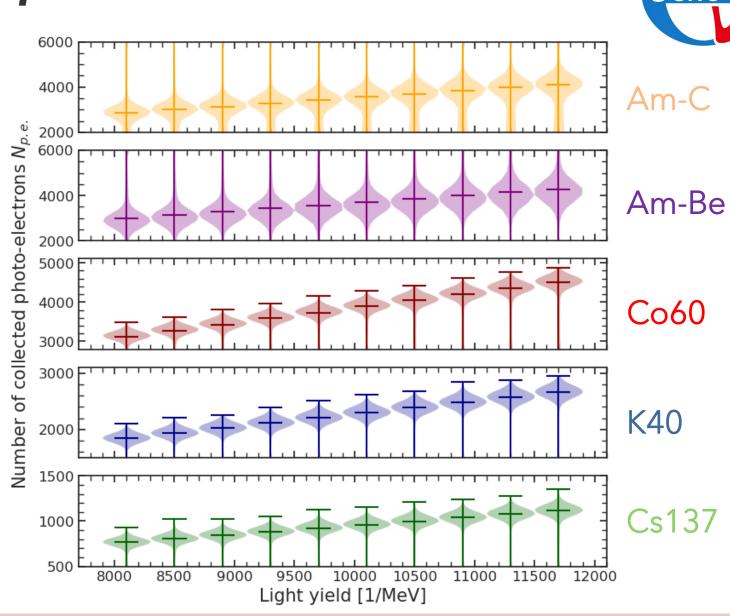
### How LS parameters impact the calibration data



### LY effect

- kB and fC are fixed:
  - $\circ$  kB = 15.45 [g/cm<sup>2</sup>/GeV]
  - $\circ$  fC = 0.525
- LY is varying
- Light yield is the most influential parameter
- All sources are highly affected

Only main peaks are shown



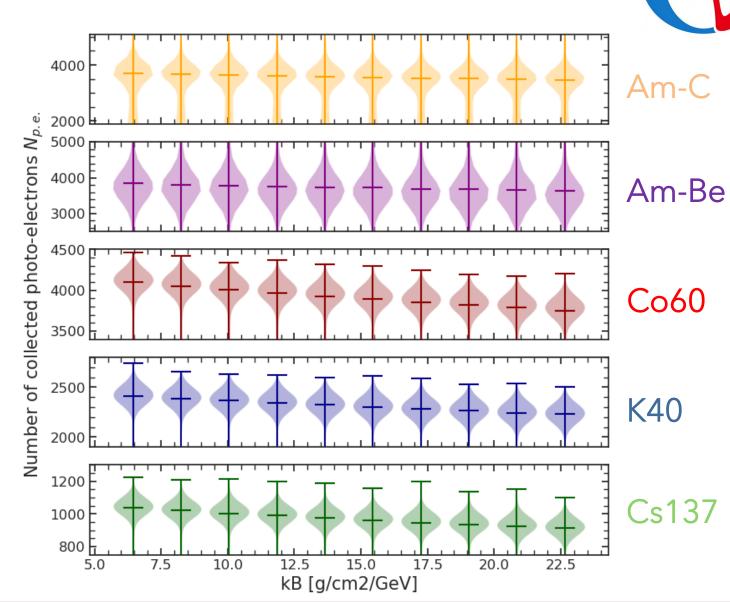
### How LS parameters impact the calibration data



### kB effect

- LY and fC are fixed:
  - LY = 10100 [1/MeV]
  - $\circ$  fC = 0.525
- kB is varying
- kB effect is smaller than LY and anticorrelated with the photo peak
- All sources are affected

Only main peaks are shown



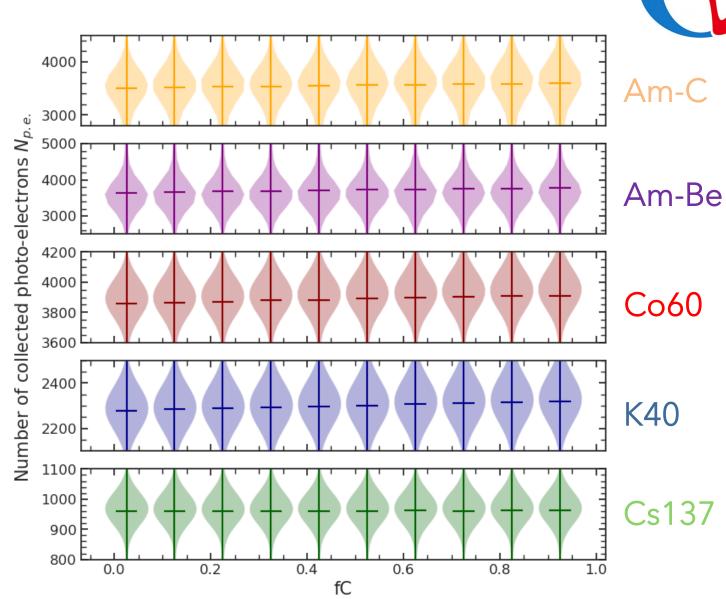
### How LS parameters impact the calibration data



### fC effect

- kB and LY are fixed:
  - $\circ$  kB = 15.45 [g/cm<sup>2</sup>/GeV]
  - O LY = 10100 [1/MeV]
- fC is varying
- fC has a minor effect to the spectra
- Cs137 is not affected at all
- Slight effect for Co60 and K40

Only main peaks are shown



## The JUNO detection process

**JUNO** will measure the antineutrinos  $(\bar{\nu}_e)$ generated in the fissions occurring in 8 nuclear cores at 52.5 km

The **detection** is based on a charged current interaction named Inverse Beta Decay (IBD) on protons (p)

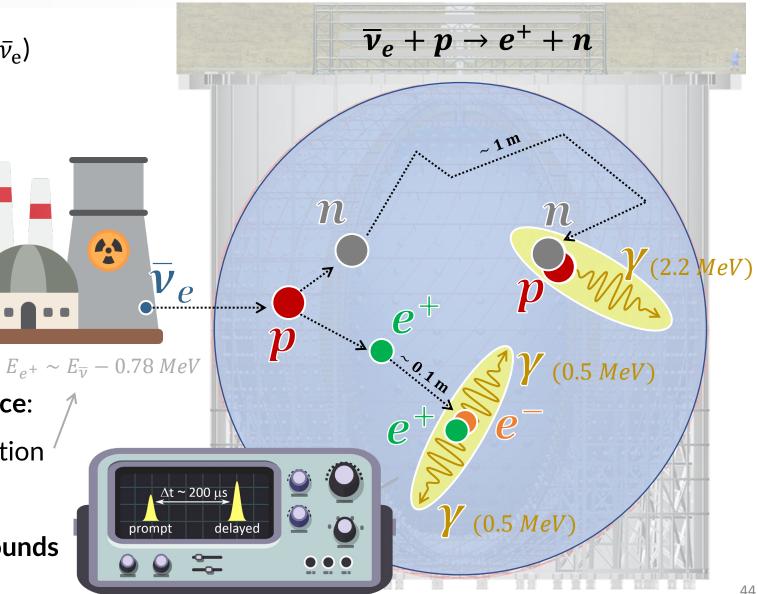
 $\rightarrow$  sensitive only to electron  $\overline{\nu}_e$ 

Detection relies on a **double coincidence**:

**prompt** signal: positron (e<sup>+</sup>) annihilation

delayed signal: neutron (n) capture

→ strong handle against most backgrounds



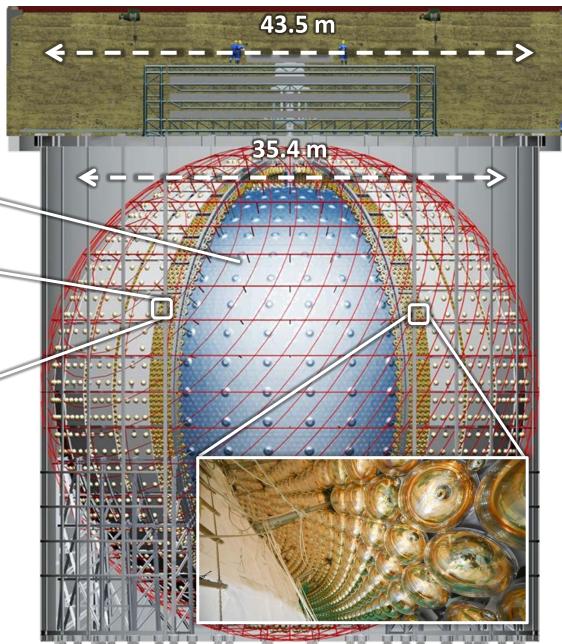
### The JUNO detector

### Main requirements:

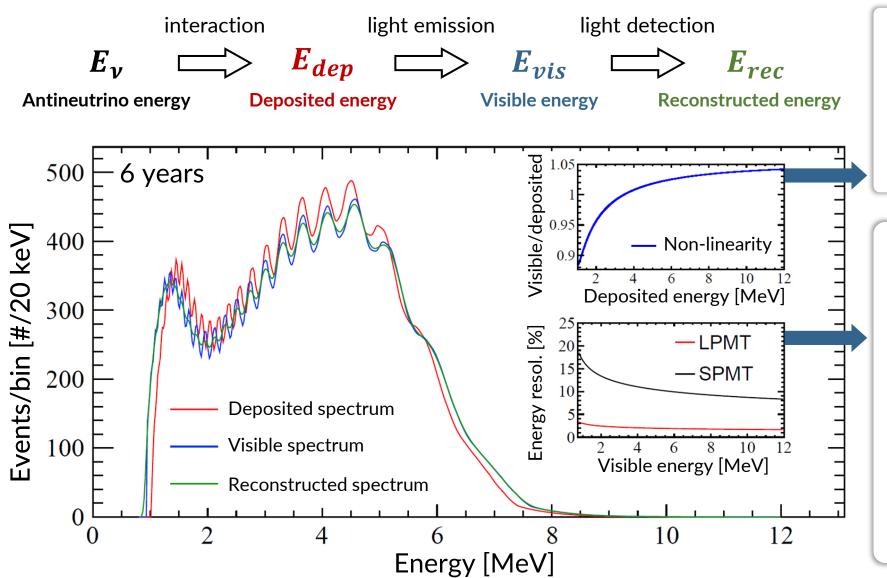
- high statistics
  - → 20 kton of liquid scintillator acrylic sphere
- <3% energy resolution @ 1 MeV</li>
  - → photocoverage ~78%
- energy-scale systematics below 1%
  - → 17612 20" Large-PMT
  - → 25600 3" Small-PMT



	Target mass [kton]	Energy resolution	Light yield [PE/MeV]
Daya Bay	0.02	8%/√E	160
Borexino	0.3	5%/√E	500
KamLAND	1	6%/√E	250
JUNO	20	3%/√E	~1600



# Detector response: what JUNO actually sees



#### **Calibration campaigns**

- automated multiple-position and multi-source calibration (link)
- **periodic calibration** campaigns
- dual-calorimetry system (link)

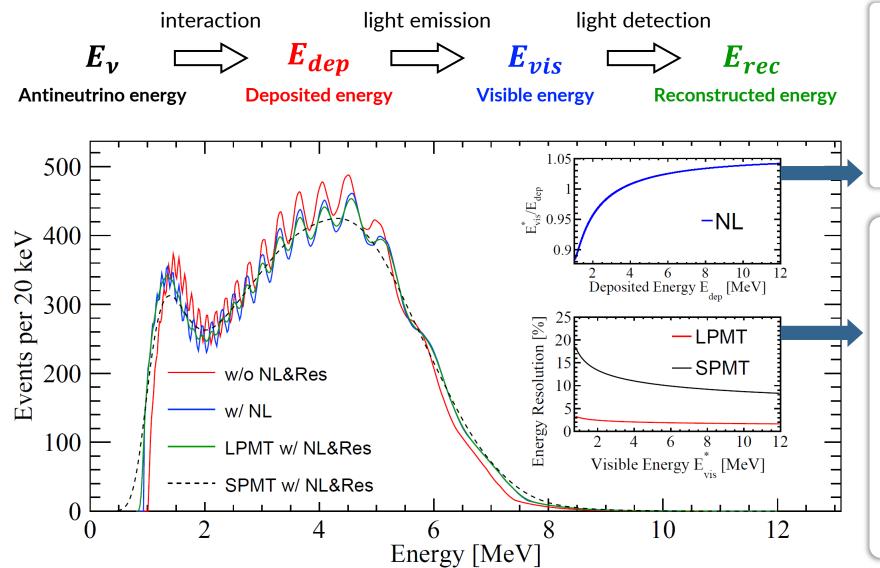
#### **Energy resolution**

$$\frac{\boldsymbol{\sigma}}{E} = \sqrt{\left(\frac{\boldsymbol{a}}{\sqrt{E}}\right)^2 + \boldsymbol{b}^2 + \left(\frac{\boldsymbol{c}}{E}\right)^2}$$

- a Stochastic term: light yield (from source calibration)
- **b** Dominated by **non-uniformity** (from multi-source calibration)
- c PMT dark noise

4

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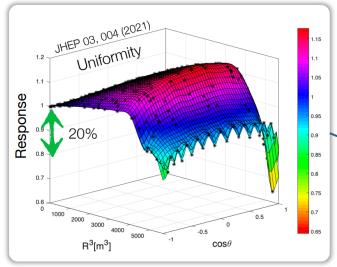
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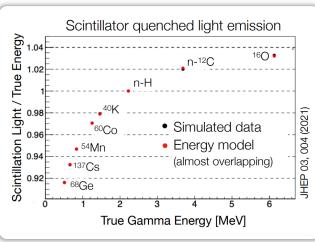
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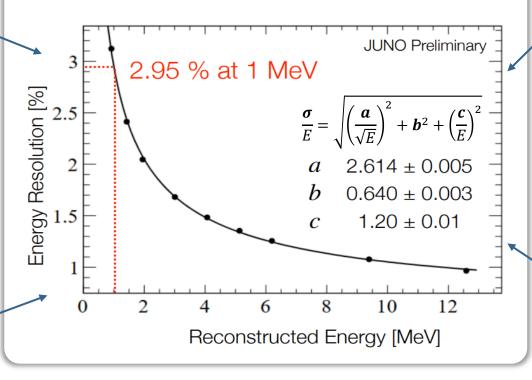
## JUNO detector response: state of the art

#### Realistic MC simulation

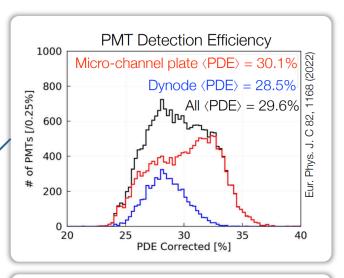


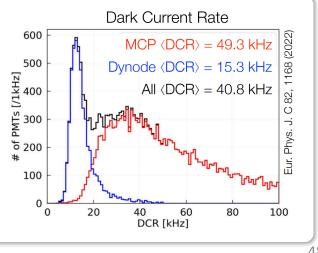


### **Updated values** based on **commissioning** data and realistic MC simulation



#### Measured data

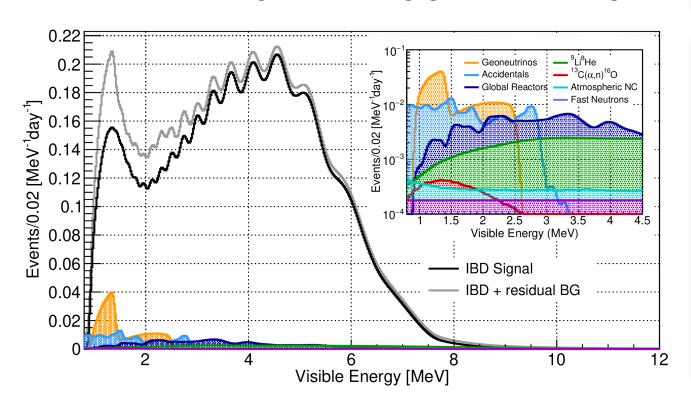




## IBD backgrounds in JUNO

JUNO employs various selection cuts to retain high efficiency and assure high purity in the IBD signal:

- Cosmogenic backgrounds → muon veto
- Accidental coincidences → fiducial volume + IBD cuts
- **Irreducible** backgrounds → **negligible** (~1/20 of signal)



IBD selection cuts	Efficiency [%]	IBD rate [day <sup>-1</sup> ]
All IBDs	100.0	57.4
Fiducial volume	91.5	52.5
IBD selection	98.1	51.1
Energy range	99.8	-
Time correlation ( $\Delta T_{p-d}$ )	99.0	-
Spatial correlation ( $\Delta R_{p-d}$ )	99.2	-
Muon veto (Time+spatial)	91.6	47.1
Combined selection	82.2	47.1

Residual backgrounds	Rate [day⁻¹]	Rate unc. [%]	Shape unc. [%]
Geoneutrinos	1.2	30	5
World reactors	1.0	2	5
Accidentals	0.8	1	negligible
<sup>9</sup> Li/ <sup>8</sup> He	0.8	20	10
Atmospheric neutrinos	0.16	50	50
Fast neutrons	0.1	100	20
<sup>13</sup> C(α,n) <sup>16</sup> O	0.05	50	50
Total background	4.11	-	-

### Detection channels in JUNO

NC recoil threshold: 200 keV

### Liquid scintillator:

### **Linear alkylbenzenes**

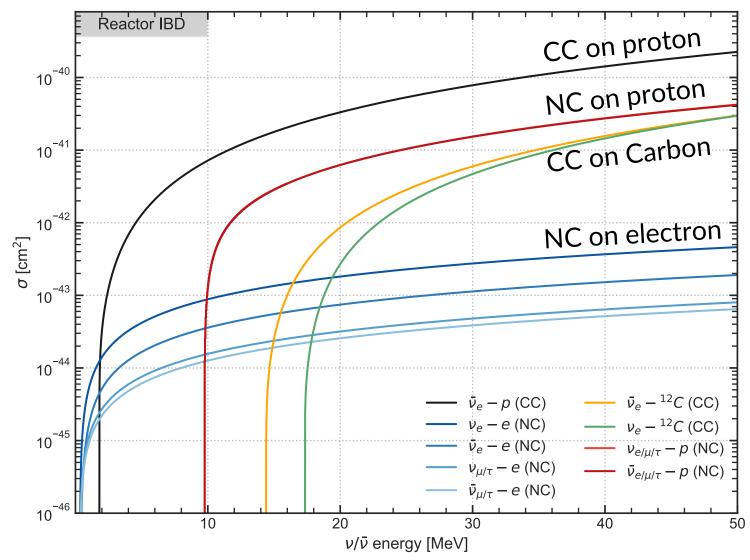
$$\overline{v}_e + p \rightarrow e^+ + n$$

$$\nu + p \rightarrow \nu + p$$

$$\nu + e \rightarrow \nu + e$$

$$- \nu_e + {}^{12}C \rightarrow e^- + {}^{12}N$$

$$- \bar{\nu}_e + {}^{12}C \rightarrow e^+ + {}^{12}B$$



# Photomultiplier Tubes



#### 5000 x 20" Hamamatsu R12860

High QE: 28.5% Fine TTS: 1.3 ns



#### 15012 x 20" NNVT MCP-PMTs

Highest QE: 30.1% Good TTS: 7.0 ns High efficiency of photon detection



#### 25600 x 3" HZC XP72B22

- Calibration of 20" PMTs' non-linearities
- Extension of dynamic range



# **Dual calorimetry system**

JUNO employs the dual calorimetry system to correct for electronics non-linearity

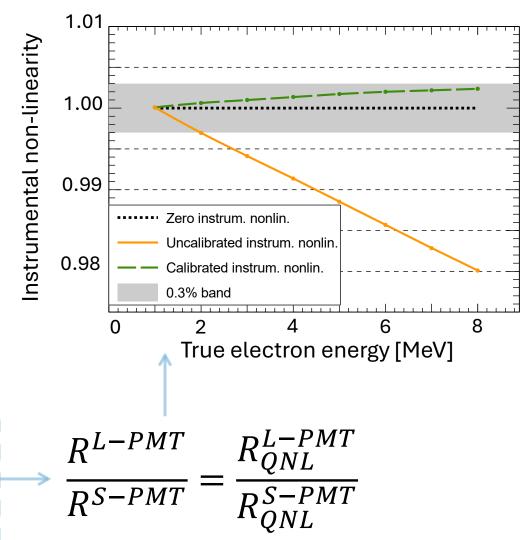
#### Sources of non-linear response:

- Non-uniformity (NU)
- Liquid scintillator non-linearity (LSNL)
- Charge non-linearity (QNL) of L-PMTs

Simulations with extreme channel-level non-linearity of 50% over 100 PE show that L-PMT response (*R*) non-linearity can be corrected using S-PMT as calibration reference:

$$R^{L-PMT} = R_{LSNL} \cdot R_{NU}^{L-PMT} \cdot R_{QNL}^{L-PMT}$$

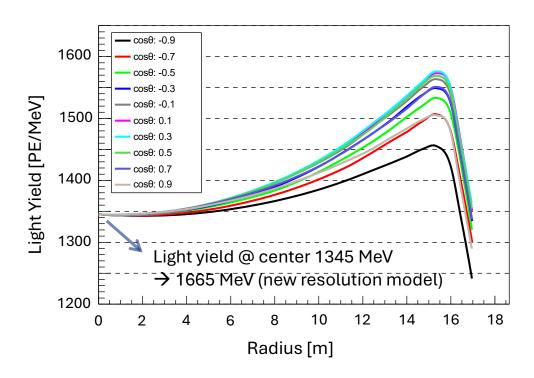
$$R^{S-PMT} = R_{LSNL} \cdot R_{NU}^{S-PMT} \cdot R_{QNL}^{S-PMT}$$



### Other non-linearities

#### **Detector non-uniformity**

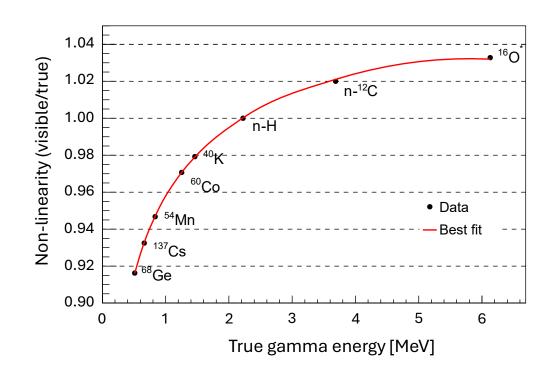
The detector response to the same charge deposition depends on the position at which the event occurs and needs to be properly characterized.



#### Liquid scintillator non-linearity

Light emission has an intrinsic non-linearity because of:

- Birks' quenching effect in scintillation photon yield;
- Velocity-dependent Cherenkov emission.



### Calibration of the JUNO detector

Radioactive sources (100-200 Hz) + Laser sources

1D: Automatic Calibration Unit (ACU)

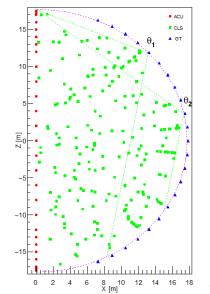
2D: Cable Loop System (CLS)

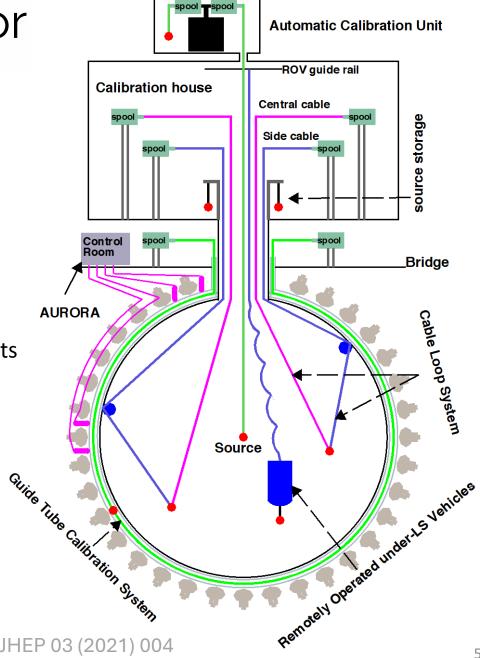
3D: Remotely Operated under-LS Vehicles (ROV)

• Boundary: Guide Tube Calibration System (GTCS)

Sources/Processes	Type	Radiation
$^{137}\mathrm{Cs}$	$\gamma$	$0.662~{ m MeV}$
$^{54}{ m Mn}$	$\gamma$	$0.835 \mathrm{MeV}$
$^{60}\mathrm{Co}$	$\gamma$	$1.173+1.333\;{ m MeV}$
$^{40}\mathrm{K}$	$\gamma$	$1.461~{ m MeV}$
$^{68}\mathrm{Ge}$	$e^{+}$	annihilation $0.511 + 0.511 \text{ MeV}$
$^{241}$ Am-Be	$n, \gamma$	${ m neutron} + 4.43 \; { m MeV} \; (^{12}{ m C}^*)$
$^{241}$ Am- $^{13}$ C	$n, \gamma$	${ m neutron} + 6.13~{ m MeV}~(^{16}{ m O}^*)$
$(\mathrm{n},\!\gamma)\mathrm{p}$	$\gamma$	$2.22~{ m MeV}$
$(\mathbf{n}, \gamma)^{12} \mathbf{C}$	$\gamma$	$4.94~{ m MeV}~{ m or}~3.68 + 1.26~{ m MeV}$

250 calibration points





## **Calibration strategy**

### Comprehensive calibration (250 points, ~48h)

→ basic understanding of the CD performance

### Monthly calibrations (~100 points, ~11h)

→ monitor non-uniformity

### Weekly calibrations (~15 points, ~2.4h)

→ track variations in LY of LS, PMT gains, and electronics

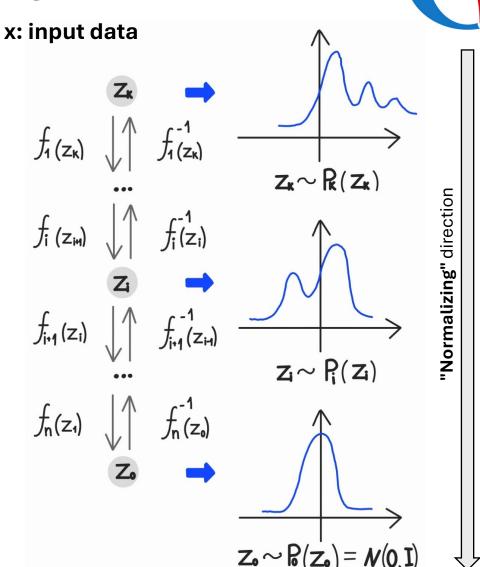
#### JHEP 03 (2021) 004

Source	Energy [MeV]	Points
Neutron (Am-C)	2.22	250
Neutron (Am-Be)	4.4	1
Laser	/	10
$^{68}{ m Ge}$	$0.511 \times 2$	1
$^{137}\mathrm{Cs}$	0.662	1
$^{54}{ m Mn}$	0.835	1
$^{60}\mathrm{Co}$	1.17 + 1.33	1
$^{40}{ m K}$	1.461	1
Total	/	/

System	Source	Points
ACU	Neutron (Am-C)	27
ACU	Laser	27
$\operatorname{CLS}$	Neutron (Am-C)	40
$\operatorname{GT}$	Neutron (Am-C)	23
Total	/	/

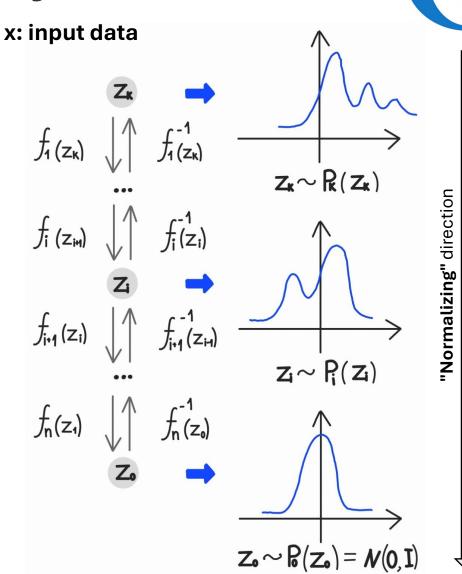
Source	Energy [MeV]	Points
Neutron (Am-C)	2.22	5
Laser	/	10
Total	/	/

- Normalizing flows [1]:
  - o Generative machine learning model
  - o Aims to explicitly model a density estimation
  - Can be generalized for modeling a conditional density
     estimation as well
  - o To obtain a value from the target distribution:
    - sample a value from the base distribution and passing it through all the flows



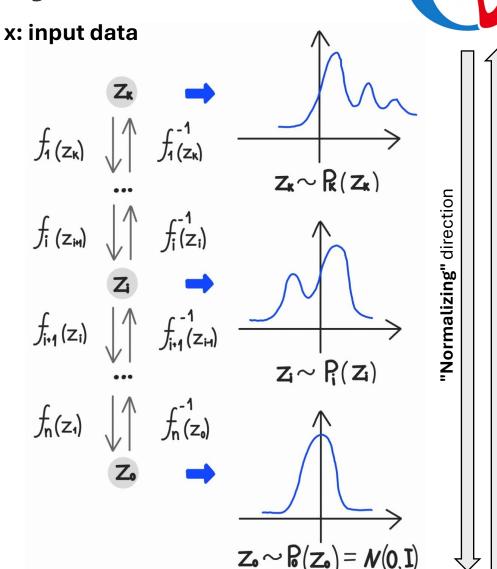
[1] R. J. Rezende et al, arxiv: 1505.05770

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- Normalizing flows are based on an idea of transforming a simple known distribution (e.g. standard Gaussian) to the complex, desired distribution by applying multiple learnable (using data) transformations
- Each transformation is called Flow and must be invertible



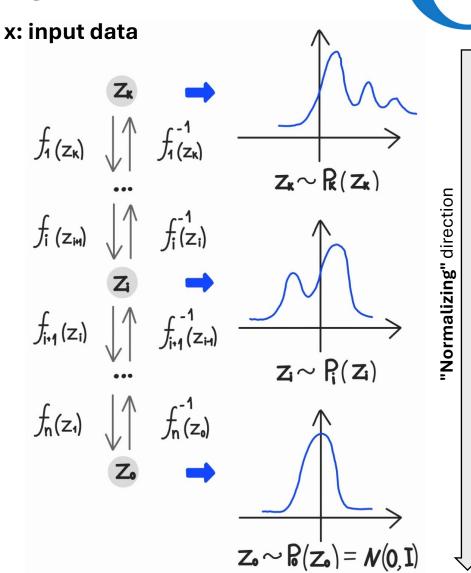
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- Normalizing flows [1]:
  - Transformations can be very diverse as long as they follow the invertibility condition
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    - $f_{\theta}(x) = x + u_{\theta} \tanh (xw_{\theta} + b_{\theta})$



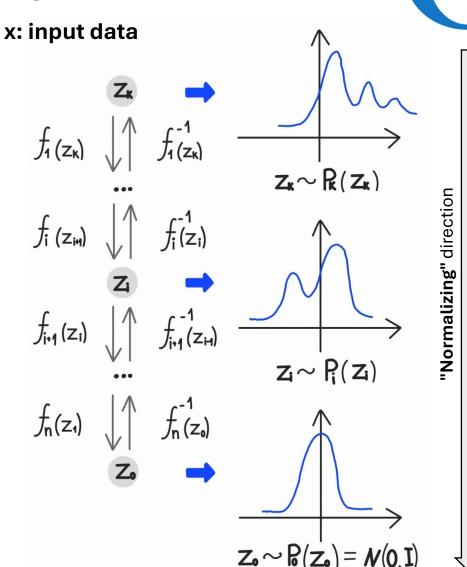
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- How to perform the inference with the model?



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- · How to perform the inference with the model?

$$\log p(x|y) = \log p(z_0) + \sum_{k=1}^{K-1} \log rac{df_{k, heta_k}(z_k)}{dz_k} + \log rac{df_{K, heta_K}(x)}{dx}$$

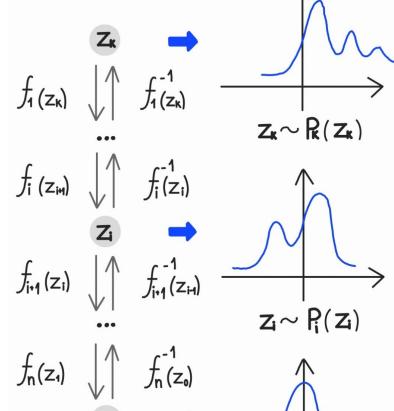
Data

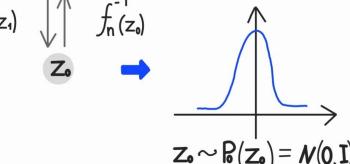
MC parameters + source type

well-known (e.g. standard Gaussian)

Computed based on the learned transformations

x: input data





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