

# Geant4 Lab Modeling Techniques

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*G4CMP Workshop 2024*

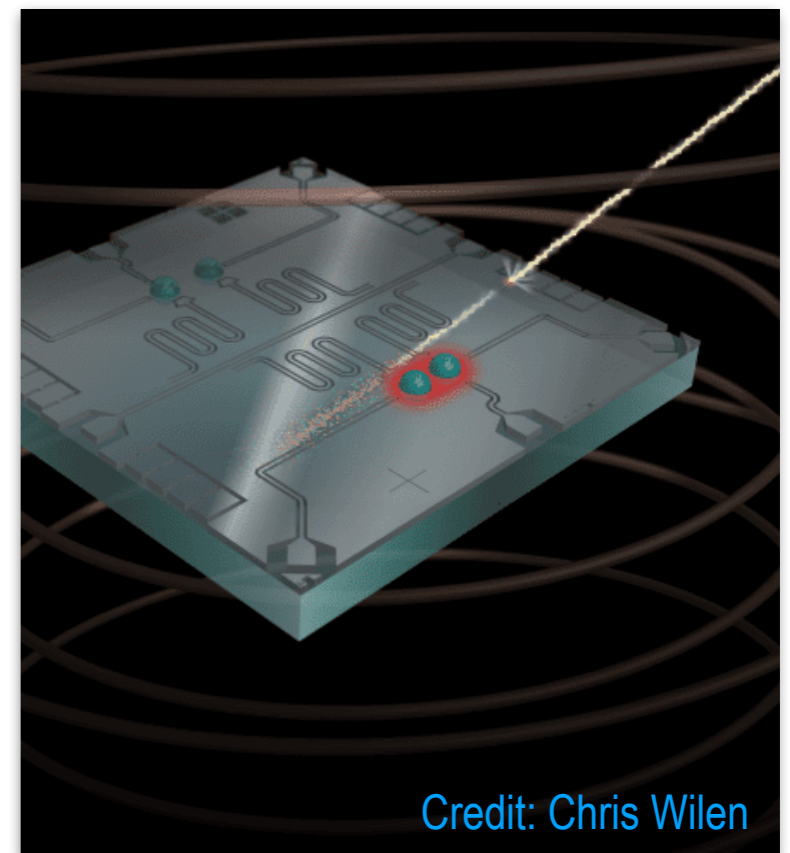
*May 29, 2024, Fermilab, Batavia, IL 60510*



# OUTLINE

- GEANT4-BASED MONTE CARLO SIMULATIONS
- OUR SIMULATION FRAMEWORK - DEMETRA
- SIMULATION INPUTS
- METHODOLOGY
- RESULTS
- COMPARISON WITH MEASUREMENTS

**Focus on superconducting qubits and simulation of ionizing radiation impacts in these devices**



# GEANT4-BASED MC SIMULATIONS

MC simulations are an important tool to:

- Predict the effect of radiation impacts in a given detector/sensor;
- Identify the major sources of ionizing radiation;
- Optimize the experimental setup;
- Study the performance of our detector.



Toolkit for the **MC simulation** of the interaction of **particles** with **matter**.

- **Event-based**, MC-driven simulation engine;
- Enables **modeling** of **complex geometries** composed of volumes with defined properties;
- Includes the ability to simulate **different radiation sources**;
- **Tracks particle interactions** within the modeled geometry.

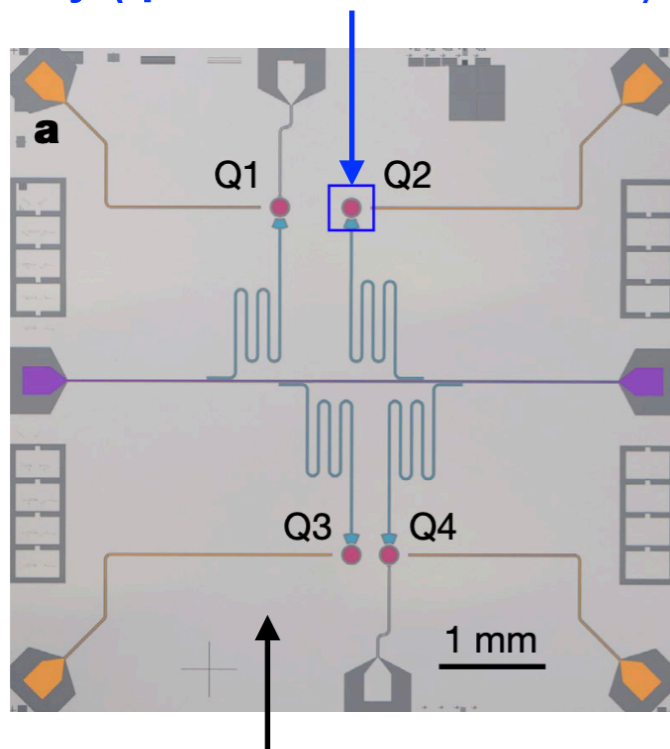
# OUR SIMULATION FRAMEWORK - DEMETRA

AIM: Predict ionizing radiation impacts rate and energy deposited on superconducting qubit chips

Geant-4 based simulation (v10.5.1), with the following inputs:

- **Geometry** of the **experimental setup** (chip, box, holder, shields, cryostat...);
- **Flux** of  $\mu$ ,  $\gamma$ ,  $n$  (measurements + literature);
- **Radioactivity** of the **setup materials** (measurements).

Direct interaction in the qubit:  
unlikely (qubit dimension  $< 100 \mu\text{m}$ )



**Substrate only active volume**  
**(single qubits NOT modeled in our simulation).**

[ C.D. Wilen et al., *Nature* **594**, 369–373 (2021) ]

Indirect interaction in the substrate ( $\sim 1 \text{ cm}^2$ )

# OUR SIMULATION FRAMEWORK - DEMETRA

Designed to implement and adapt to **various cryostats** (Wisconsin, Rome, Gran Sasso Lab) and **chips** (Wisconsin, Rigetti, Fermilab).

**Article**

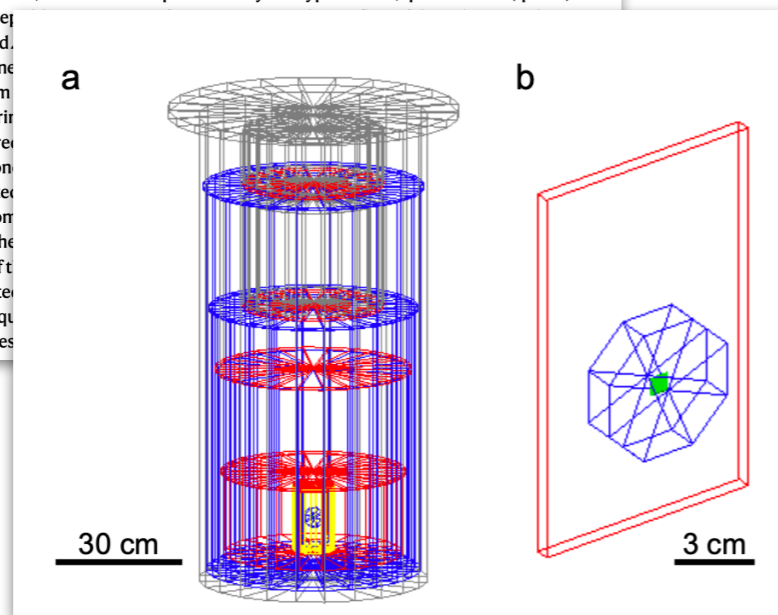
## Correlated charge noise and relaxation errors in superconducting qubits

<https://doi.org/10.1038/s41586-021-03557-5>  
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C. D. Wilen<sup>1,2</sup>, S. Abdullah<sup>1</sup>, N. A. Kurinsky<sup>2,3</sup>, C. Stanford<sup>4</sup>, L. Cardani<sup>5</sup>, G. D'Imperio<sup>6</sup>, C. Tomei<sup>7</sup>, L. Faoro<sup>1,6</sup>, L. B. Ioffe<sup>7</sup>, C. H. Liu<sup>8</sup>, A. Opremcak<sup>1</sup>, B. G. Christensen<sup>1</sup>, J. L. DuBois<sup>9</sup> & R. McDermott<sup>1,2</sup>

The central challenge in building a quantum computer is error correction. Unlike classical bits, which are susceptible to only one type of error, quantum bits (qubits) are susceptible to both bit-flip and phase errors. These errors can be correlated across the system, making them more difficult to detect and correct. In this paper, we study the impact of correlated charge noise and relaxation errors on the performance of superconducting qubits. We show that these errors can lead to significant errors in the computation, and we propose a method to mitigate them. Our results show that the errors are correlated across the system, and that the errors are more significant in the presence of noise. Robust quantum computing strategies are needed to overcome these challenges.

**WISCONSIN**



Eur. Phys. J. C (2023) 83:94  
<https://doi.org/10.1140/epjc/s10052-023-11199-2>

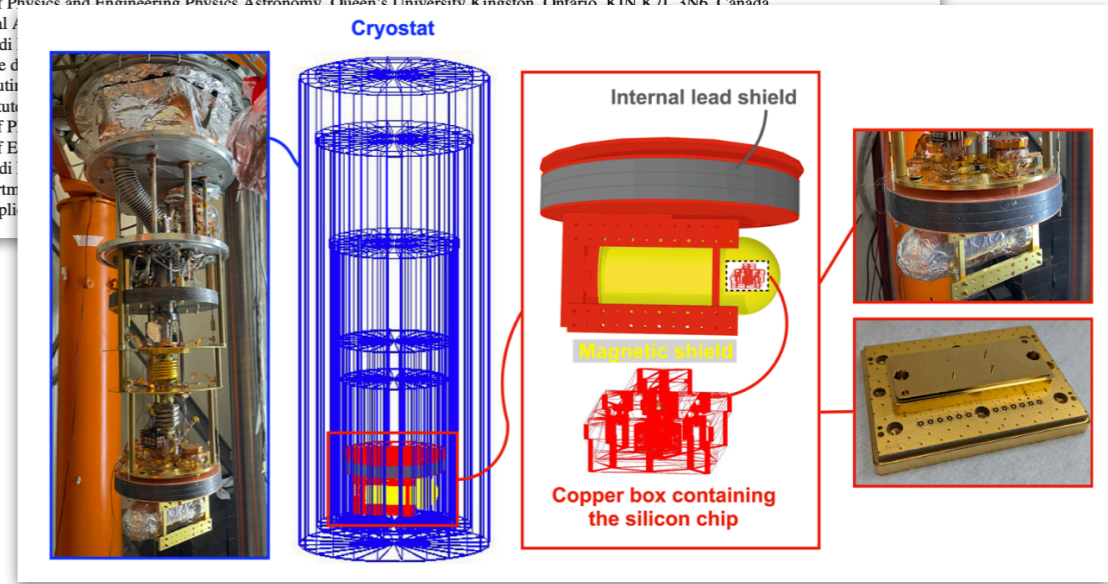
THE EUROPEAN PHYSICAL JOURNAL C

Regular Article - Experimental Physics

## Disentangling the sources of ionizing radiation in superconducting qubits

L. Cardani<sup>1,a</sup>, I. Colantoni<sup>1,2</sup>, A. Cruciani<sup>1</sup>, F. De Dominicis<sup>3,4,b</sup>, G. D'Imperio<sup>1</sup>, M. Laubenstein<sup>4</sup>, A. Mariani<sup>1,c</sup>, L. Pagnanini<sup>3,4,5</sup>, S. Pirro<sup>4</sup>, C. Tomei<sup>1</sup>, N. Casali<sup>1</sup>, F. Ferroni<sup>1,3</sup>, D. Frolov<sup>6</sup>, L. Gironi<sup>7,8</sup>, A. Grassellino<sup>6</sup>, M. Junker<sup>4</sup>, C. Kopas<sup>9</sup>, E. Lachman<sup>9</sup>, C. R. H. McRae<sup>10,11,12</sup>, J. Mutus<sup>9</sup>, M. Nastasi<sup>7,8</sup>, D. P. Pappas<sup>9</sup>, R. Pilipenko<sup>5</sup>, M. Sisti<sup>8</sup>, V. Pettinacci<sup>1</sup>, A. Romanenko<sup>6</sup>, D. Van Zanten<sup>6</sup>, M. Vignati<sup>1,13</sup>, J. D. Withrow<sup>14</sup>, N. Z. Zhelev<sup>15</sup>

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**GRAN SASSO LAB (LNGS)**

**Can accommodate other configurations upon request**

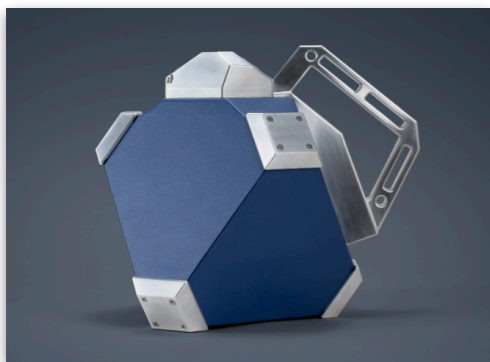
# SIMULATION INPUTS - MEASUREMENTS OF IONIZING RADIATION SOURCES

Dedicated tools and facilities to measure fluxes from “far” sources and internal contaminations of materials (“close” sources)

## “Far” sources



NaI(Tl) scintillation detector for gammas



DIAMON spectrometer for neutrons

## “Close” sources



- **S T E L L A (SubTerraanean Low-Level Assay) facility @LNGS;**
- **HPGe detectors.**



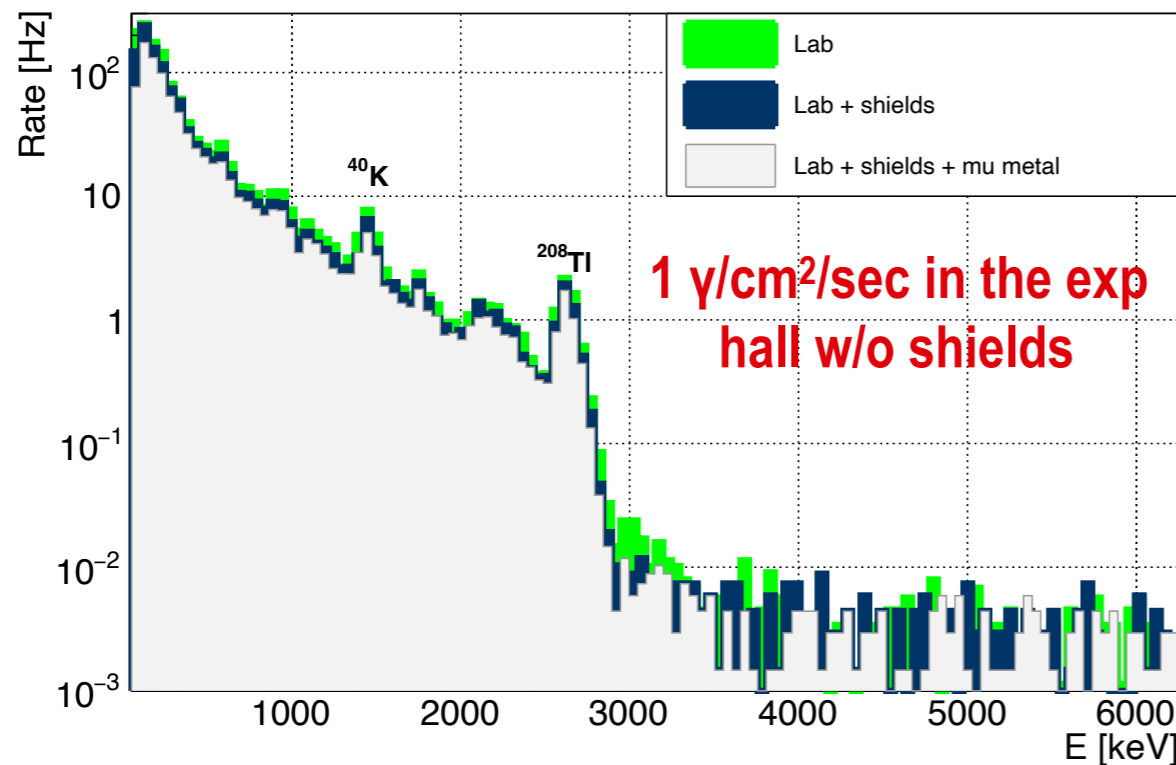
- **Chemistry Lab @LNGS;**
- **ICP-MS.**

**Provide accurate and reliable data for our simulation**

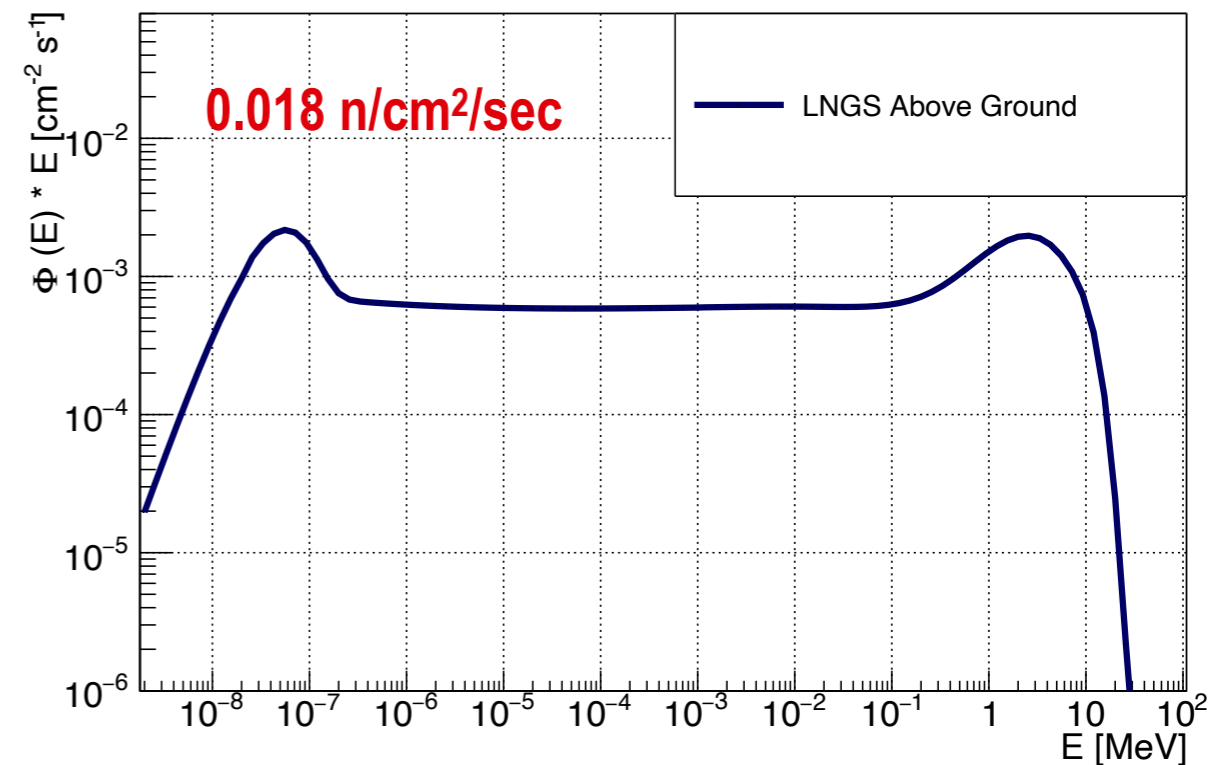
# SIMULATION INPUTS - “FAR” SOURCES

- **Muons** → literature [JMP A. Vol. 33, No.30, (2018)] (**sub-dominant underground**);
- **Gammas** → measurements @ underground cryogenic facility of LNGS and in other above-ground labs;
- **Neutrons** → measurements @ different locations above-ground (**sub-dominant underground**).

Energy spectrum of environmental  $\gamma$ s measured underground @LNGS with different shielding conditions



Energy spectrum of neutrons measured above-ground @LNGS



[ Cardani et al., *Eur. Phys. J. C* **83**, 94 (2023) ]

**Similar spectral shapes but different fluxes expected in other laboratories**

# SIMULATION INPUTS - “CLOSE” SOURCES

Measurements of **radioactive isotopes activities** in all the setup components with High-Purity Germanium (HPGe) detectors @INFN-LNGS STELLA underground facility.

Component	$^{232}\text{Th}$ [mBq/kg]	$^{238}\text{U}$ [mBq/kg]	$^{235}\text{U}$ [mBq/kg]	$^{40}\text{K}$ [mBq/kg]	$^{137}\text{Cs}$ [mBq/kg]	
PCB	<b><i>A</i></b>	<b>(18000 ± 1000)</b>	<b>(11500 ± 400)</b>	<b>(710 ± 110)</b>	<b>(12000 ± 1000)</b>	<b>&lt; 30</b>
A-MAGNETIC PCB	<i>A*</i>	(5410 ± 330)	(4200 ± 200)	(230 ± 50)	(4200 ± 500)	< 40
COPPER BOX + COPPER FINGER	<i>B</i>	< 1.5	< 1.2	< 4	< 9	< 0.6
MAGNETIC SHIELD	<i>C</i>	< 8.4	< 8.3	< 8.4	< 35	< 2.7
SMA ADAPTERS	<i>D</i>	(46 ± 13)	(42 ± 10)	(70 ± 30)	(240 ± 90)	< 10
COPPER COAX CABLES	<i>E</i>	(54 ± 12)	(44 ± 11)	(34 ± 17)	(740 ± 130)	< 12
RADIALL SWITCH	<i>F</i>	(1880 ± 100)	(1340 ± 60)	(130 ± 30)	(2200 ± 300)	< 11.2
SINGLE-JUNCT CIRCULATOR	<i>G*</i>	< 310	< 330	< 410	< 2000	< 60
DUAL-JUNCT CIRCULATOR	<i>H*</i>	< 250	< 380	< 380	< 2600	< 60
TRIPLE-JUNCT ISOLATOR	<i>I</i>	< 190	< 240	< 220	< 2000	< 50
XMA ATTENUATORS	<i>J</i>	< 52	(200 ± 20)	< 47	< 140	< 13
K&L LOW PASS FILTERS	<i>K</i>	(23 ± 4)	< 9.1	(60 ± 10)	< 100	< 1.9
NiTi COAX CABLES	<i>L</i>	< 750	< 1000	< 380	< 7000	< 230
CRYO AMPLIFIER	<i>M</i>	< 890	< 1000	< 850	< 10000	< 210
CuBe COAX CABLES	<i>N</i>	(240 ± 40)	< 78	(350 ± 90)	< 500	< 20
EPOXY GLUE	<i>O*</i>	< 40	< 50	< 50	< 25	< 10
CRYOGENIC GREASE	<i>P*</i>	(53 ± 4)	(47500 ± 2800)	(350 ± 30)	(290 ± 40)	< 2.2

**Most radioactive component**

[ Cardani et al., *Eur. Phys. J. C* **83**, 94 (2023) ]



# SIMULATION GEOMETRY - A SPECIFIC CASE

## LNGS CRYOSTAT

### 2 LAYERS MAGNETIC SHIELDING

- **Outer layer:** 55.6 cm (OD) x 91.3 cm, 1.5 mm-thick Permimphy;
- **Inner layer:** 51 cm (ID) x 89 cm, 1.5 mm-thick Permimphy.

### RADIATION SHIELDING

1 round of 10 x 66.5 cm<sup>2</sup>, 2 cm-thick Cu bars

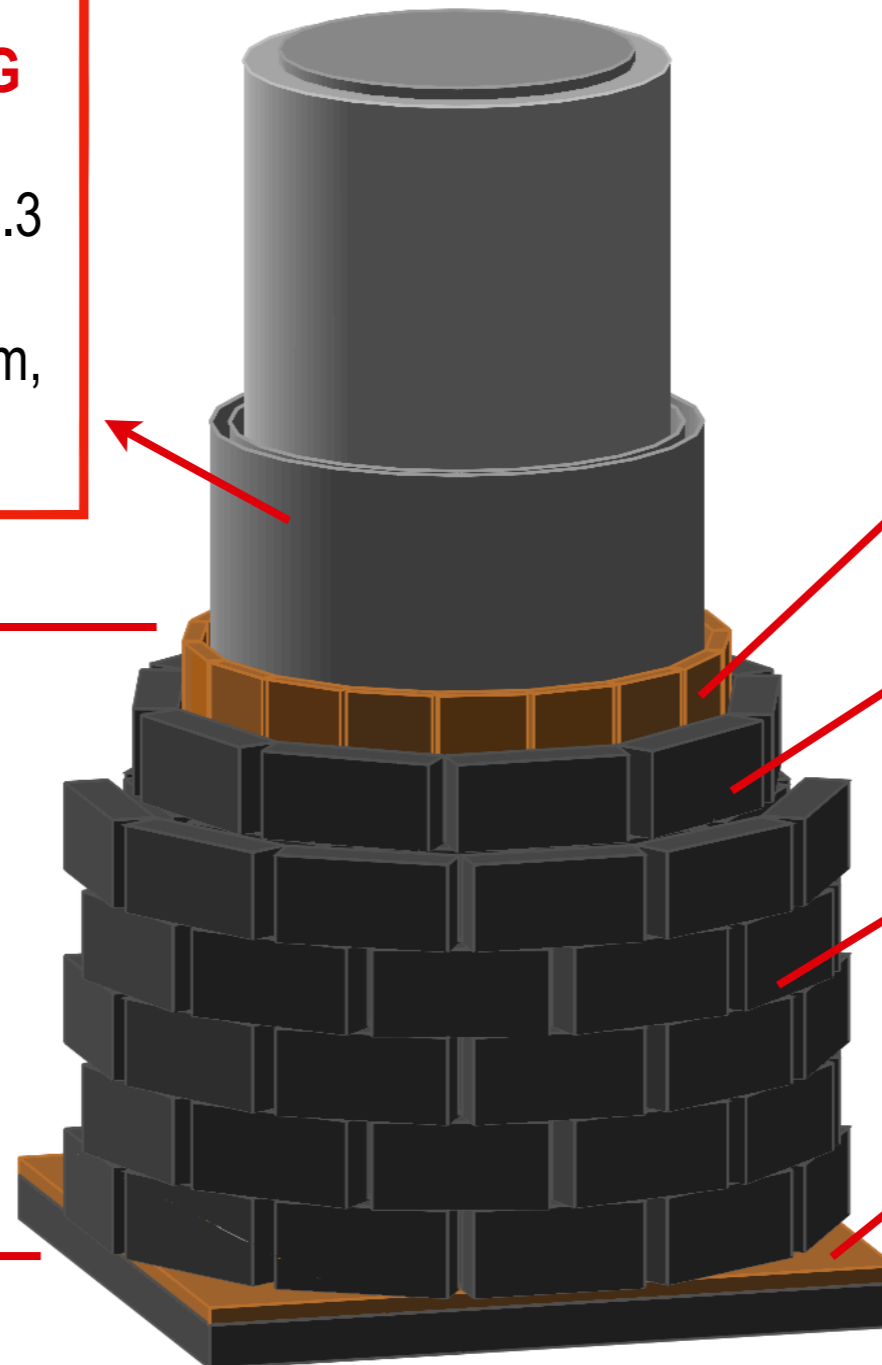
1 round of 10 x 20 cm<sup>2</sup>, 5 cm-thick Pb bricks

½ round of 10 x 20 cm<sup>2</sup>, 5 cm-thick Pb bricks

80 x 80 cm<sup>2</sup>, 2 cm-thick Cu

80 x 80 cm<sup>2</sup>, 5 cm-thick Pb

73.5 cm



# SIMULATION GEOMETRY - A SPECIFIC CASE

## LNGS CRYOSTAT

48.1 cm (OD) x 119.5 cm **cryostat**  
with internal vessels

3 cm-thick **Pb internal shield**

**CryoPerm® magnetic shield**

Gold-plated copper holder

30.23 x 30.23 x 6.3 mm<sup>3</sup>  
**gold-plated copper box**  
hosting the chip

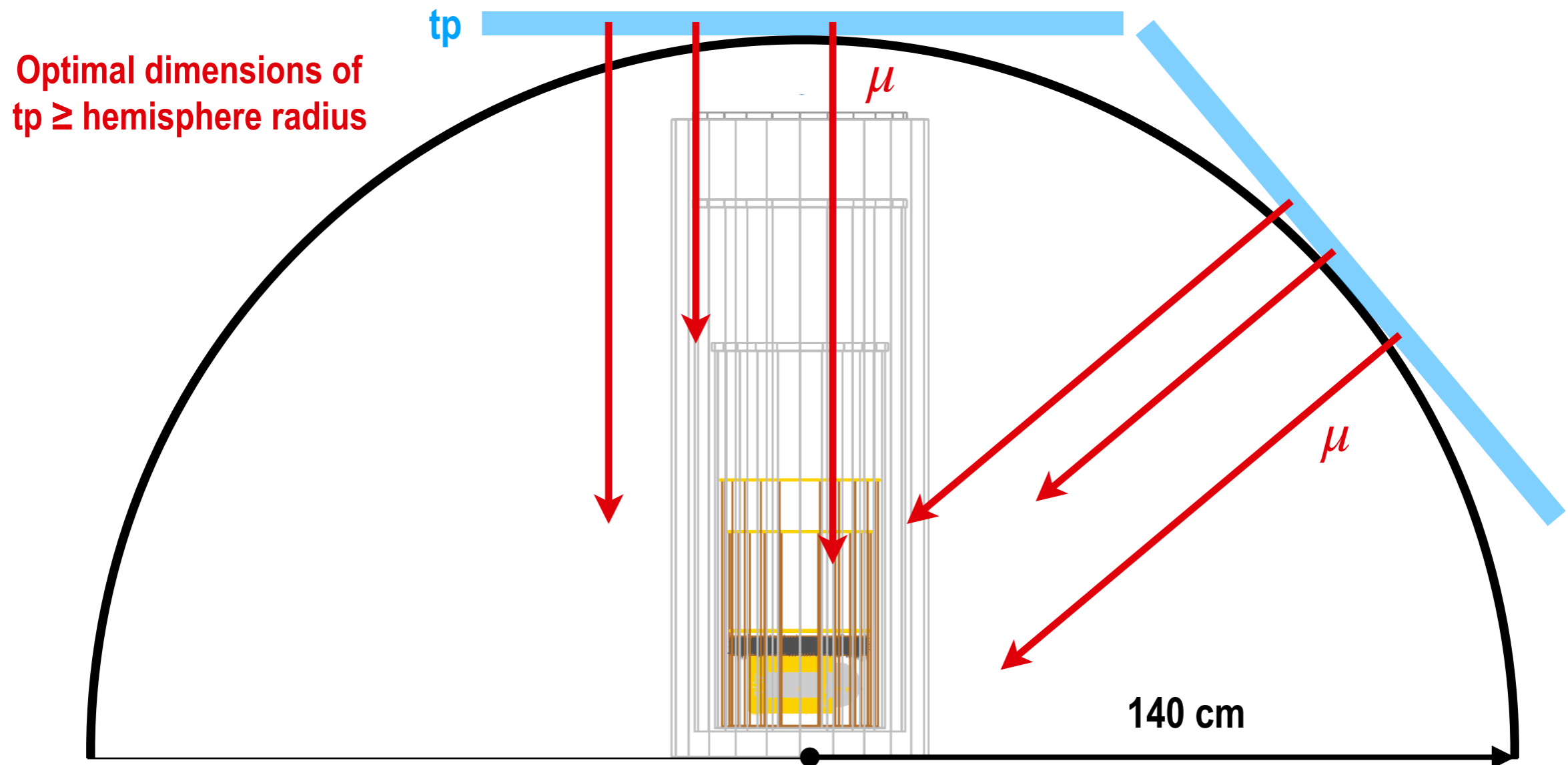
## SUPERCONDUCTING CHIP

- 7.5 x 7.5 mm<sup>2</sup>, 432 μm-thick **HEMEX Sapphire substrate**;
- **Nb** 160 nm-thick (**bottom**) layer;
- **Au** 10 nm-thick (**top**) layer.

# METHODOLOGY

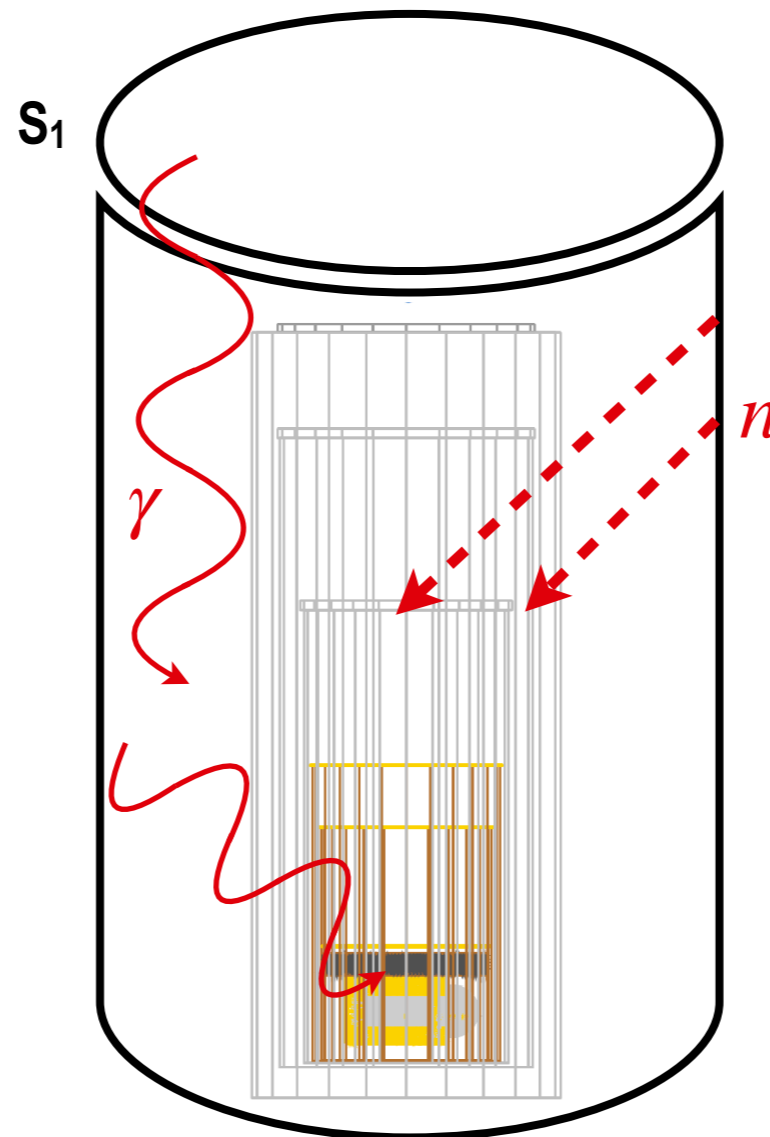
# SIMULATION STRATEGY - ATMOSPHERIC MUONS

- **Positions** randomly generated on a hemisphere surrounding the cryostat, according to a  **$\cos^2$  distribution**;
- For every sampled position, **muons** perpendicularly generated from a **(140x140) cm<sup>2</sup> tangent-plane (tp)** to the hemisphere.



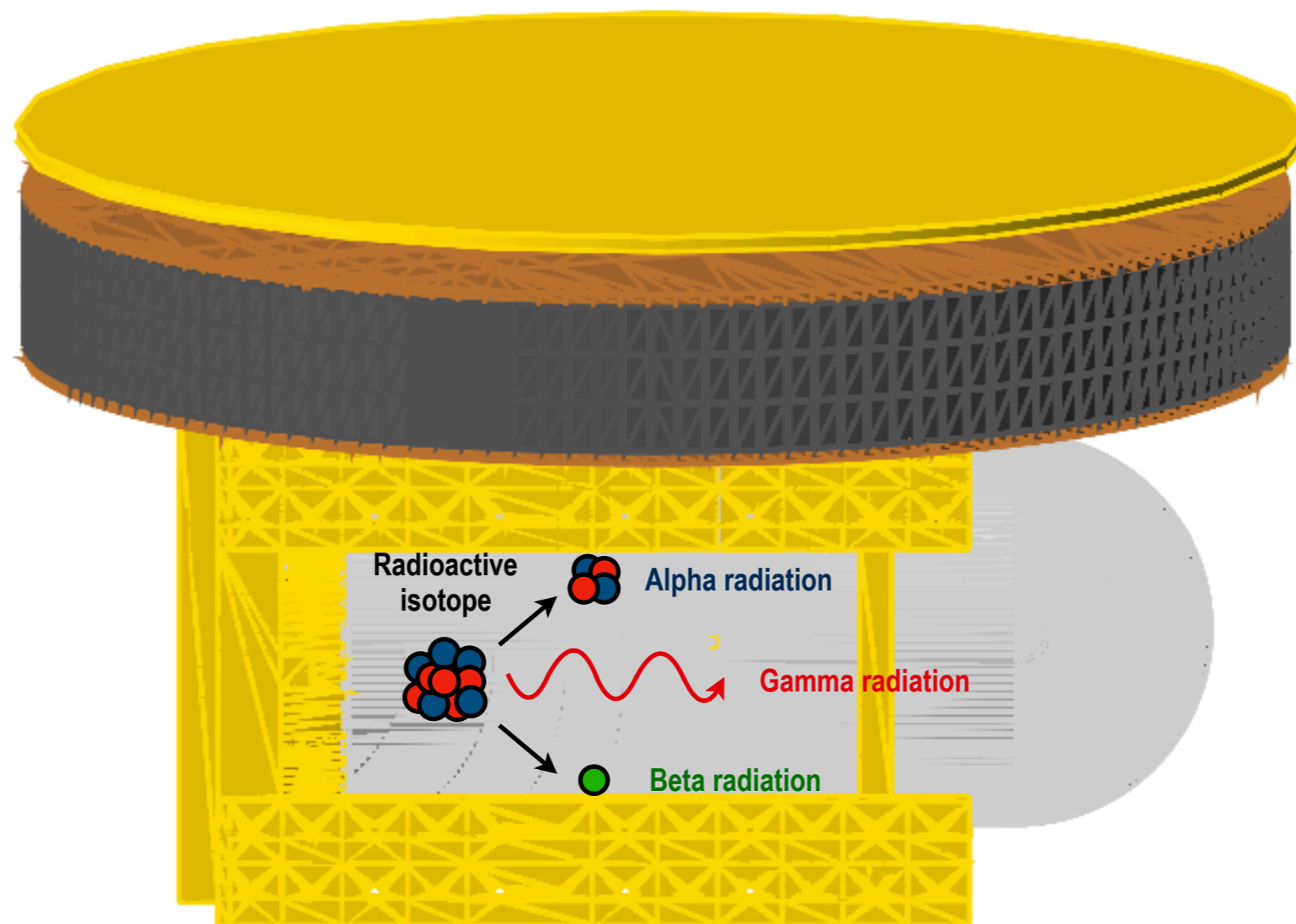
# SIMULATION STRATEGY - ENVIRONMENTAL GAMMAS AND NEUTRONS

- **Gammas** and **neutrons** randomly (and uniformly) generated from a **cylindrical surface ( $S_1$ )** based on measured spectra with isotropic momentum distribution;
- Interaction rate in the substrate estimated by scaling the number of recorded events to flux measurements.

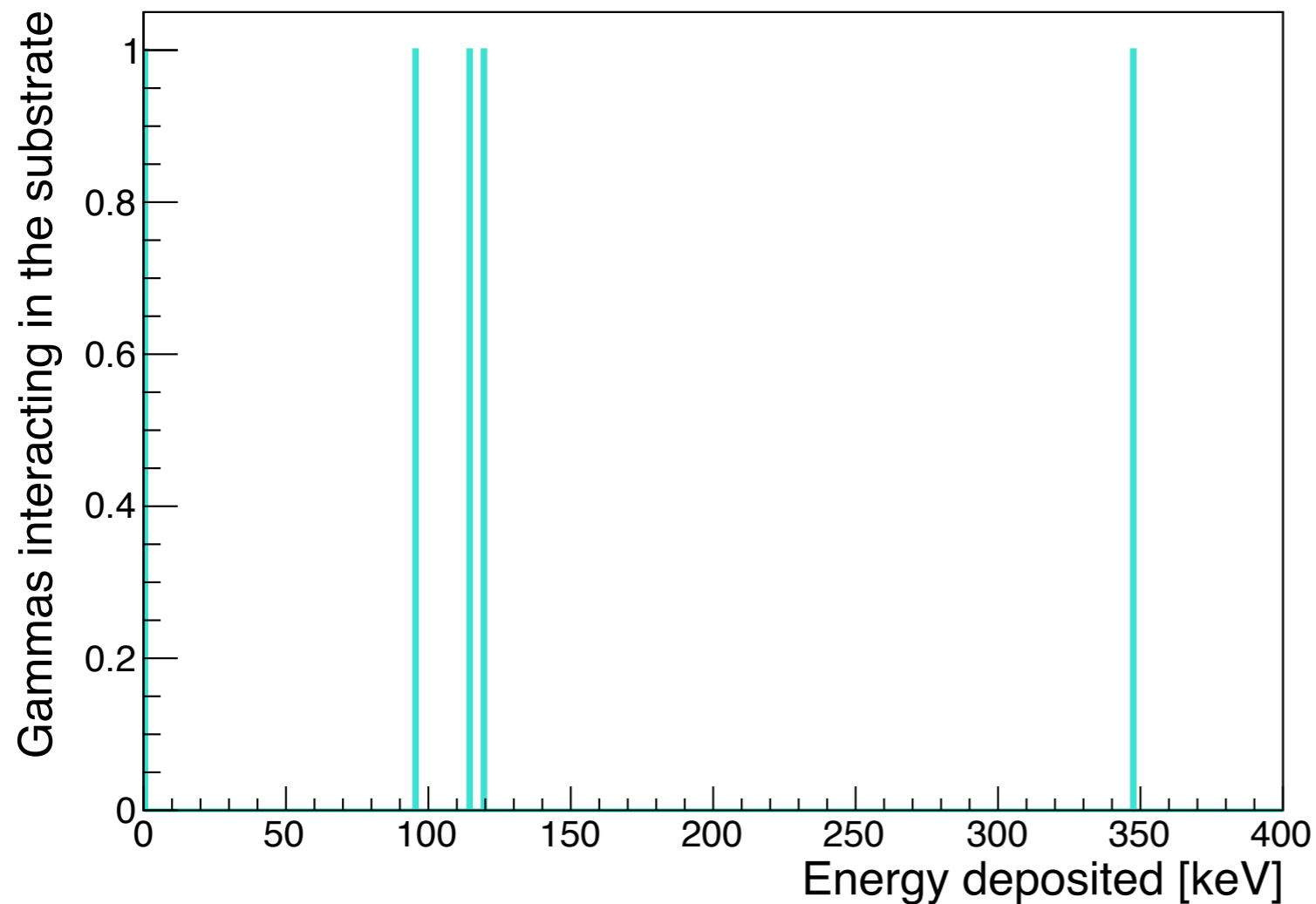


# SIMULATION STRATEGY - CLOSE SOURCES OF RADIOACTIVITY

- **Radioactive decays** of relevant isotopes ( $^{40}\text{K}$ ,  $^{232}\text{Th}$  and  $^{238}\text{U}$  chains) uniformly distributed within the **volumes of the setup components**;
- Interaction rate in the substrate estimated by scaling the number of recorded events to measured isotope activities.



# ENVIRONMENTAL GAMMAS - SIMULATION CHALLENGE



- Number of generated events:

$1e^8$

- Gammas interacting in the substrate (no shield):

5

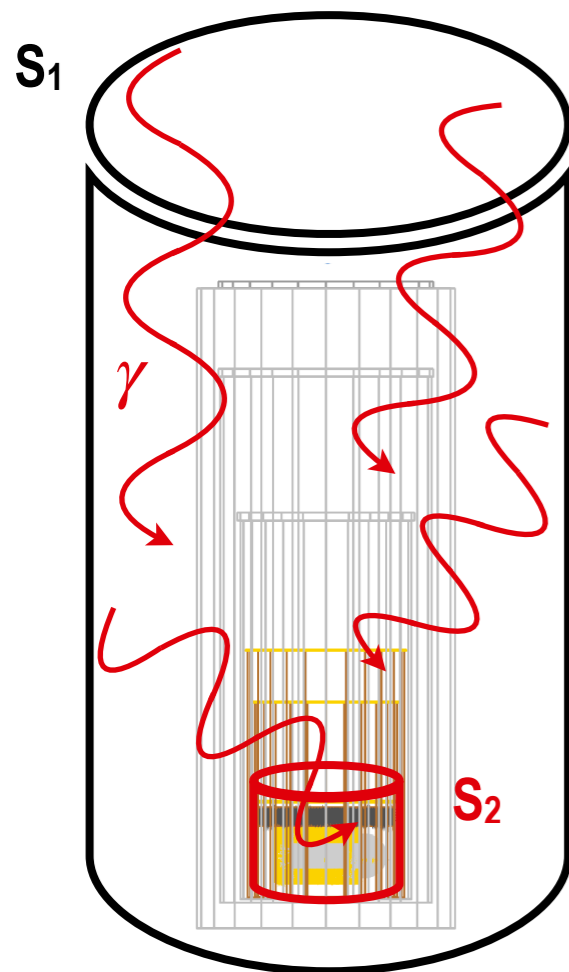
**Statistics is too low!!**

**5 gammas interacting in the substrate every 100 million**

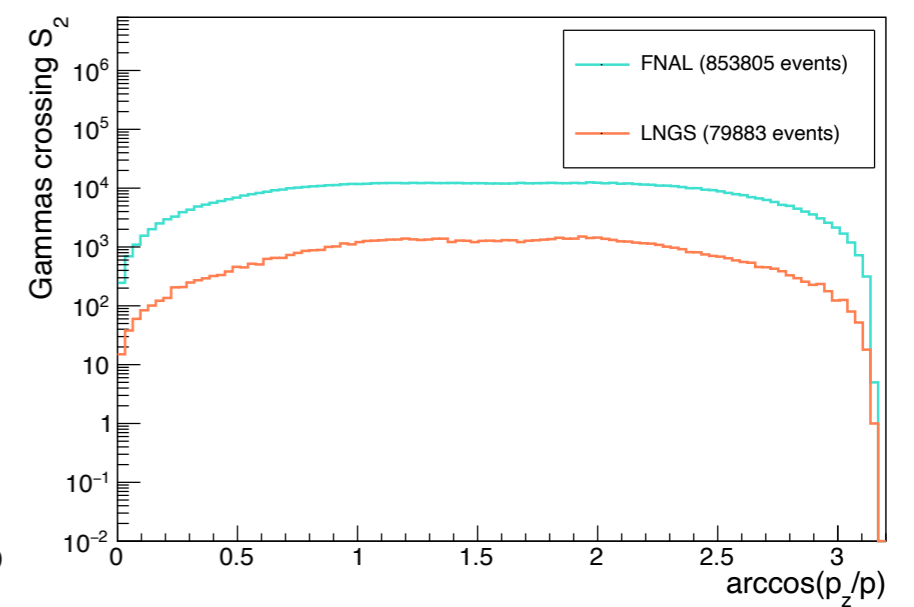
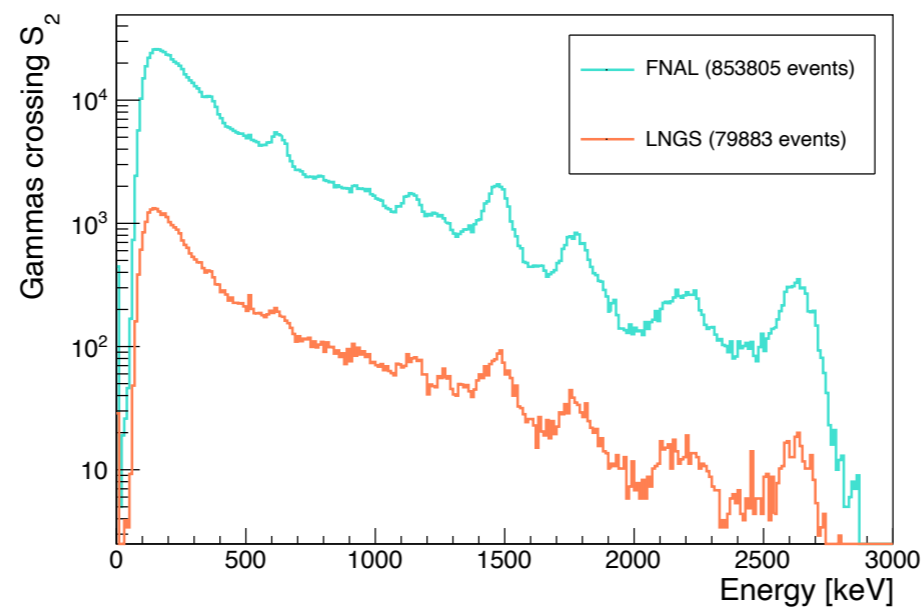
# ENVIRONMENTAL GAMMAS - SIMULATION SOLUTION

**Environmental gammas can be simulated in TWO STEPS:**

- **Gammas** randomly (and uniformly) generated with isotropic momentum distribution from a **cylindrical surface ( $S_1$ )** based on measured spectrum with isotropic momentum distribution;
- **Energy** and **momentum** of  $\gamma$ s crossing a smaller **cylindrical surface ( $S_2$ )** recorded to start a **2nd generation**, according to measured energy and angular distributions in  $S_2$ ;
- Interaction rate in the substrate estimated by scaling recorded event counts to flux recorded in  $S_2$  (requires geometry correction factor).



**Energy and angular distributions of  $\gamma$ s crossing  $S_2$**

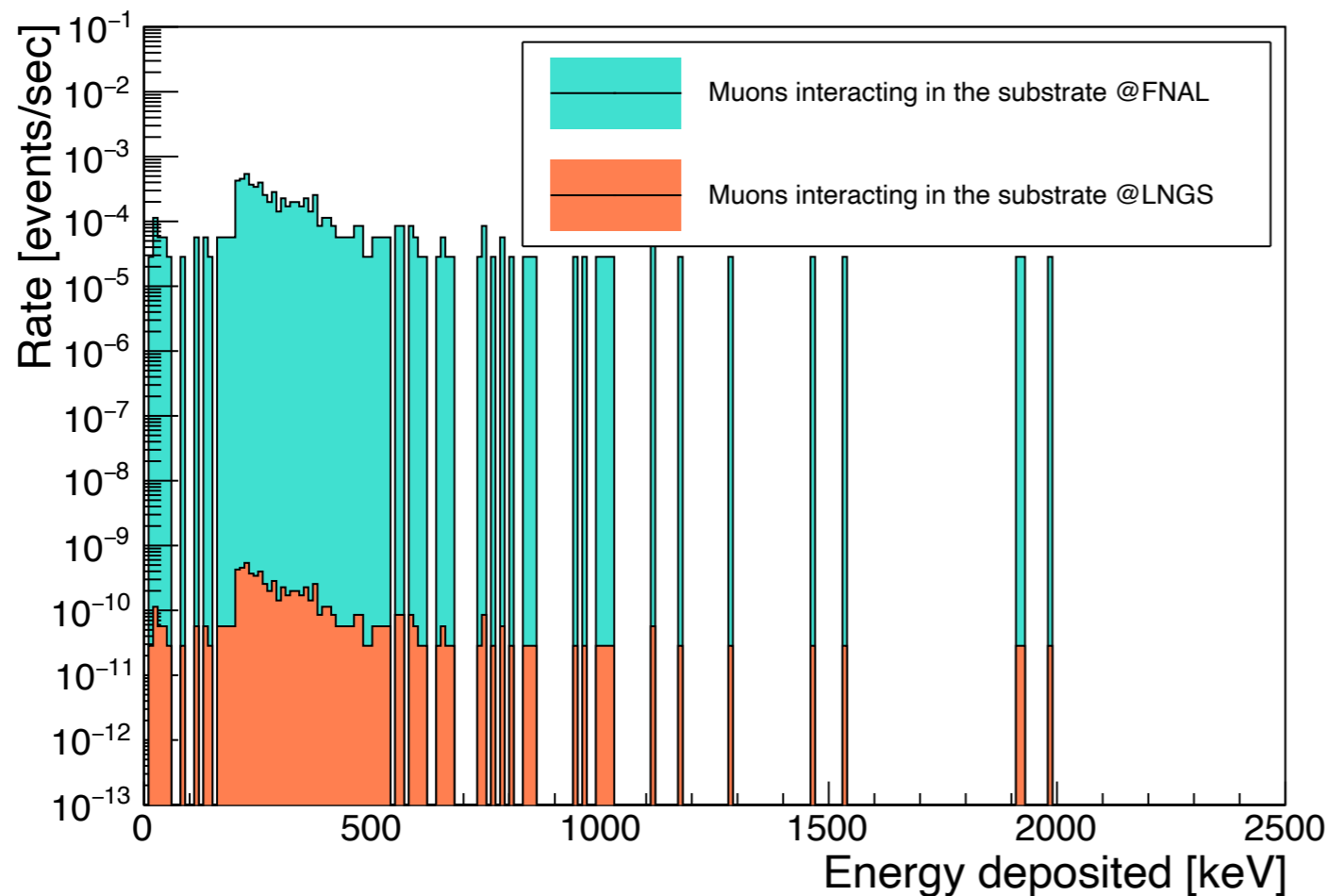




# **SIMULATION RESULTS**

# SIMULATION RESULTS - ATMOSPHERIC MUONS

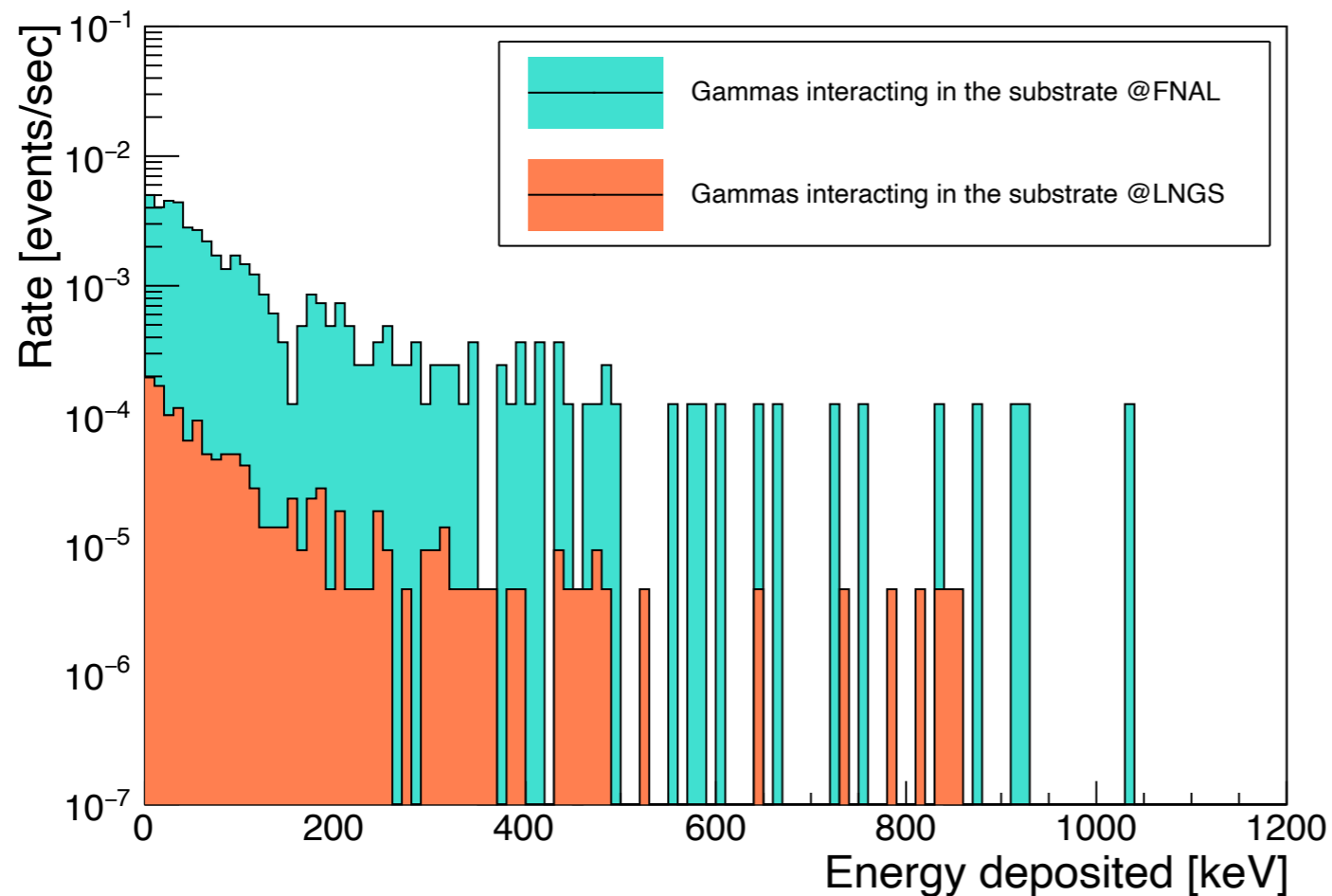
	FNAL (no shield)	LNGS (Cu + Pb shield)
<b>Flux in exp hall [<math>\mu/\text{cm}^2/\text{min}</math>]</b>	1 (literature)	$1\text{e}^{-6}$ (literature)
<b>Number of generated events</b>	$11.5\text{e}^6$	$11.5\text{e}^6$
<b>Simulation equivalent time [sec]</b>	$352\text{e}^2$	$352\text{e}^8$
<b><math>\mu\text{s}</math> interacting in the substrate [events/sec]</b>	$(8.0 \pm 0.5) \times 10^{-3}$	$(8.0 \pm 0.5) \times 10^{-9}$



- $\sim 1 \mu / 125 \text{ sec @FNAL};$
- $\sim 1 \mu / 4 \text{ years @LNGS.}$

# SIMULATION RESULTS - ENVIRONMENTAL GAMMAS

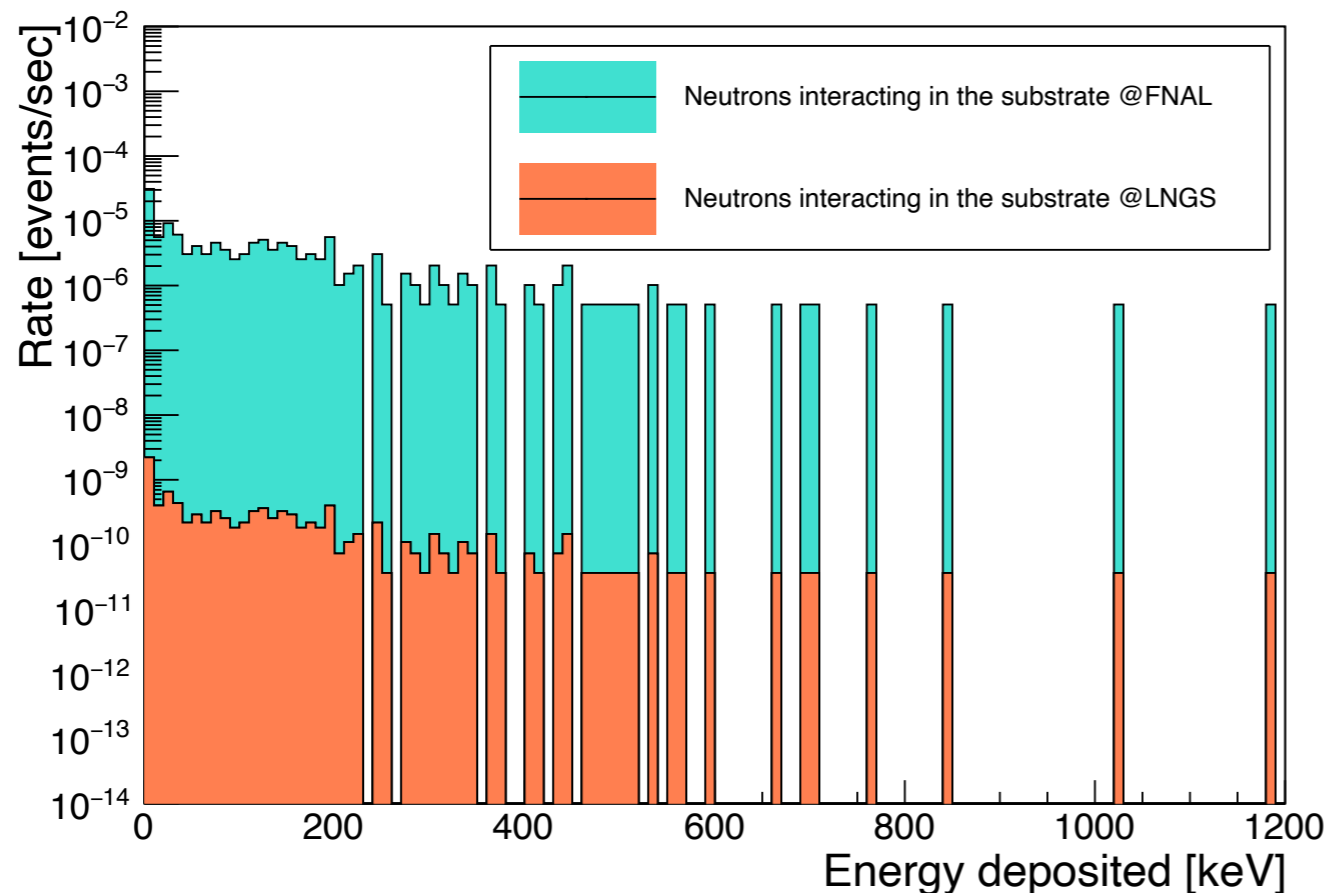
	FNAL (No shield)	LNGS (Cu + Pb shield)
Flux of $\gamma$ s crossing S <sub>2</sub> [ $\gamma/\text{cm}^2/\text{s}$ ]	~1.5	$5.6e^{-2}$
Number of generated events	$1e^8$	$1e^8$
Simulation equivalent time [sec]	$163e^2$	$438e^3$
<b><math>\gamma</math>s interacting in the substrate [events/sec]</b>	$(46 \pm 2) \times 10^{-3}$	$(1.3 \pm 0.1) \times 10^{-3}$



- ~1  $\gamma$  / 22 sec @FNAL;
- ~1  $\gamma$  / 769 sec @LNGS.

# SIMULATION RESULTS - NEUTRONS

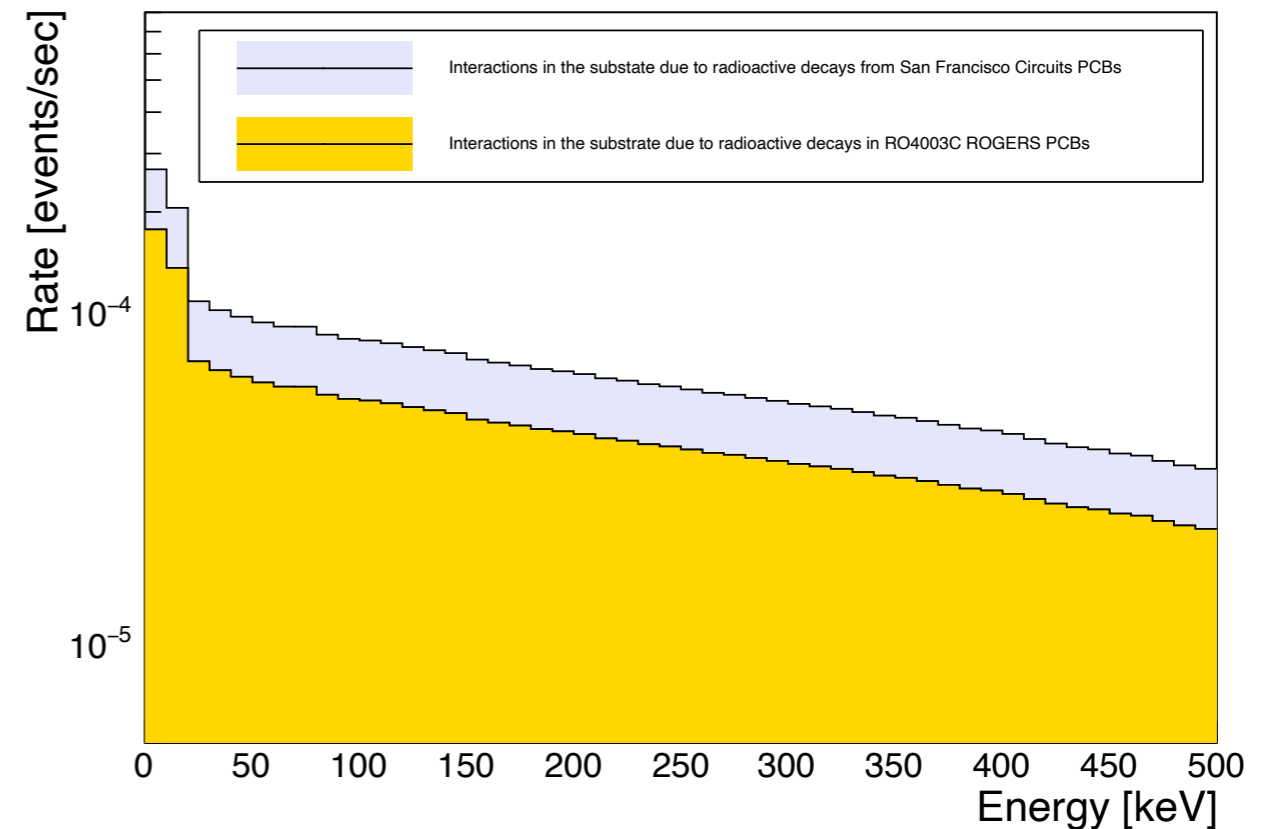
	<b>FNAL (No shield)</b>	<b>LNGS (Cu + Pb shield)</b>
<b>Flux in exp hall [n/cm<sup>2</sup>/sec]</b>	0.014 (averaging measured fluxes in “standard” labs)	1e <sup>-6</sup> (measured)
<b>Number of generated events</b>	13e <sup>8</sup>	13e <sup>8</sup>
<b>Simulation equivalent time [sec]</b>	191e <sup>4</sup>	267e <sup>8</sup>
<b>ns interacting in the substrate [events/sec]</b>	$(1.0 \pm 0.3) \times 10^{-4}$	$(7.0 \pm 0.5) \times 10^{-9}$



- ~1 n / 3 hours @FNAL;
- ~1 n / 4.5 years @LNGS.

# SIMULATION RESULTS - CLOSE SOURCES OF RADIOACTIVITY

Component	Description	Rate [events/sec]
A	PCB	$[3 - 4.5] \times 10^{-3}$
B	Box	$[1 - 6] \times 10^{-6}$
B*	Holder	$[2 - 4] \times 10^{-7}$
C	Magnetic Shield	$[2 - 9] \times 10^{-7}$
D	SMA	$(2.0 \pm 0.4) \times 10^{-8}$
E	Cu coax cables	$(3.0 \pm 0.6) \times 10^{-8}$
F	Cryogenic switch	$(1.0 \pm 0.2) \times 10^{-5}$
G	Circulator	$< 8 \times 10^{-7}$
H*	Dual-junct. circulator	$< 2 \times 10^{-6}$
I*	Triple-junct. isolator	$< 2 \times 10^{-6}$
J	Attenuators	$[0.5 - 1] \times 10^{-8}$
K	Low Pass Filter	$(1.0 \pm 0.2) \times 10^{-8}$
L	NbTi cables	$< 4 \times 10^{-7}$
M	Cryogenic amplifiers	$< 2 \times 10^{-8}$
N	Cu-Be cables	$< 1 \times 10^{-9}$

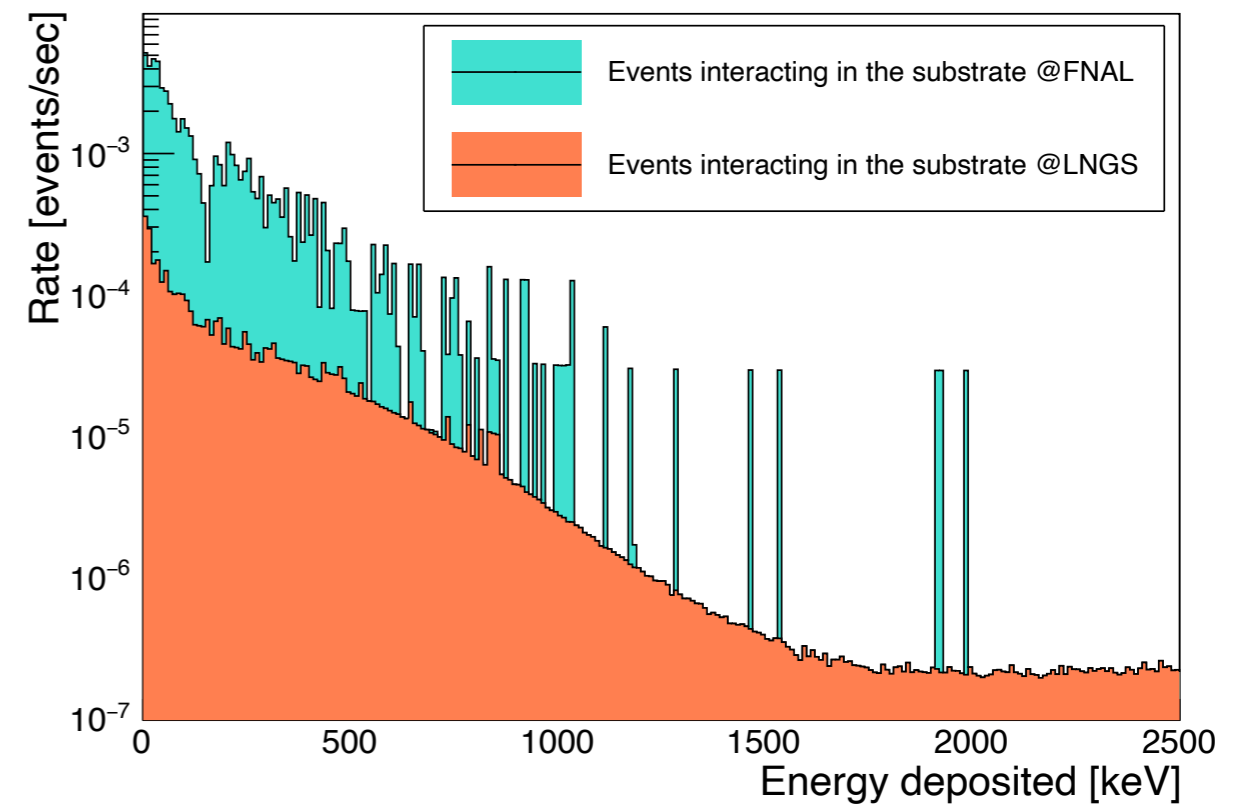


**Only the PCB has a significant impact:  
~ 1 event / 280 sec**

**Assumed equal contributions for FNAL and LNGS**

# SIMULATION RESULTS - SUMMARY

Source	Rate in the substrate [events/sec]	
	FNAL (No shield)	LNGS (Cu + Pb shield)
Lab's gammas	$(46 \pm 2) \times 10^{-3}$	$(1.3 \pm 0.1) \times 10^{-3}$
Muons	$(8.0 \pm 0.5) \times 10^{-3}$	$(8.0 \pm 0.5) \times 10^{-9}$
Neutrons	$(1.0 \pm 0.3) \times 10^{-4}$	$(7.0 \pm 0.5) \times 10^{-9}$
Close sources	$(3.0 \pm 0.7) \times 10^{-3}$ (PCB dominated)	$(3.0 \pm 0.7) \times 10^{-3}$ (PCB dominated)
<b>Total</b>	$(57 \pm 3) \times 10^{-3}$	$(4.3 \pm 0.8) \times 10^{-3}$



- ~1 event / 17 sec @FNAL;
- ~1 event / 233 sec @LNGS.

# COMPARING SIMULATION WITH MEASUREMENTS

# MEASUREMENTS WITH RADIOACTIVE SOURCES



$^{232}\text{Th}$



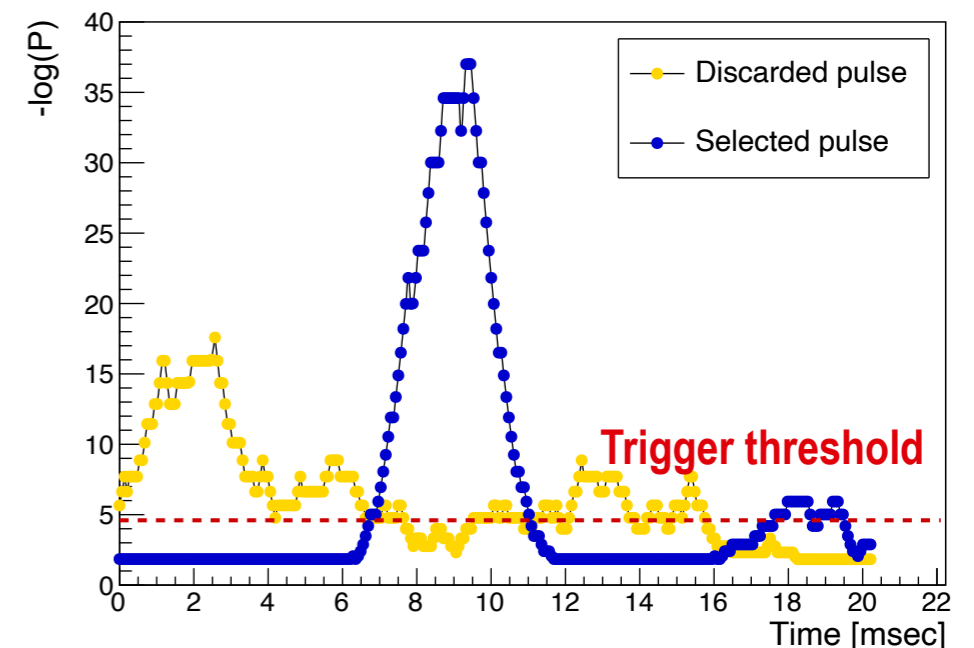
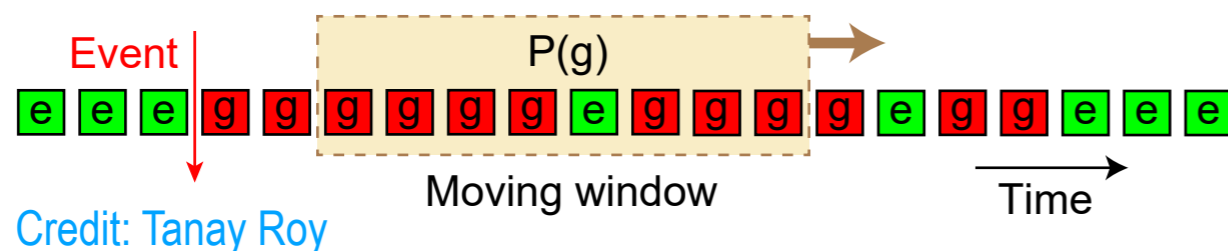
- Superconducting qubits exposed to Thorium radioactive sources with increasing activity levels;
- Sources positioned between the cryostat and the copper bars, approximately at the same height as the chip.

[Talk by Tanay Roy at RISQ 2024 on Thursday](#)

LNGS FACILITY

[ De Dominicis et al., [arXiv:2405.18355 \(2024\)](#) ]

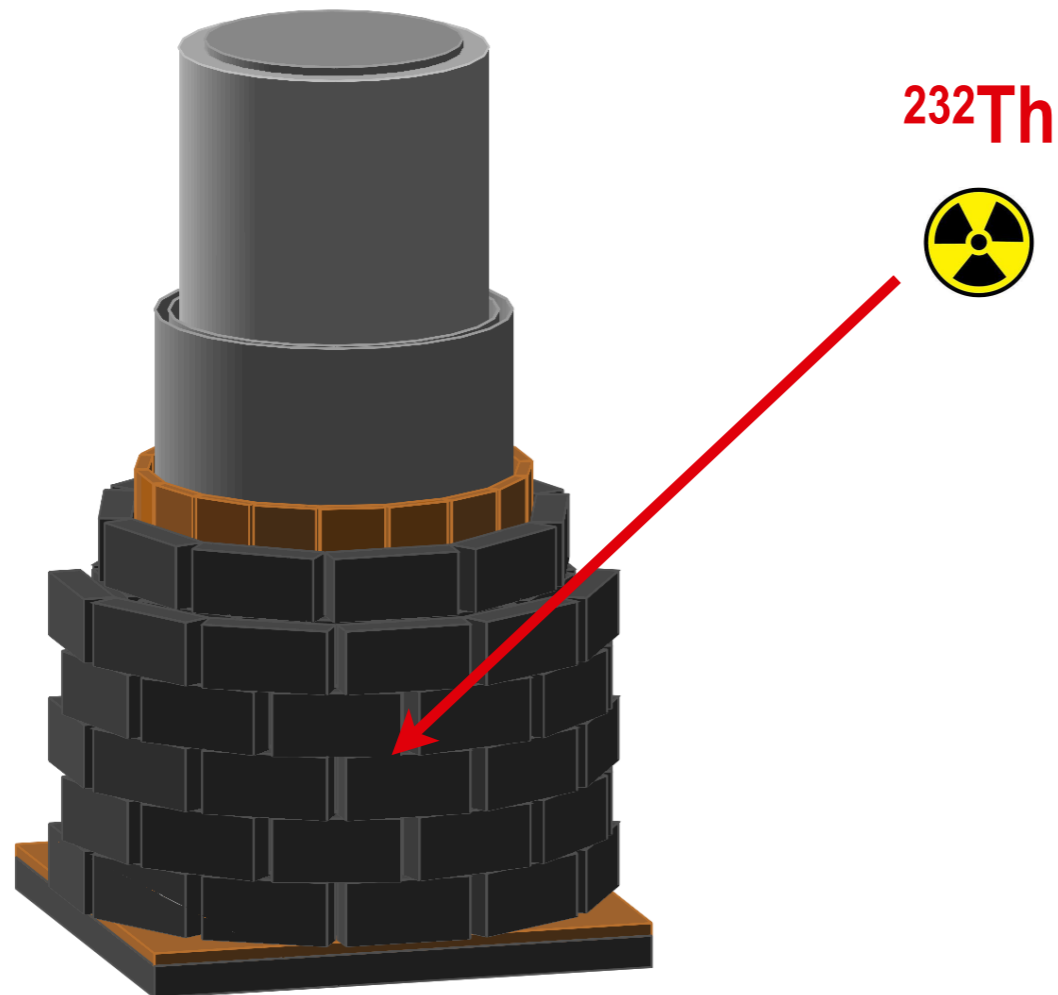
- Fast decay detection protocol for single qubit;
- Pulses selected based on the probability of observing a certain stream of  $|e\rangle$  and  $|g\rangle$  states





# SIMULATION OF RADIOACTIVE SOURCES

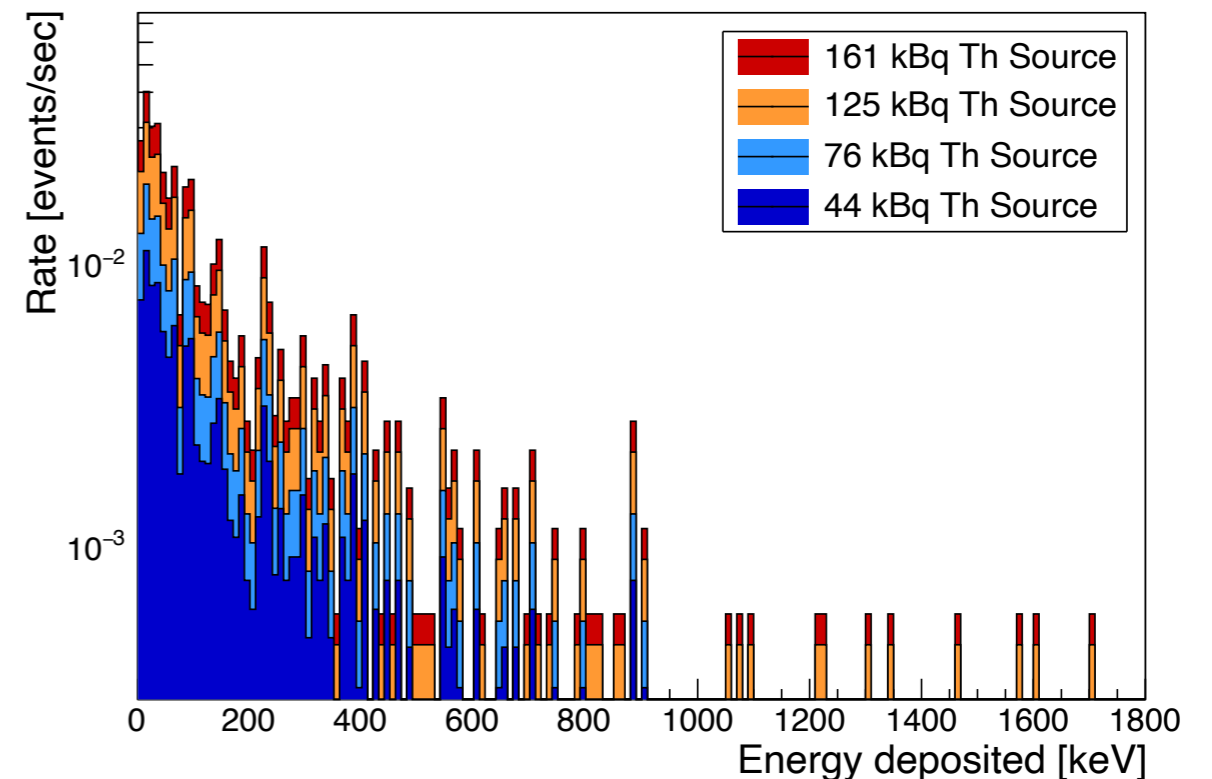
- Radioactive decays generated from a **point-like  $^{232}\text{Th}$  radioactive source**, considering only gamma emitters in the chain:  $^{228}\text{Ra}$ ,  $^{228}\text{Ac}$ ,  $^{212}\text{Pb}$ ,  $^{212}\text{Bi}$ ,  $^{208}\text{Tl}$ .



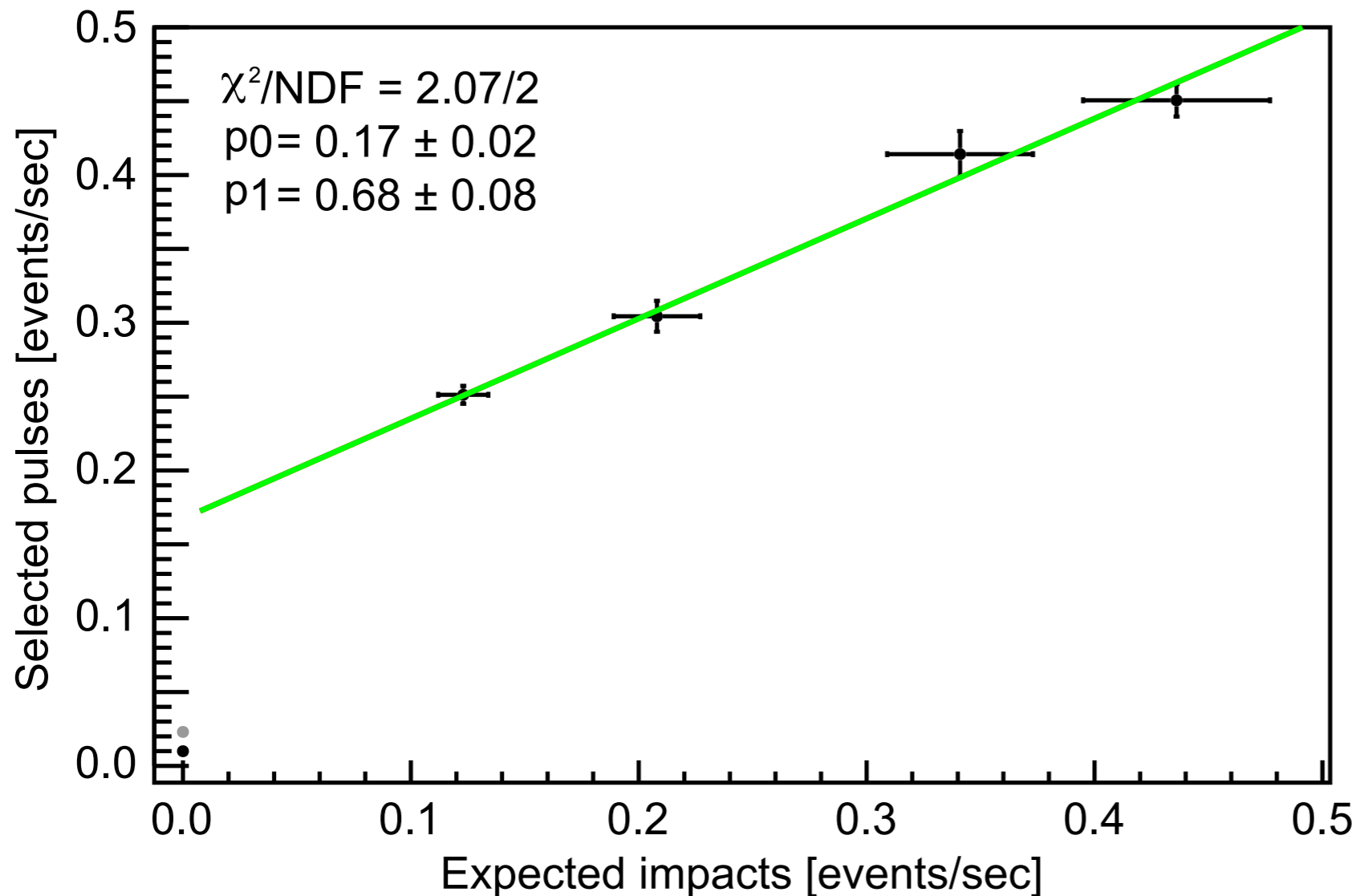
**From 1 event / 8 sec to 1 event / 2 sec**

[ De Dominicis et al., *arXiv:2405.18355* (2024) ]

Source Activity [kBq]	Rate in the substrate [events/sec]
44.2	$0.12 \pm 0.01$
75.9	$0.20 \pm 0.02$
125.4	$0.34 \pm 0.03$
161.0	$0.43 \pm 0.04$



# SIMULATION VS. MEASUREMENTS



- $p_0$  = “background” rate
- $p_1$  = detection efficiency

Expected background rate  
( $< 0.01$  events/sec)

$<$

Measured “background” rate  
(0.17 events/sec)

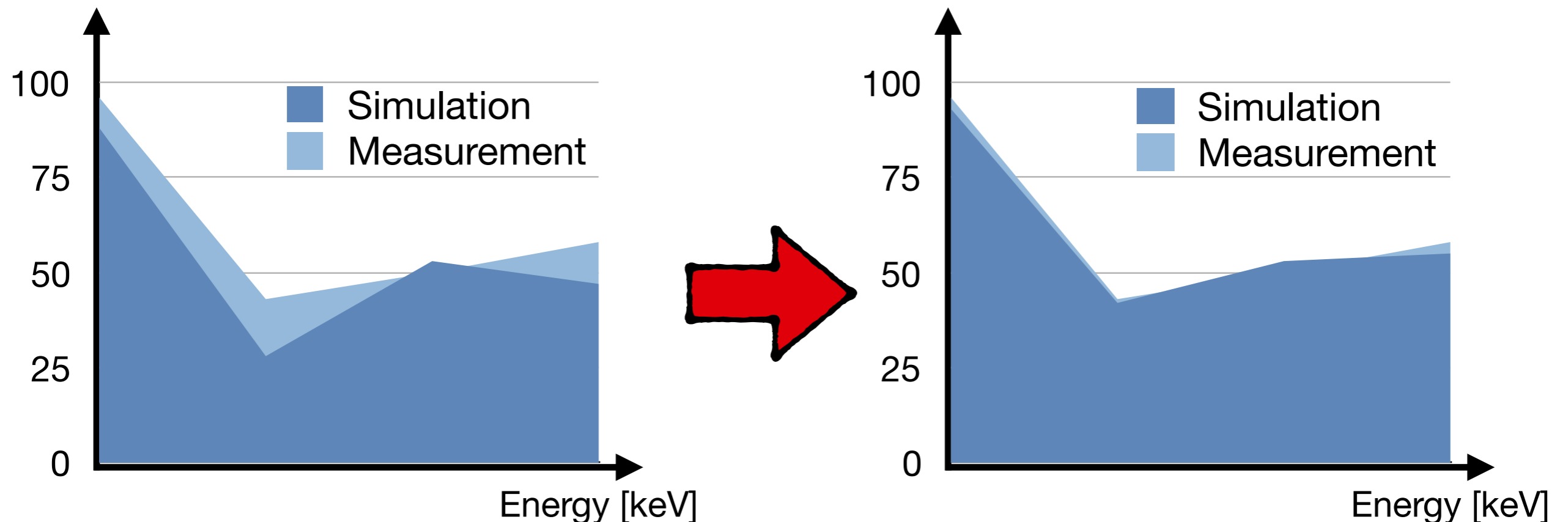
[ De Dominicis et al., *arXiv:2405.18355* (2024) ]

**Excess noise or unpredicted effect??**

**Charges and phonons modeling would be very helpful,  
along with additional measurements!**

# CONCLUSIONS

- **Superconducting quantum devices** are currently a **highly relevant topic** of research;
- Can be used both for **quantum computing** and **sensing** (such as light dark matter detectors);
- Measurements have revealed **unexpected additional counts** compared to **simulated data**;
- **Deepening our understanding** is **crucial** for all applications;
- **Urgent need for increasingly accurate MC simulations**;
- Comparative analysis with **G4CMP** results would **significantly contribute** to **advancing** this understanding.



**THANKS FOR YOUR ATTENTION!**

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