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Monte-Carlo simulations and Nuclear Spectroscopy for Muon Capture Experiments

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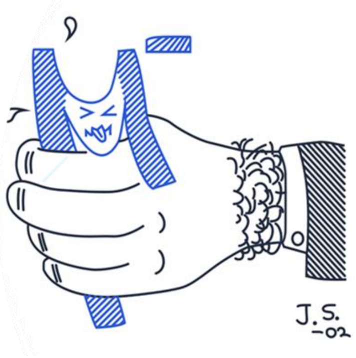
List of contents

- **Short Theoretical introduction.**
- **Advantages of using Monte-Carlo codes like MCNP6.**
- **Steps for Monte-Carlo Simulations.**
- **MONUMENT experiment and Muon-Beam Profile.**
- **Monte-Carlo Simulation of MONUMENT experiment.**
- **Simulations of the Induced Secondary Particles.**
- **Simulations of the Calibration Sources.**
- **Separating Spectrum into its Components and Isotopes Production.**
- **More for Near Future.**

Motivation

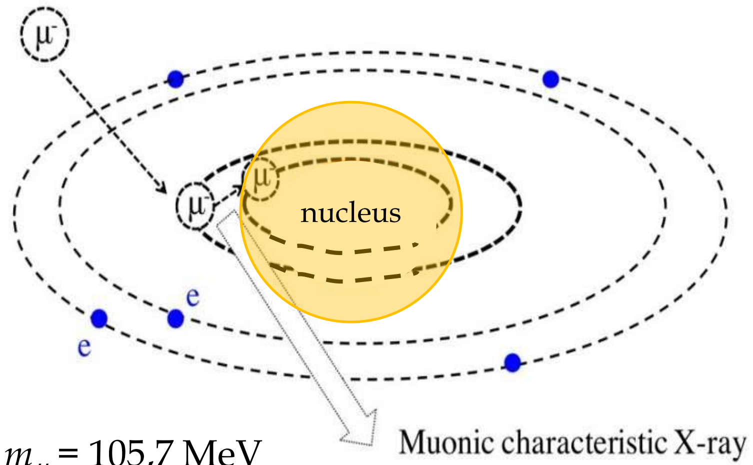
- Verification of the accuracy of theoretical calculations of nuclear matrix elements (including for $0\nu\beta\beta$-decay)
- Verification of the suppression of the parameter g_A

$$|\mathbf{NME}_{0\nu}|^2 \cong \left|M^{0\nu}_{GTGT}\right|^2 = (g_{a,0\nu})^4 \left|\Sigma_{J^\pi}\left(\langle 0_f^+ \middle| O^{0\nu}_{GTGT} \middle| 0_i^+ \rangle\right)\right|^2$$



- Obtaining total and partial rates of ordinary muon capture (OMC
- Filling the atlas of meso-X-ray spectra *(https://muxrays.jinr.ru/index.html)*
- Using OMC to study the astrophysical properties of neutrinos (100Mo)

(10.1103/PhysRevC.99.024327)



m_μ = 105,7 MeV

ν_μ $\tau_{dec} = 2.2\mu s$

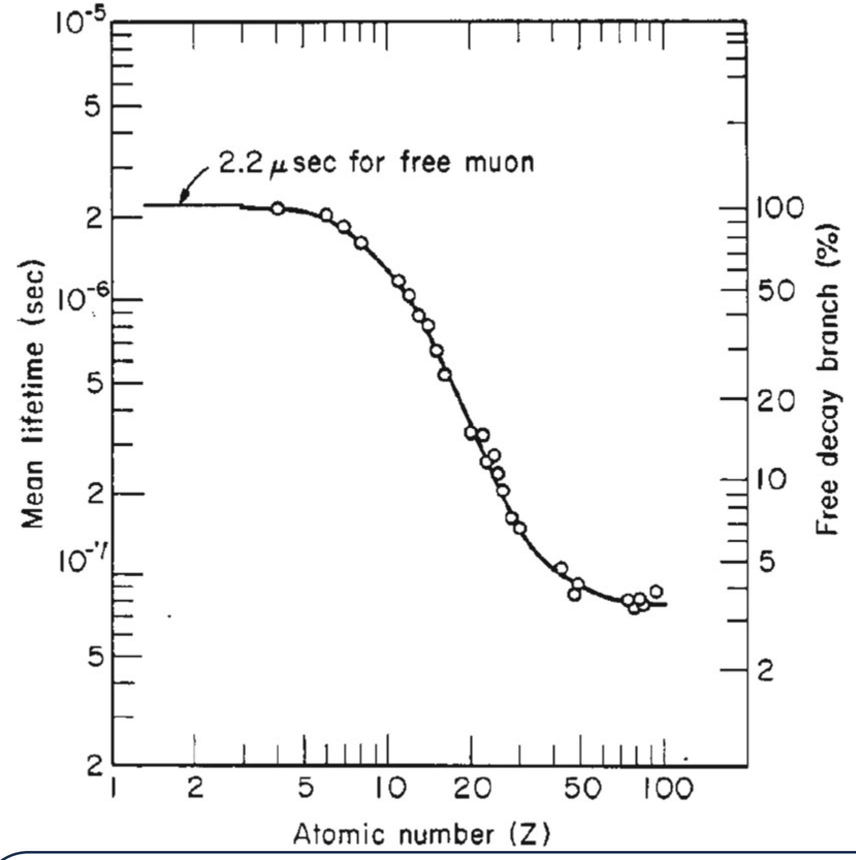
$(A, Z) + \mu^- \rightarrow (A, Z\text{-}1)^* + \nu_\mu$

$Z\text{-}1) + \gamma$

$\rightarrow (A\text{-}1, Z\text{-}1) + \gamma + n$

$\rightarrow (A\text{-}2, Z\text{-}1) + \gamma + 2n$

Motivation



The mean lifetime of negative muons inside a material of atomic number Z and the corresponding percentage of remaining ordinary muon decays.

10.1140/epjp/s13360-020-00777-y

The capture rate of the muon capture reaction varies depending on the nucleus forming the muonic atom

$$\frac{1}{\tau_{\text{total}}} = \Lambda_{\text{cap}} + \frac{Q}{\tau_{\mu^+}},$$

where τ_μ is the lifetime of the muon ~ 2.2 μs, and *Q is a Huff factor*, which takes into account a reduction in the muon decay rate due to the atomic binding energy

The capture rate can be expressed by Primakoff formula:

$$\Lambda_{\text{cap}}(A, Z) = Z_{\text{eff}}^4 X_1 \left[1 - X_2 \left(\frac{A-Z}{2A}\right)\right]$$

The parameters X1 and X2 are coefficients obtained from a global fit of the experimental data, where X_1= 170 s^{-1} and X_2= 3.125

https://arxiv.org/pdf/2501.05897v2

List of contents

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- Steps for Monte-Carlo Simulations.
- MONUMENT experiment and Muon-Beam Profile.
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Advantages of using Monte-Carlo codes like MCNP6

- In general, Monte Carlo Transport Codes like *MCNP6* plays a pivotal role in simulating and optimizing experiments. Its ability to model particle interactions, complex geometries, and detector systems makes it an indispensable tool for researchers in this field.

- MCNP6 facilitates the simulation of muon transport, capture, and decay within target materials.

- Additionally, *MCNP6* enables the design and optimization of experimental setups by simulating detector responses, energy deposition, background radiation which can be suppressed (including natural background, Compton, Bremsstrahlung and other background-induced radiations when the beam is on), ensuring accurate measurements and reducing systematic uncertainties.

- The code is also valuable for studying rare phenomena, such as nuclear recoil effects and isotopic shifts, and for separating contributions from different nuclear isotopes in complex samples. Its versatility and accuracy make *MCNP6* an essential tool for advancing muonic X-ray experiments.

List of contents

Steps for Monte-Carlo Simulations

1. The geometry and materials of all components of the MONUMENT experiment have been written and constructed employing many codes and softwares: **MCNP6** + **Phig3D-PHITS** + **TopMC**. As a beginning, simulations were applied to the experiment carried out in 2021 at PSI using **BaCO3** target with ~95% enrichment of Ba-136.

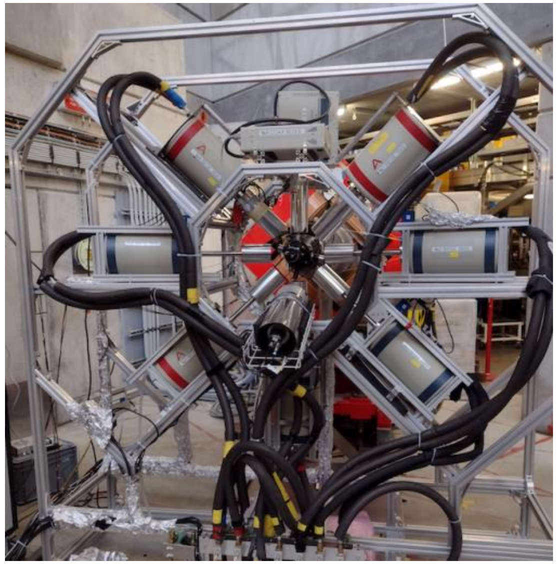
2. The full input-files for Monte-Carlo code MCNP6 have been written for different calculations: muon-beam profile simulations; simulations to get all generated-particles during the muon-irradiation; simulations of the background (terrestrial background); the cosmic-rays background; simulations of the generated isotopes in the Target and the Detector and their gamma-intensities; and other related simulations.

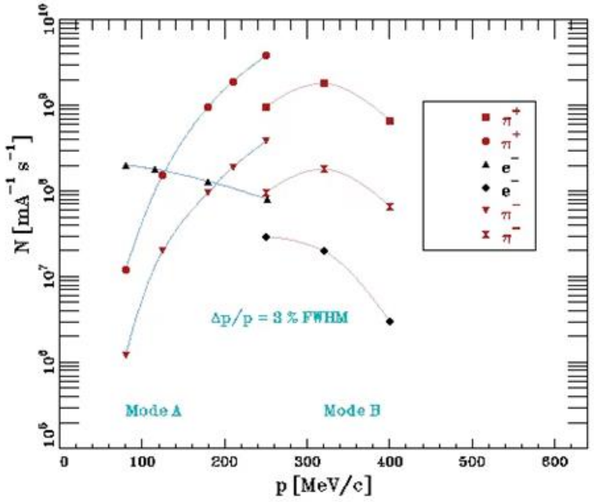
3. Getting results (mentioned in the previous paragraph) after processing the data resulting from simulations. The simulated results were compared with the experimental ones.

4. Conducting the simulations using MCNP6 code on the JINR Cluster and Cloud with more Cores and RAMs resources to accelerate simulations (not all types of simulations!).

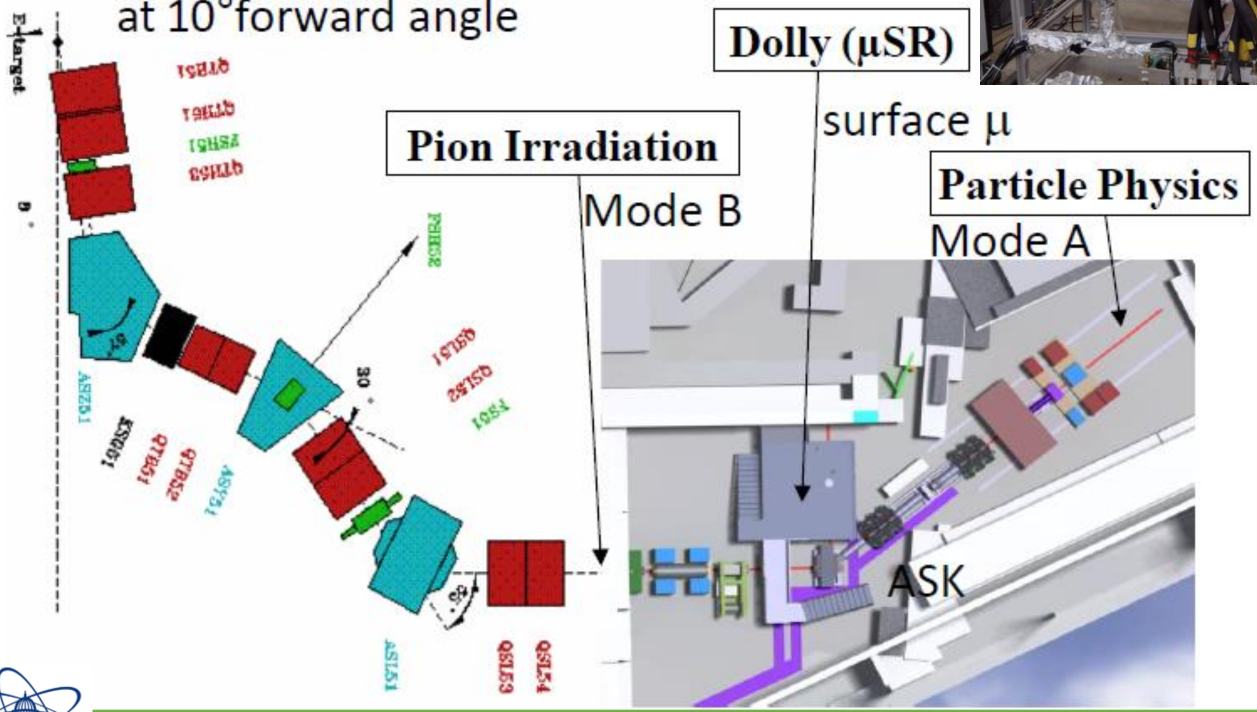
List of contents

MONUMENT experiment @ πE1 beamline (PSI, Switzerland)



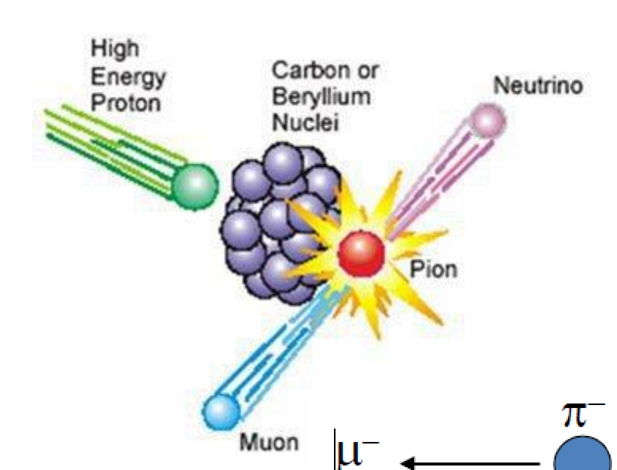


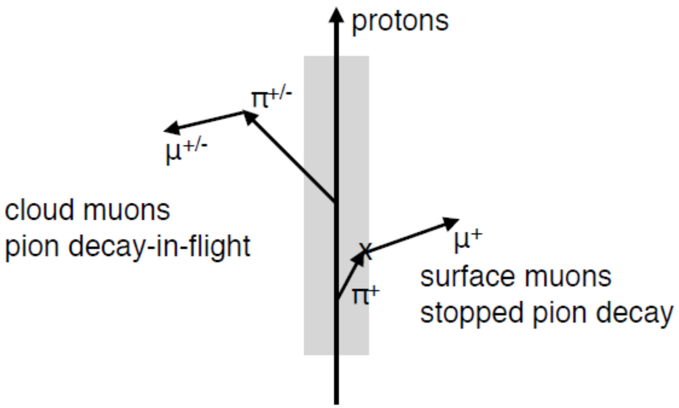
These Pions Produce Muon-Beam With momentum: 33-40 MeV/c



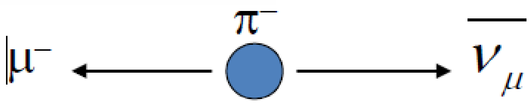
Purpose	OMC targets (enrichment)	Year/Status
experimental input for DBD NME calculations	^{76}Se (99.97%)	**2021** / analysis and publication
experimental input for DBD NME calculations	^{136}Ba (95.27%)	**2021** / analysis and publication
experimental input for astrophysics investigations with SN	^{100}Mo (97.3%)	**2022** / started data analysis
Nuclear spectroscopy, total cap. rates, yields	^{nat}Mo	**2022** / started data analysis
testing nuclear shell model (SM) calculations	^{48}Ti (99.9%)	**2023** / started data analysis
experimental input for DBD NME calculations, ab-initio calculations	^{96}Mo, ^{12}C, ^{13}C, ^{56}Fe	**2026-2028** / in preparation

MONUMENT experiment @ πE1 beamline (PSI, Switzerland)

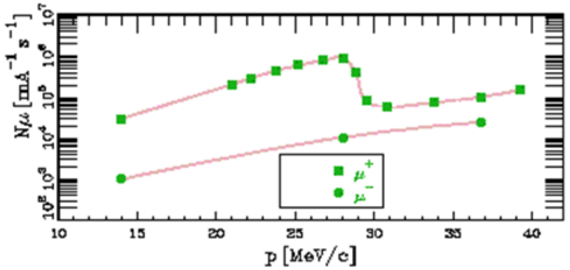


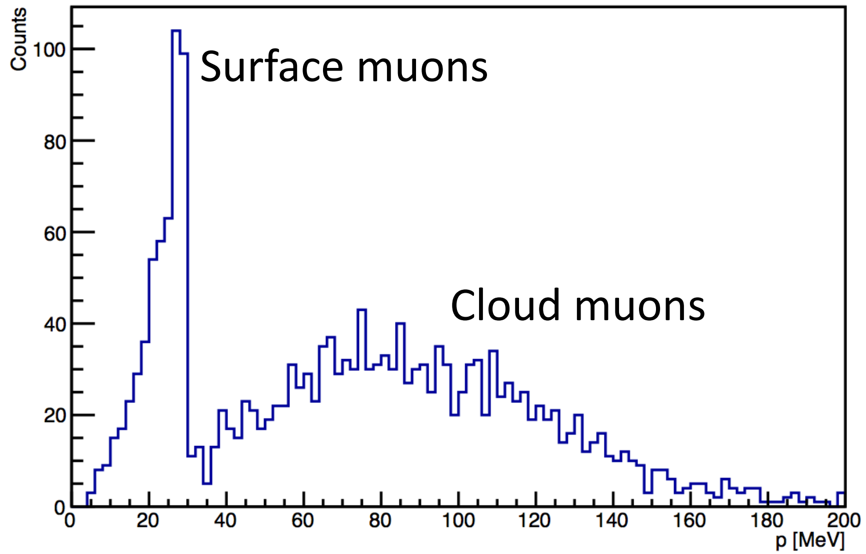


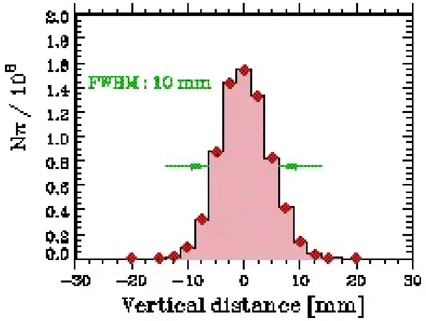
- Single pion production at 290 MeV proton energy (LAB)
- Low-energy muon beam lines typically tuned to surface μ+ at ~ 28 MeV/c
- Note: surface μ —> polarized positively charged muons (spin antiparallel to the momentum)
- Contribution from cloud muons at similar momentum about 100x smaller
- **Negative muons only available as cloud muons**

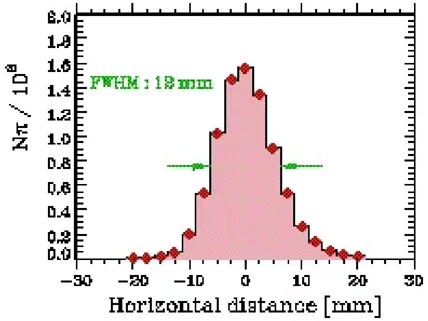


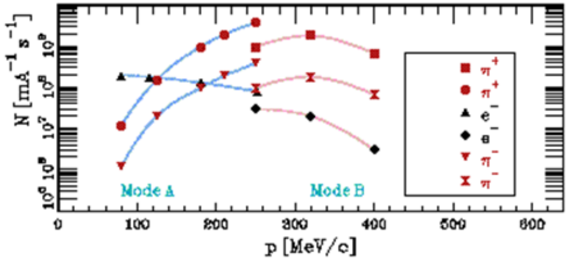
- Negative muons only available as clouds muons
- almost 100% polarized



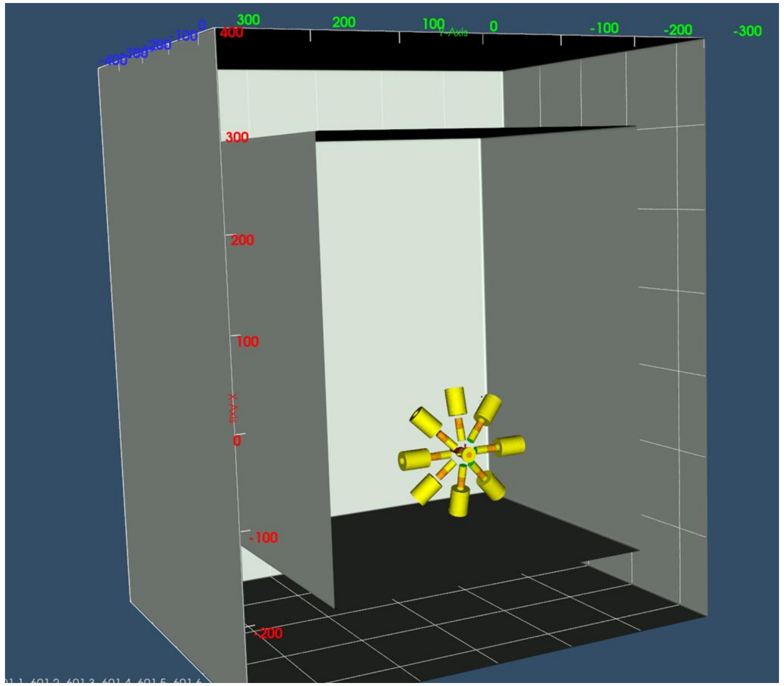


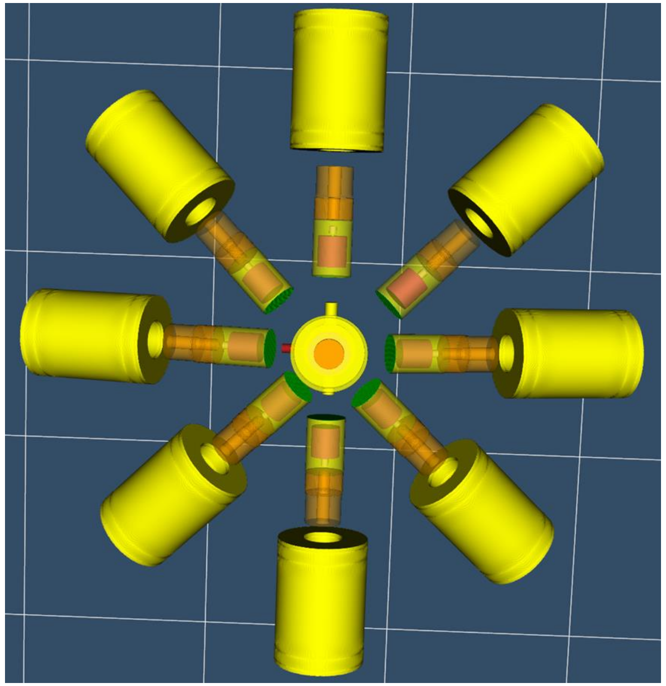
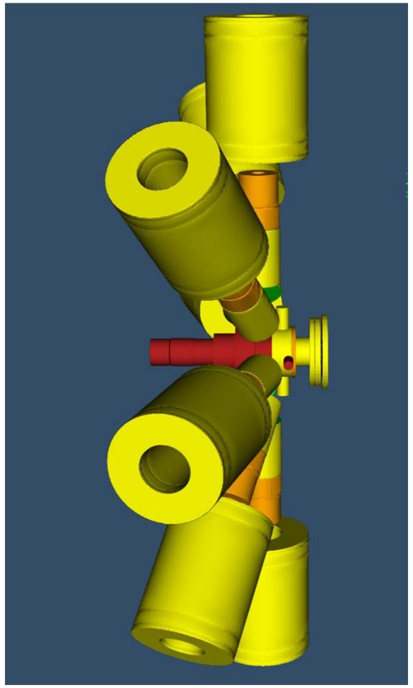






List of contents



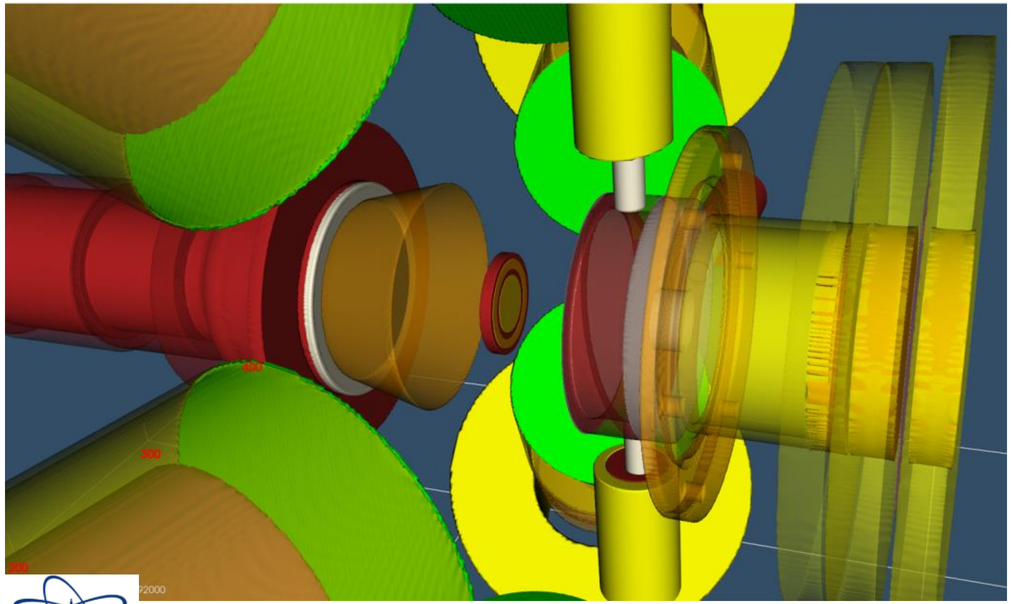
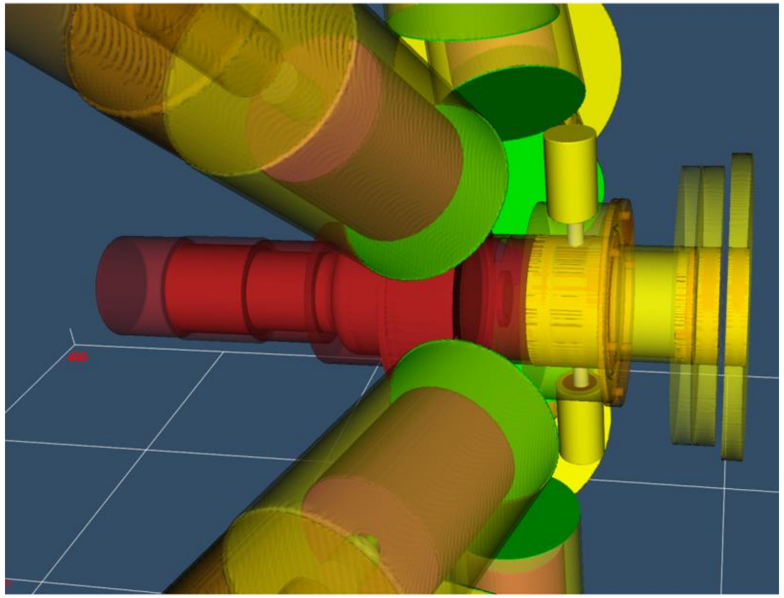
Geometry of MONUMENT-Experiment described in the MCNP-input file and generated using Phig3D-PHITS program.

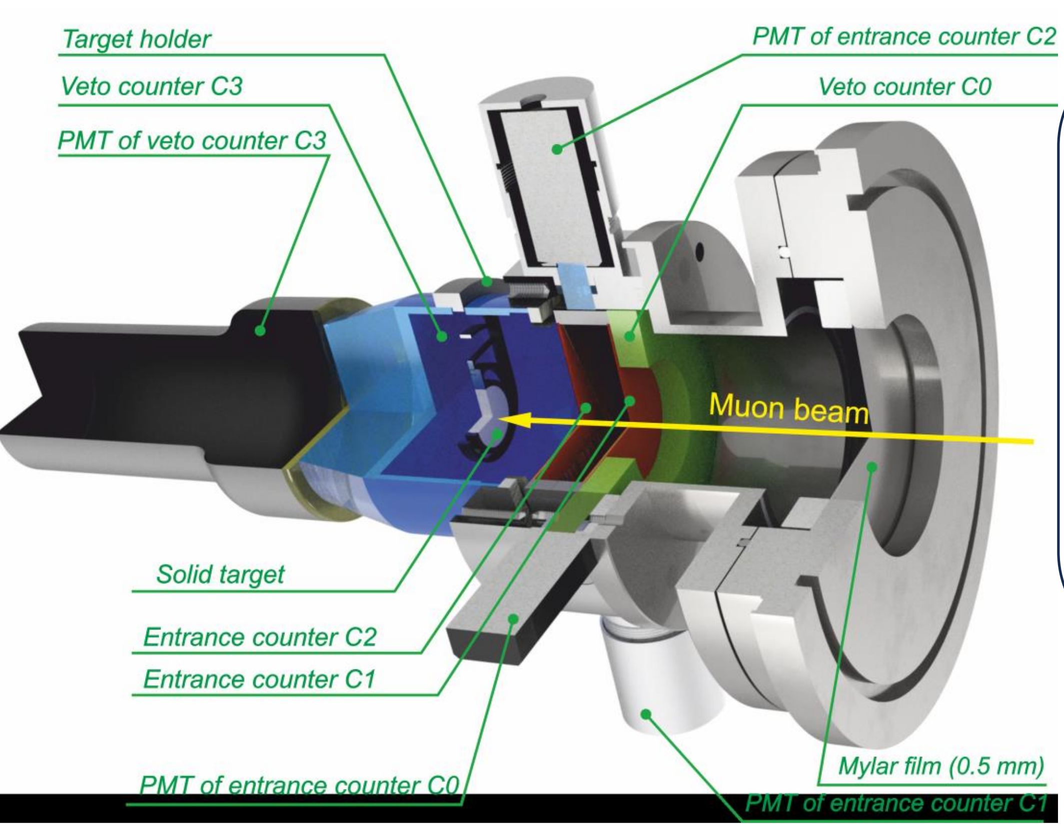
<u>The following codes and programs were used to obtain the geometry:</u>

- **MCNP6** (Monte Carlo N-Particle Transport is a general-purpose, continuous-energy, generalized-geometry, time-dependent, Monte Carlo radiation transport code designed to track many particle types over broad ranges of energies and is developed by Los Alamos National Laboratory.)

- **Phig3D-PHITS** (Particle and Heavy Ion Transport code System) is a general purpose Monte Carlo particle transport simulation code developed under collaboration between JAEA, RIST, KEK and several other institutes)

- **TopMC** (Multi-Functional Program for Neutronics Calculation, Nuclear Design and Safety Evaluation, which has been developing by FDS



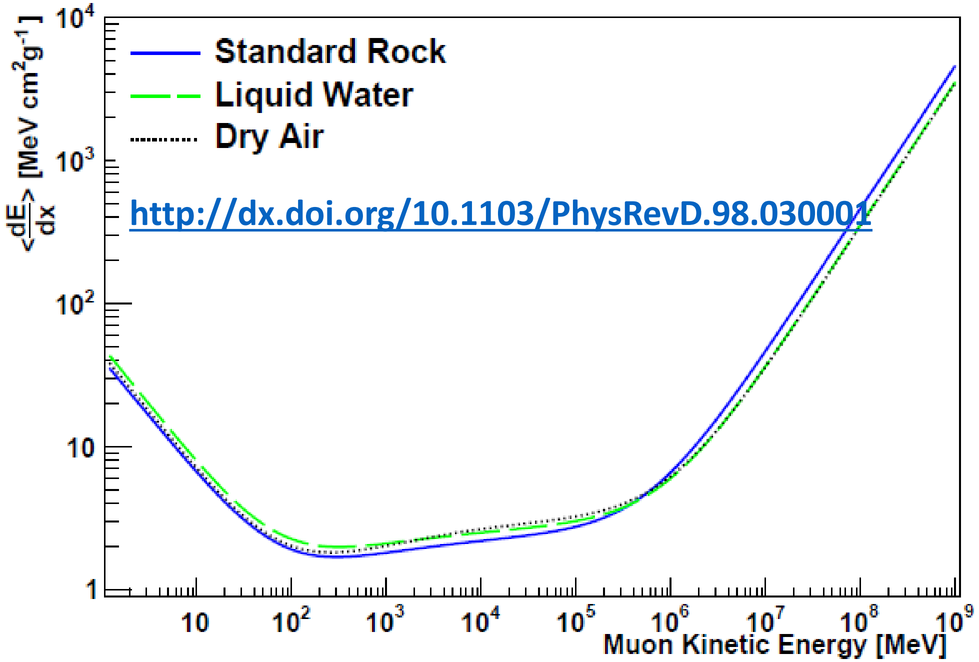
The Target Assembly with the scintillation counters **C0**, **C1**, **C2** and **C3**

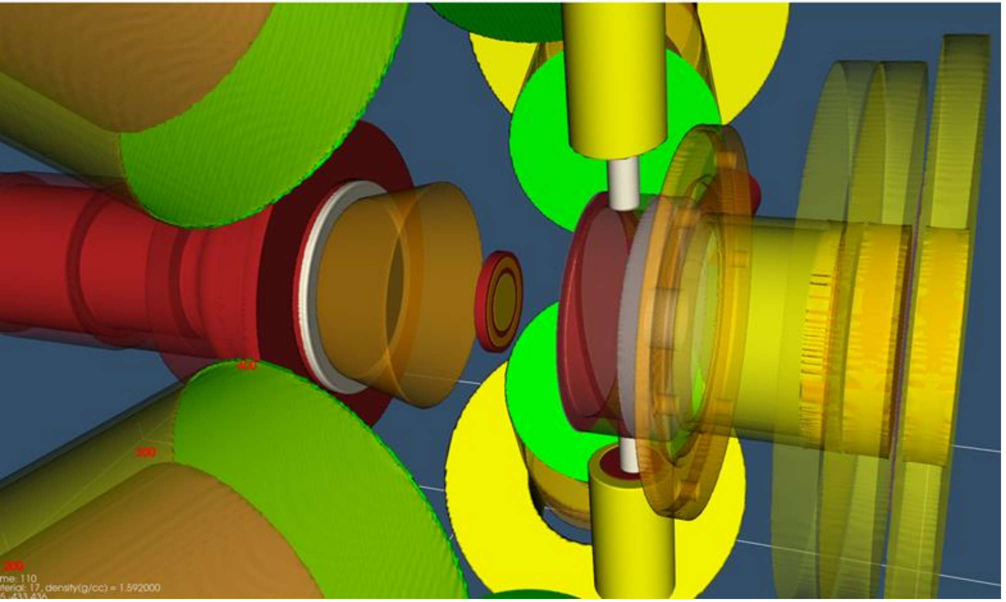
The muon trigger system combined with the target unit consists of:

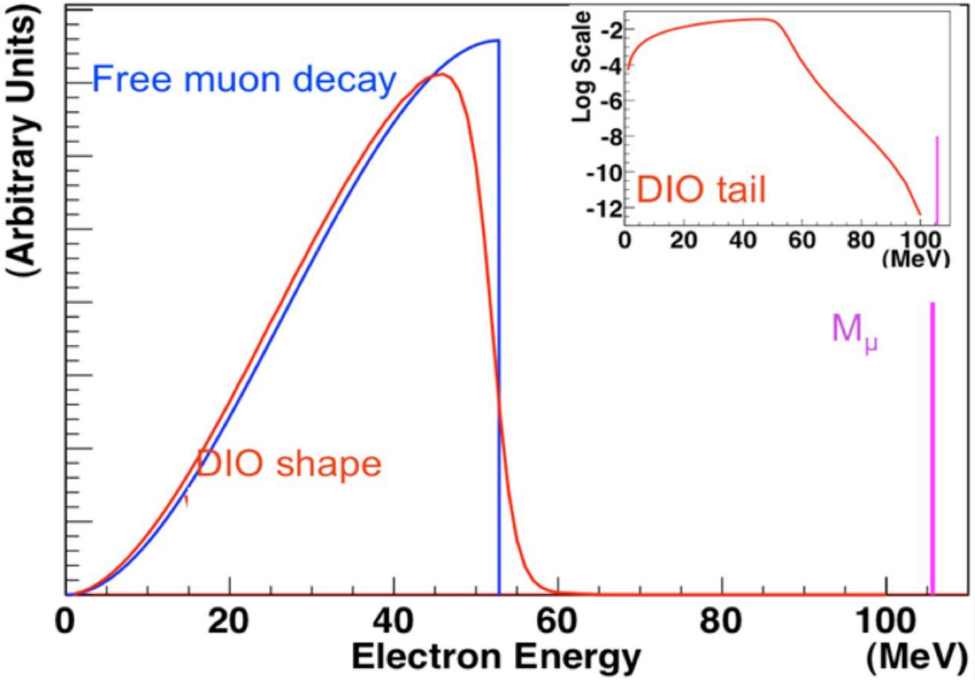
- An active muon veto counter **C0** (10 mm thickness), placed at the entrance of the target enclosure;
- Two thin (0.5 mm) pass-through counters **C1** and **C2** ;
- The actual target volume surrounded by a cup-like counter **C3** .

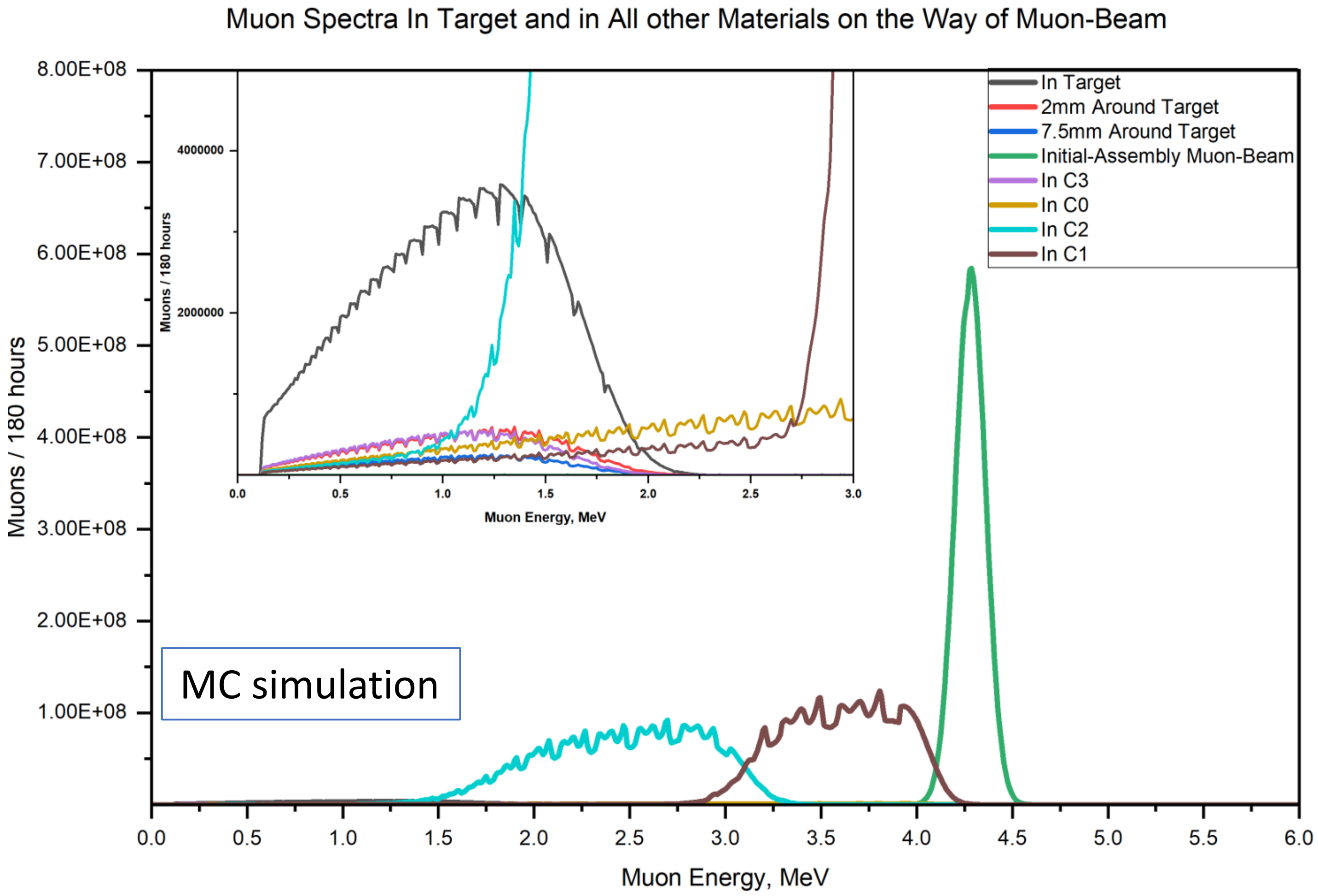
The four muon counters are defining μ-stop trigger

The stopping power for muons in C1, C2 for 1 mm thickness = 1.5 MeV

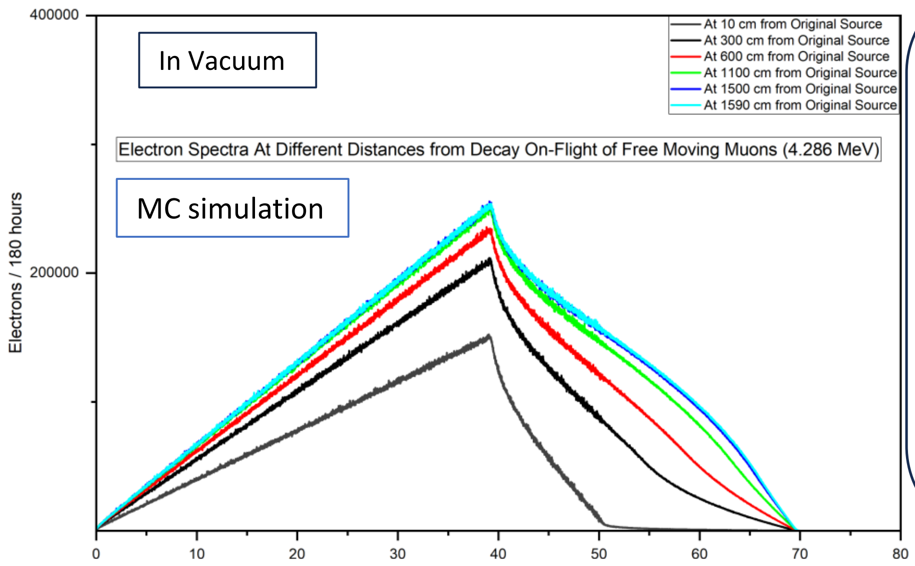








The muons decreases in numbers after **C2** by about 22% (8.1% from the free Muon Decay-on-Flight, and 13.9% lost in the materials before Target), and the muon-energy was shifted by scattering.

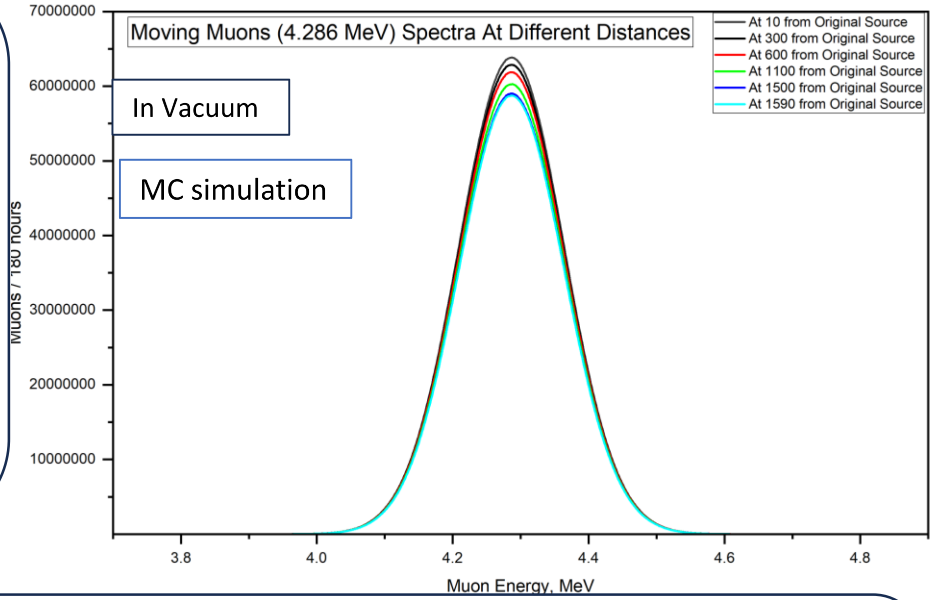


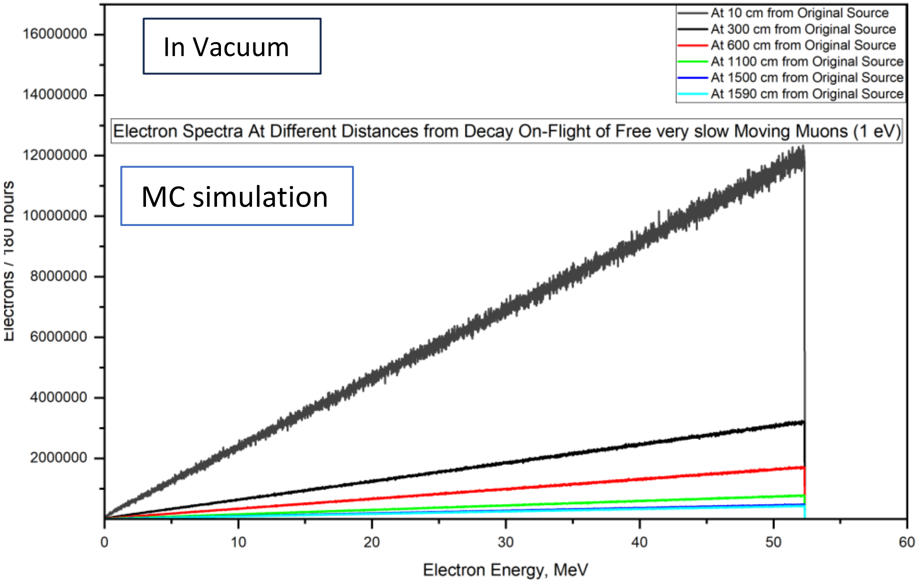
The probability a muon does **not** decay during the flight is (*Lorentz factor γ≈1.04*):

$$P_{\text{surv}} = \exp\Big(-\frac{t_{\text{flight}}}{\tau_{\text{lab}}}\Big).$$

$$P_{\text{surv}} = \exp\Big(-\frac{192.9\ \text{ns}}{2286\ \text{ns}}\Big) = \exp(-0.0844) \approx 0.9190.$$

So ≈ **91.9%** of the muons survive to the target; ≈ **8.1%** decay in flight (*In agreement with MCNP result*)





The two Electrons spectra are different for three tightly-coupled reasons: the Michel spectrum in the muon rest frame, the Lorentz boost to the lab, and the downstream, on-axis detector geometry (distance/acceptance). MCNP6 is showing all three at work:

1) Start from the same rest-frame physics For an unpolarized muon at rest, the electron energy follows the Michel spectrum the electron energy in the muon rest frame:

2) A moving muon boosts energies and collimates angles If the muon moves with β, γ the lab energy is:

$$\frac{dN}{dE_*} \propto E_*^2\left(3 - 2\frac{E_*}{E_{\max}}\right), \qquad 0 \le E_* \le E_{\max} \approx 52.83\ \text{MeV},$$

PDG "Muon Decay Parameters" (2020), Eq. 58.3

$$E = \gamma\,(E_* + \beta\, p_* \cos\theta_*),$$

Jackson Classical Electrodynamics (3rd ed.)

- **Forward endpoint (hard edge)**

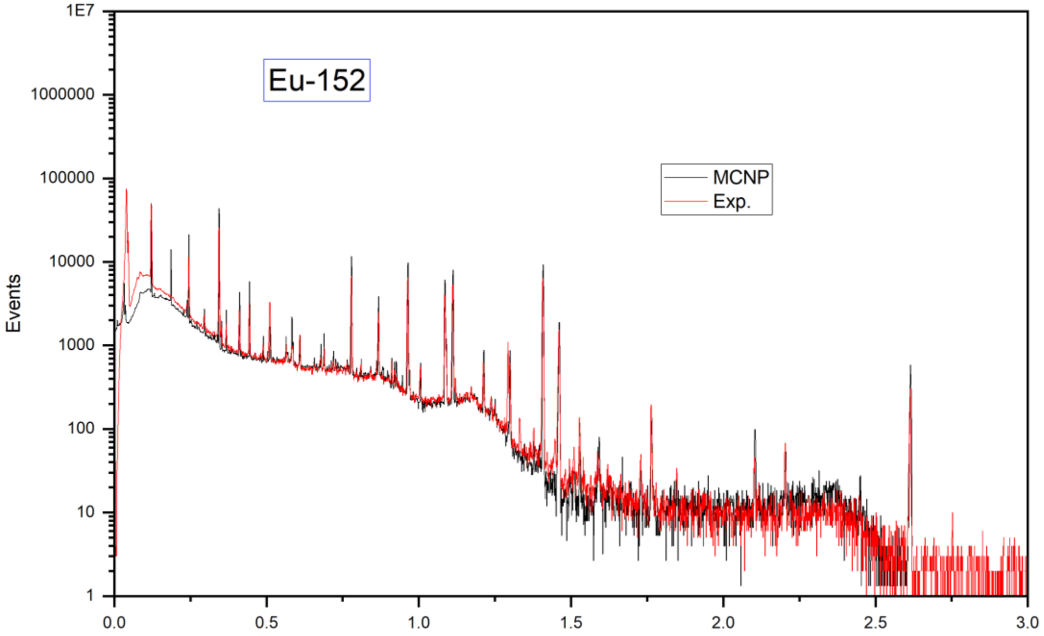
  $E^{\text{lab}}_{\max} \approx \gamma(1+\beta)E_{\max} \approx 1.0406 \times 1.2765 \times 52.83\ \text{MeV} \approx \mathbf{70\ MeV}.$

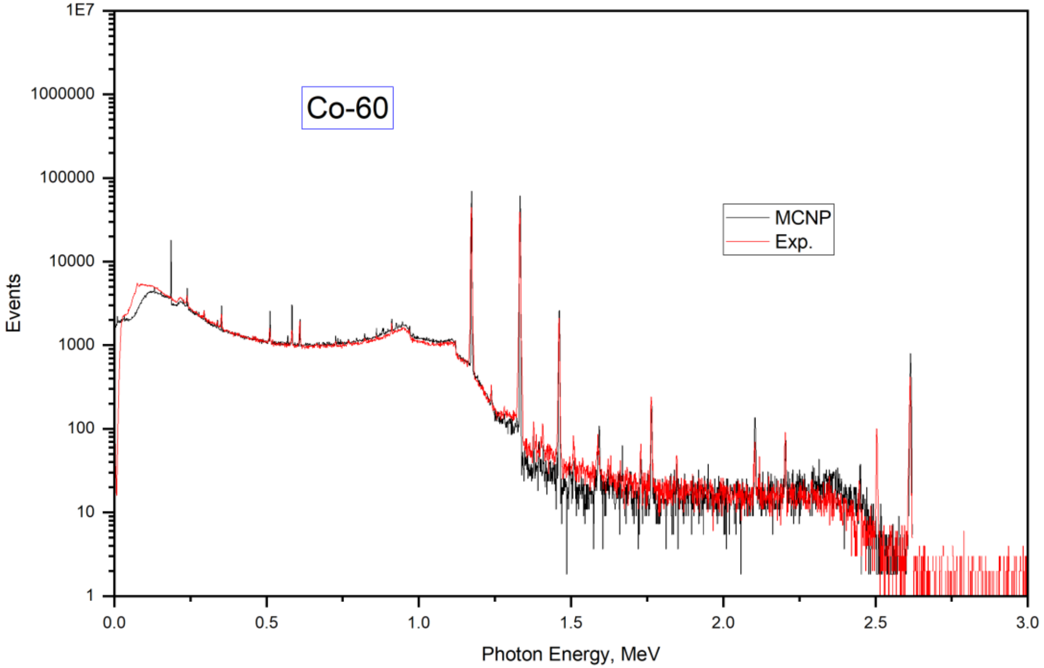
- **Soft edge for electrons that can still reach a downstream on-axis plane**

  The lowest lab energies that can hit a plane *in front* of the muon come from the *same* high-energy electrons emitted **backward** in the muon frame but still bent forward by the boost:

  $E^{\text{lab}}_{\min} \approx \gamma(1-\beta)E_{\max} \approx 1.0406 \times 0.7235 \times 52.83\ \text{MeV} \approx \mathbf{40\ MeV}.$

List of contents





Agreement: **Very close**, small deviations at low energies (<200 keV) likely due to electronic noise, detector threshold effects, or incomplete modeling of scattering in nearby structures.

What the Comparison Tells us

- **MCNP6 is accurately modeling:**
  - Detector geometry and material response.
  - Photon transport and interaction physics.
  - Energy resolution (a ***Gaussian Energy Broadening function (GEB)*** was applied).
- **Deviations mainly arise from:**
  - Detector geometry (real detector housing, Endcap distance, real value of active volume, … *maybe not accurate as shown in the detector certificate*!.
  - Pile-up and dead time in experiment not included in MCNP (***can be simulated later***)
  - Statistical fluctuations (both measurement and simulation).
  - Coincidence summing effects (very relevant for Eu-152) (***can be simulated later***).

Together, these calibration checks give confidence that MCNP6 setup can reliably model γ-ray transport and detector response, which is crucial before applying it to more complex muonic x-ray and capture studies.

List of contents

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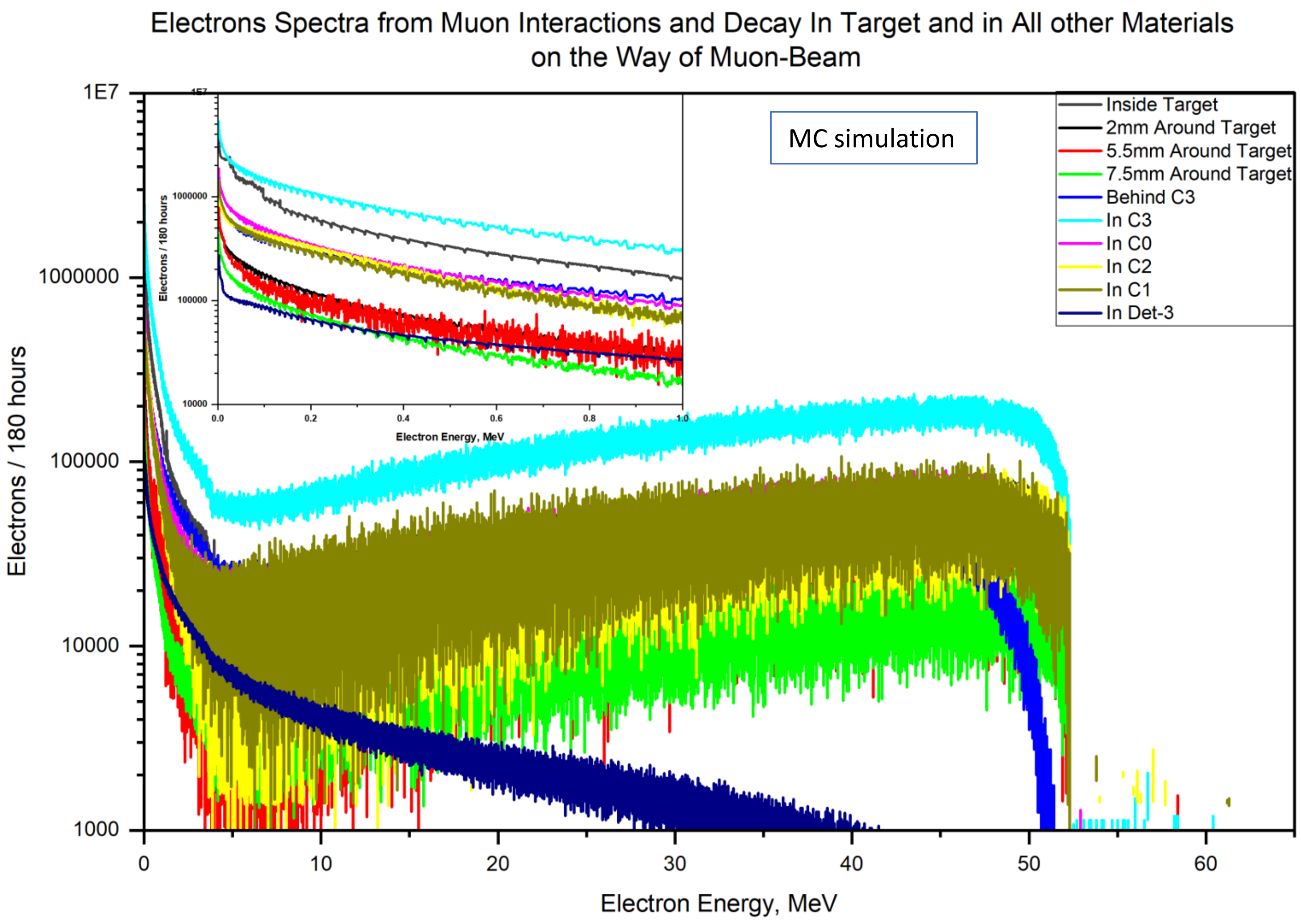
Secondary induced-particles can interact with all parts of the experiment and induce isotopes mainly important at Target and Detector, and can have considerable contributions of background.



Real physics shaping the spectra:

- inside **$BaCO_3$_Target**: decay-in-orbit (DIO) continuum up to ~52.8 MeV (slightly smeared by binding/recoil) + low-energy electrons from capture de-excitation (conversion/Auger/Compton) → the steep <1 MeV rise. in plastics/Mylar/air: mainly DIO electrons that were born or propagated there, softened by ionization losses and multiple scattering. Differences between “In target / around target / C0-C3 / behind C3 / detector” are just how many μ^- stop/decay in each place and how those electrons survive to the tally plane.

Code/transport texture on top of that (the little teeth/ripples):

- MCNP6 uses condensed-history charged-particle transport. When the step size and soft–hard split (production cut for δ-rays) change with energy, one can get small, quasi-periodic notches in finely binned spectra. Those aren’t cross-section resonances; they’re numerical/acceptance aliasing and will diminish if we tighten transport parameters or widen bins slightly.

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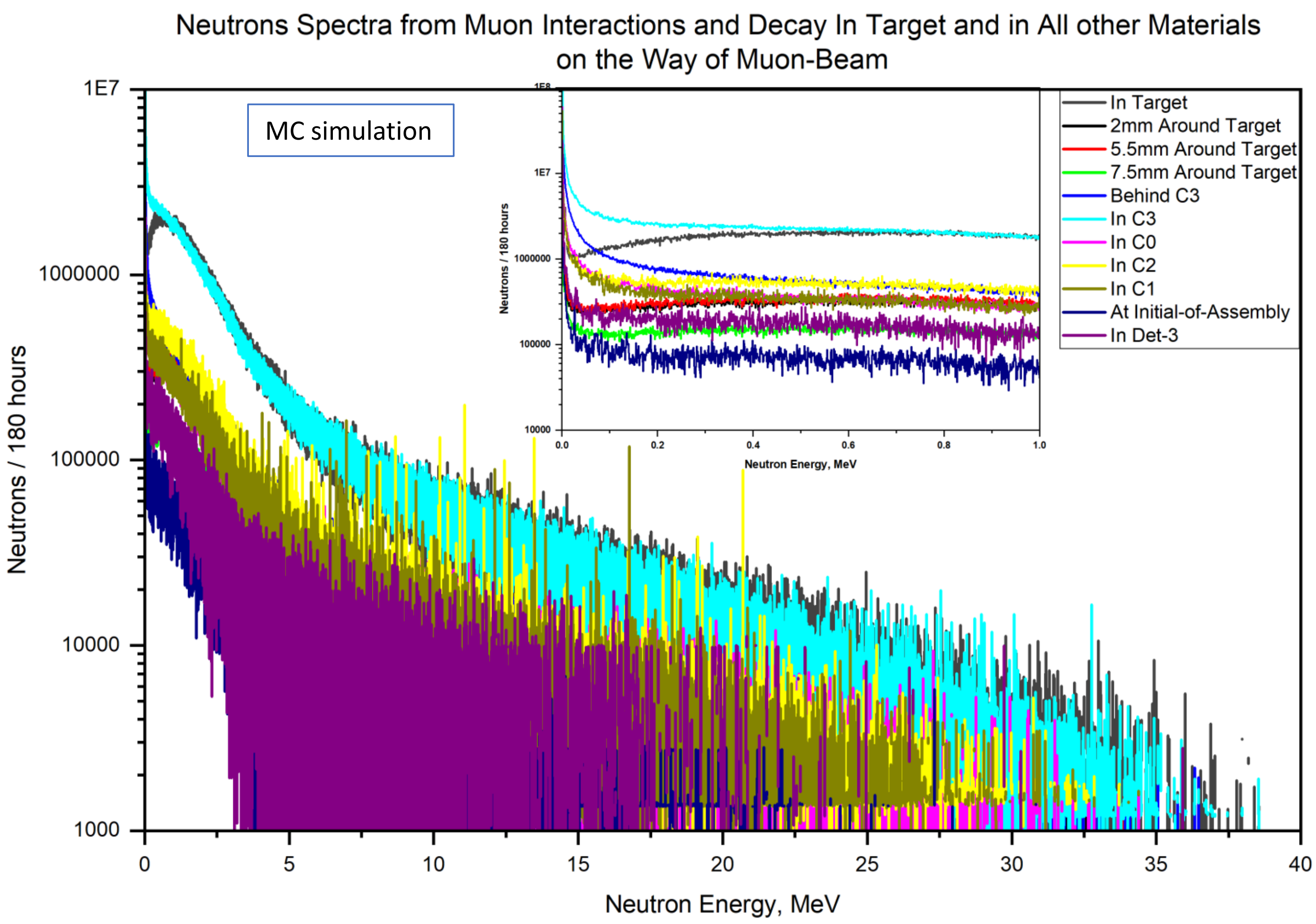


Physics mechanisms producing neutrons from stopped μ^-

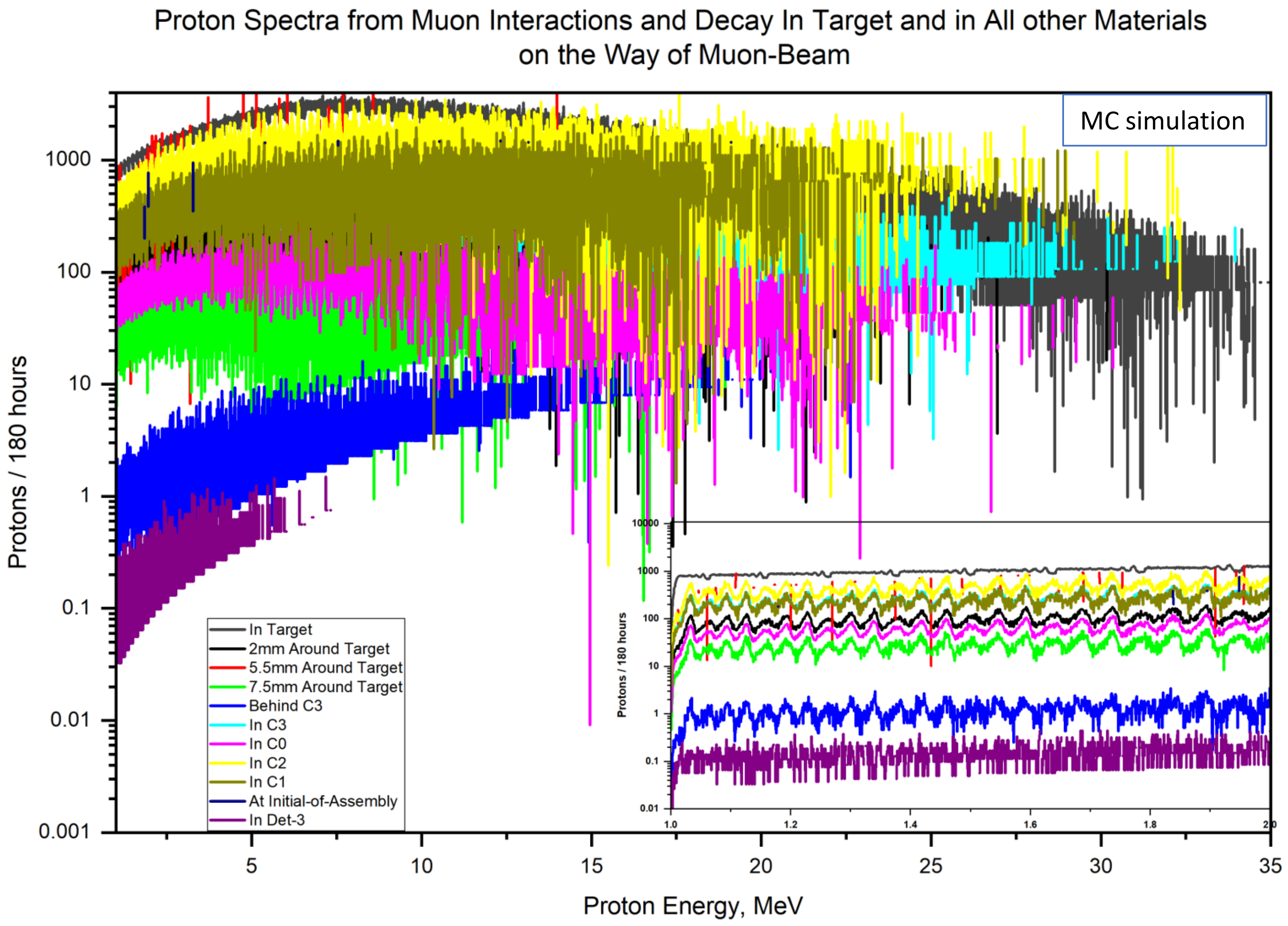
1. Muon nuclear capture (dominant in heavy nuclei like Ba): Reaction: $\mu^- + (A,Z) \rightarrow \nu_\mu + (A,Z-1)^*$. The daughter nucleus is highly excited (~15–20 MeV typical excitation energy). De-excitation occurs by emission of neutrons, protons, deuterons, alphas, and γ's, but neutrons dominate because they are uncharged and have the lowest emission barrier. This is the main source of the broad continuum we see from ~1 MeV up to ~30–40 MeV.

2. Muon-induced fission-like or pre-equilibrium processes (less likely in Ba but possible): The nuclear excitation can also lead to multi-nucleon emission (2n, np, etc.), which broadens the high-energy neutron tail.

3. Muon decay in orbit (DIO): Normally produces only an electron and neutrinos, not neutrons. But the electron can induce bremsstrahlung → low-energy neutrons. Contribution is small compared to capture, but sub-MeV neutrons can partly come from this secondary channel.

4. Secondary reactions in other materials (C0, C1, Mylar, etc.): Fast neutrons emitted in the target can scatter and degrade in surrounding materials. We'll see this as flattened, softer distributions in "around target / behind C3 / detector" curves.

Secondary induced-particles can interact with all parts of the experiment and induce isotopes mainly important at Target and Detector, and can have considerable contributions of background.



Origins of protons from muon interactions:

When a negative muon stops in matter and reaches the **1s-orbit**, two main processes happen:

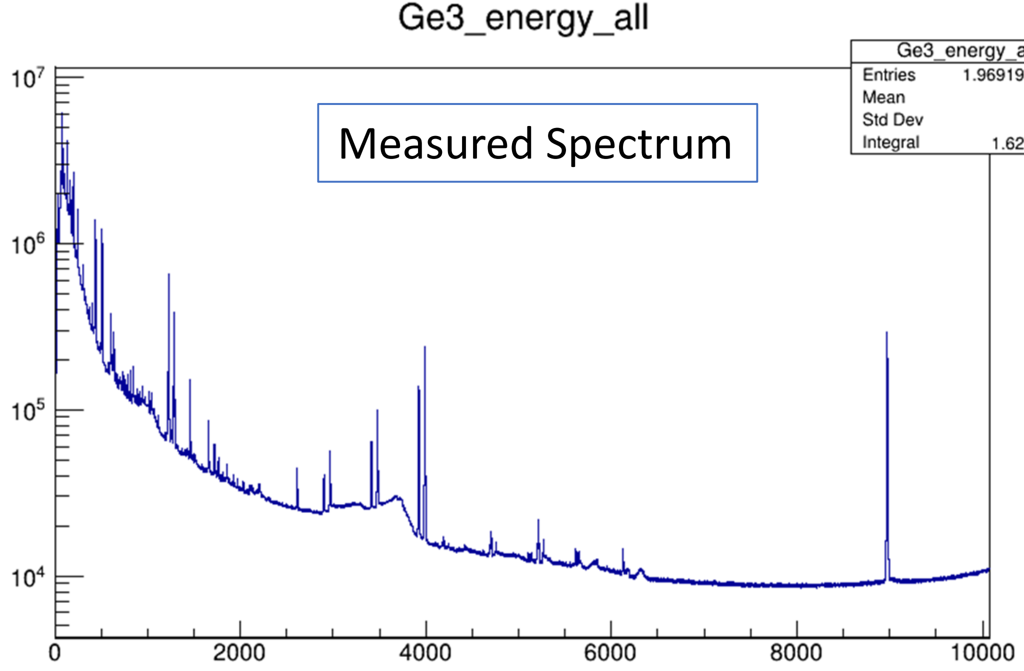
Muon Decay in Orbit (DIO):

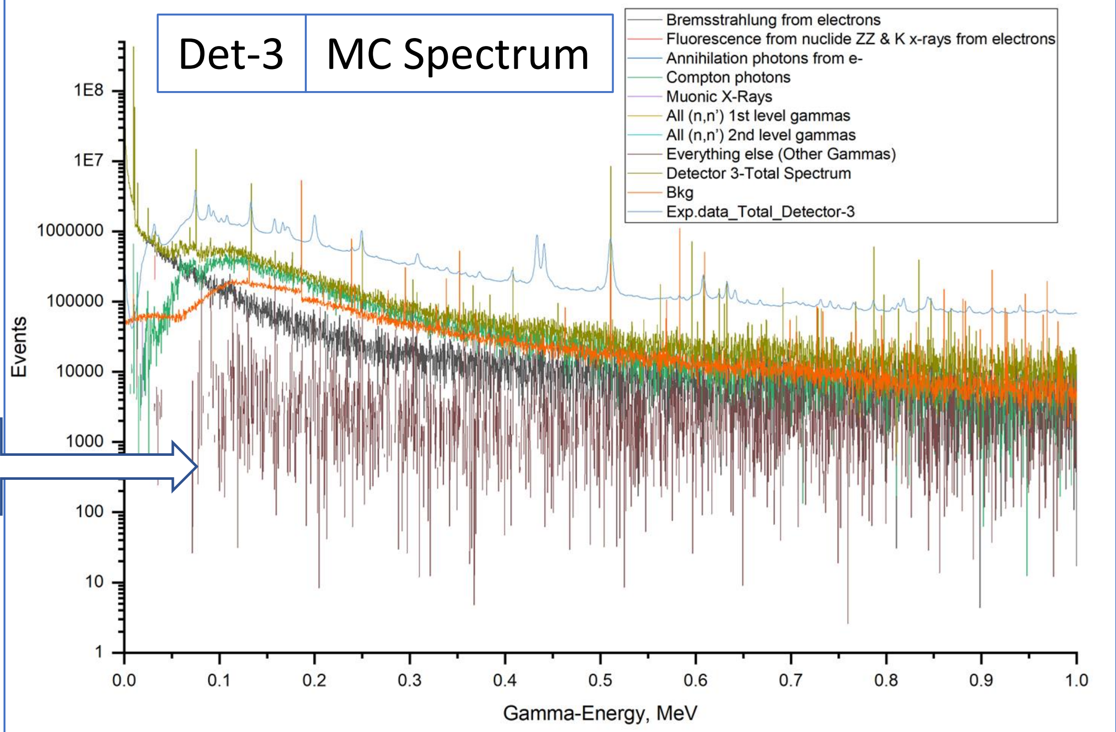
$\mu^- \rightarrow e^- + \bar{\nu}_e + \nu_\mu$ This process does not directly produce protons. But the energetic decay electron can induce secondary ionization, delta-rays, or knock-on protons in light materials (like C, O, Mylar). Contribution: small, low-energy protons (a few MeV max).

Muon Nuclear Capture (dominant in Ba):

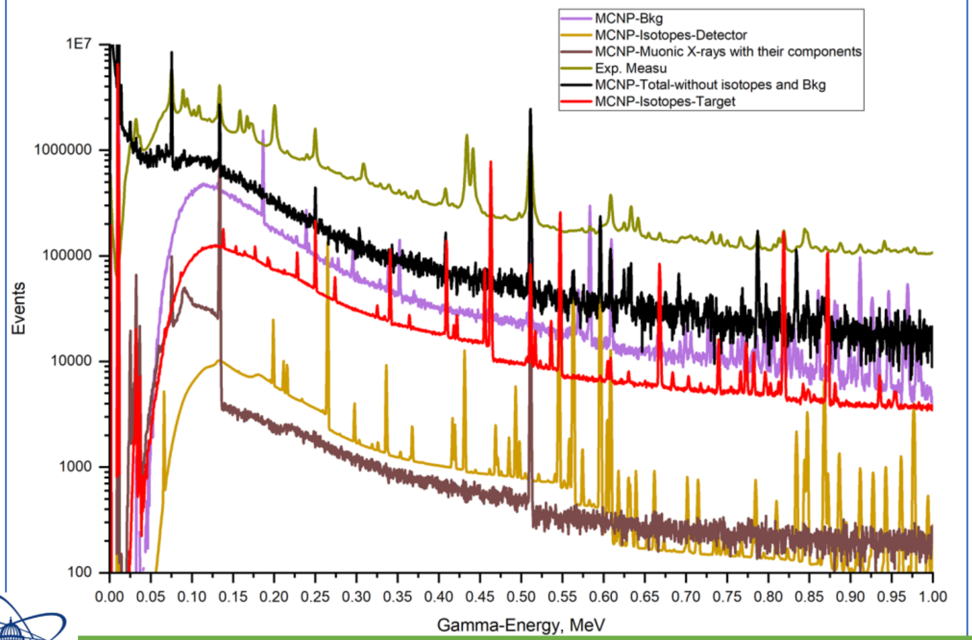
$\mu^- + p \rightarrow n + \nu_\mu$ Converts a proton in the nucleus into a neutron. The residual nucleus is left highly excited, often above particle emission threshold. It then de-excites by emitting: Neutrons (dominant, as you saw in your neutron spectrum), Protons, Deuterons, tritons, alphas, gammas (smaller fractions). These emitted protons are called muon-induced nuclear evaporation products.

List of contents





More Statistics needed, more time



The MCNP events: In the Energy Range [0, 10 MeV]

MC spectrum events = 1.21 x 10^9

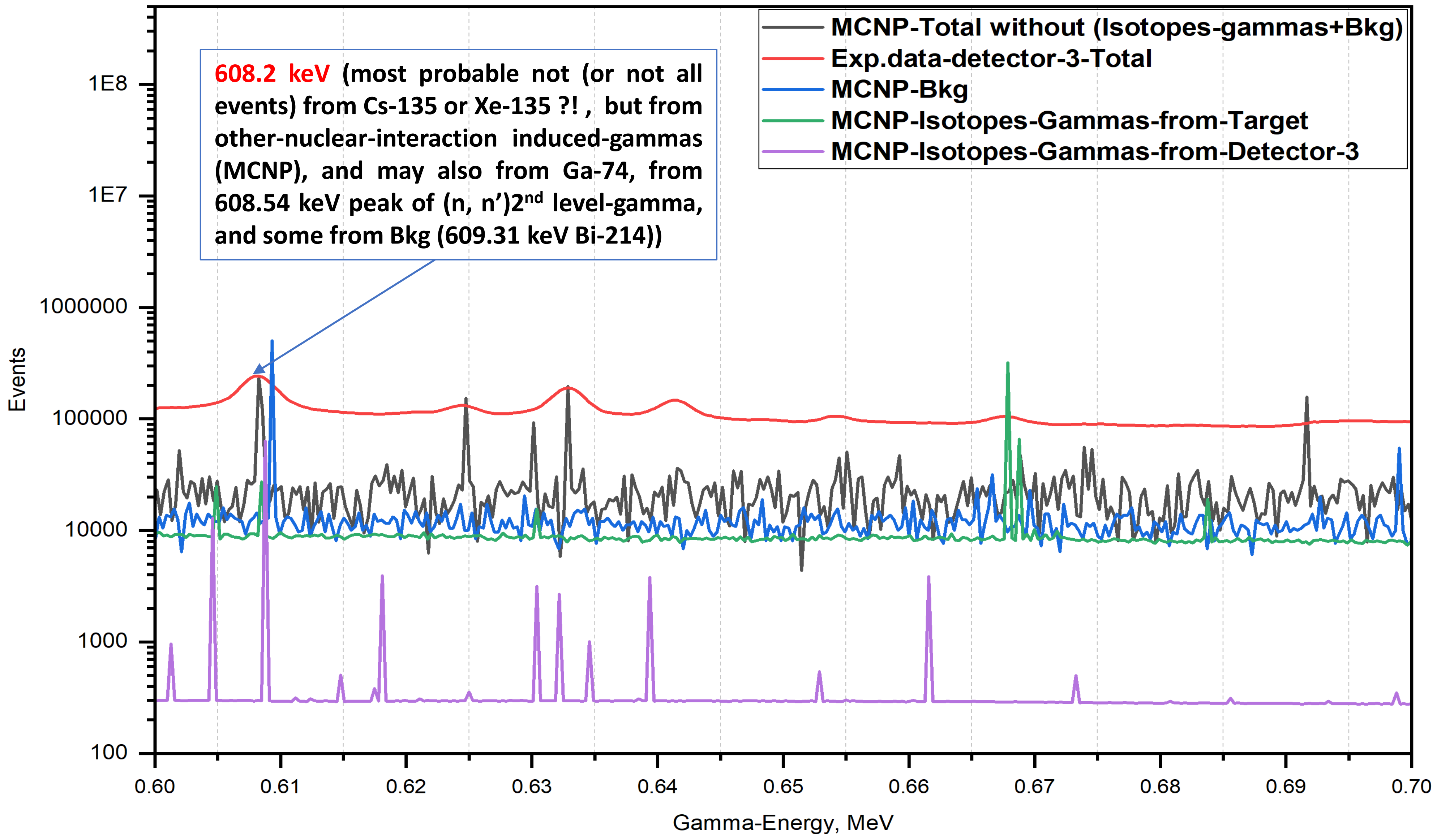
MC Natural Background events = 1.04 x 10^8

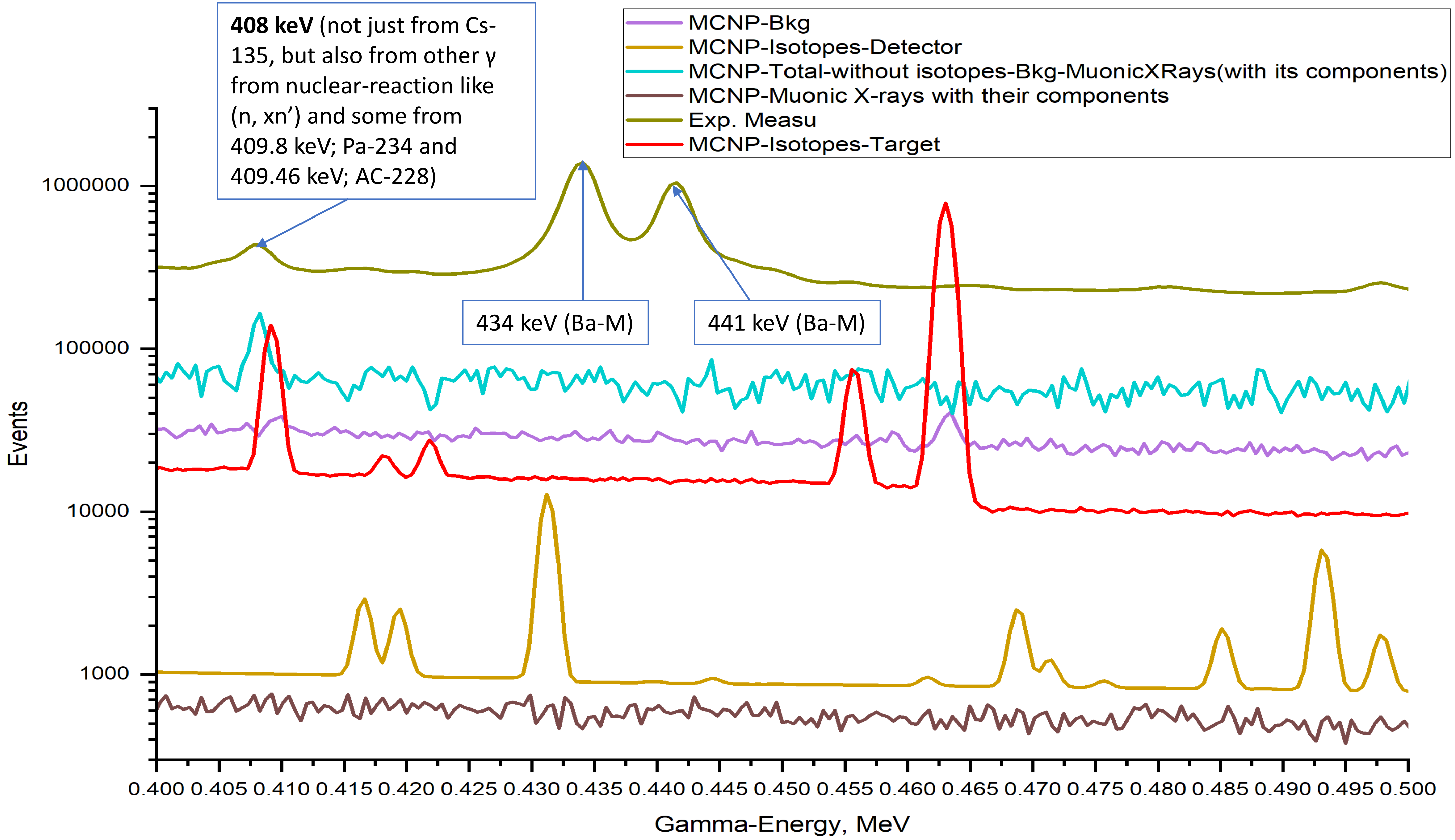
MC Induced Background events = 3.18 x 10^8

(*not included in the spectrum*)

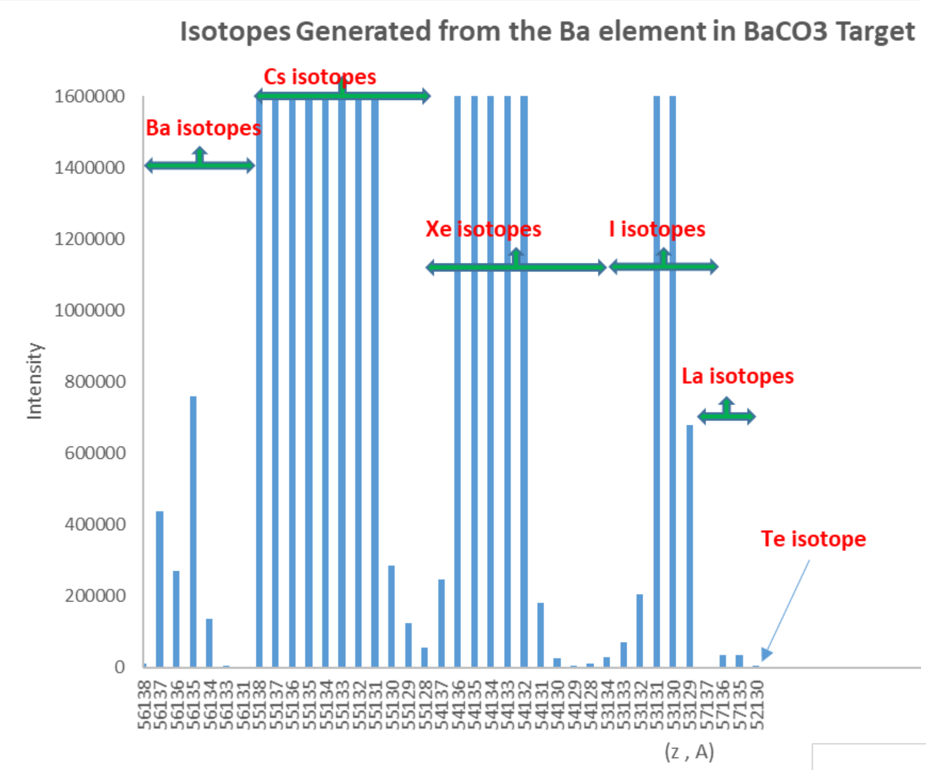
MC Sum Events (180 hours) = **1.632 x 10^9**

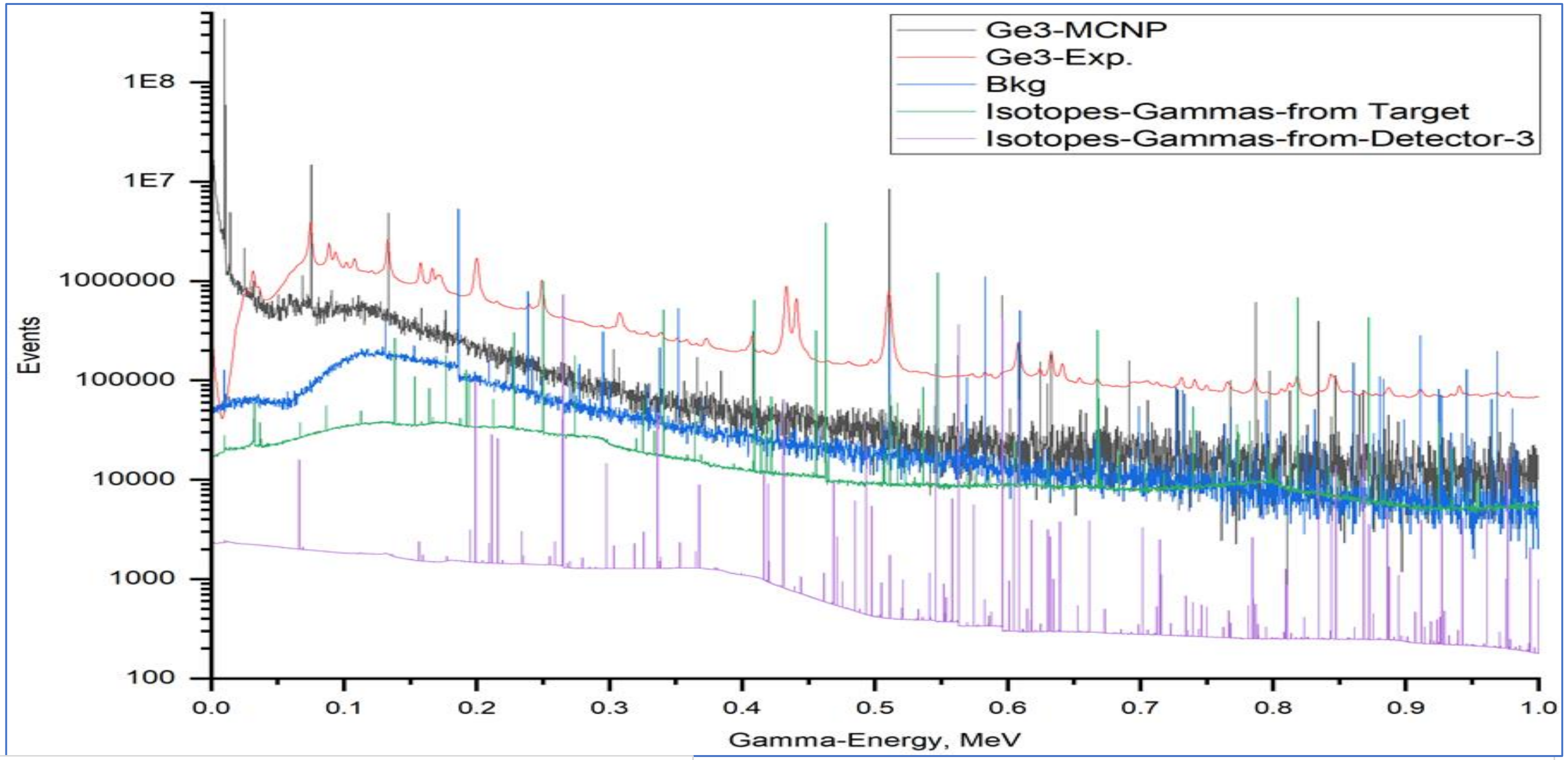
Exp. Events (180 hours) = **1.627 x 10^9**

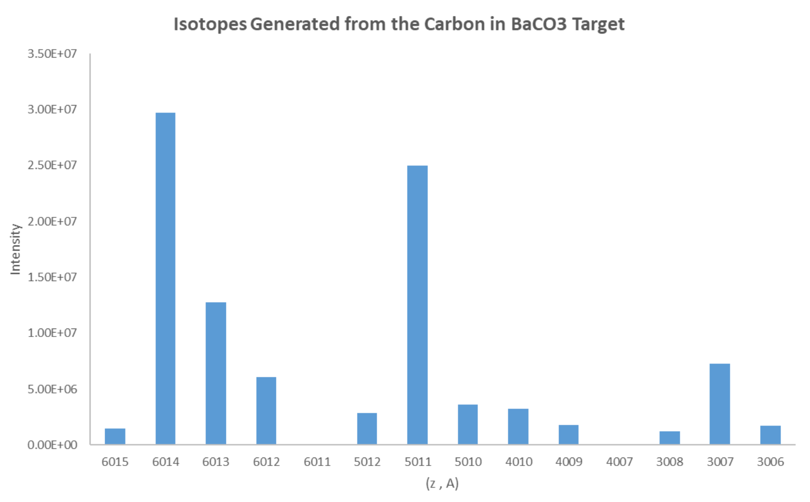

608.2 keV (most probable not (or not all events) from Cs-135 or Xe-135 ?! , but from other-nuclear-interaction induced-gammas (MCNP), and may also from Ga-74, from 608.54 keV peak of (n, n')2nd level-gamma, and some from Bkg (609.31 keV Bi-214))
MCNP-Total without (Isotopes-gammas+Bkg)
Exp.data-detector-3-Total
MCNP-Bkg
MCNP-Isotopes-Gammas-from-Target
MCNP-Isotopes-Gammas-from-Detector-3
Events
1E8
1E7
1000000
100000
10000
1000
100
0.60
0.61
0.62
0.63
0.64
0.65
0.66
0.67
0.68
0.69
0.70
Gamma-Energy, MeV

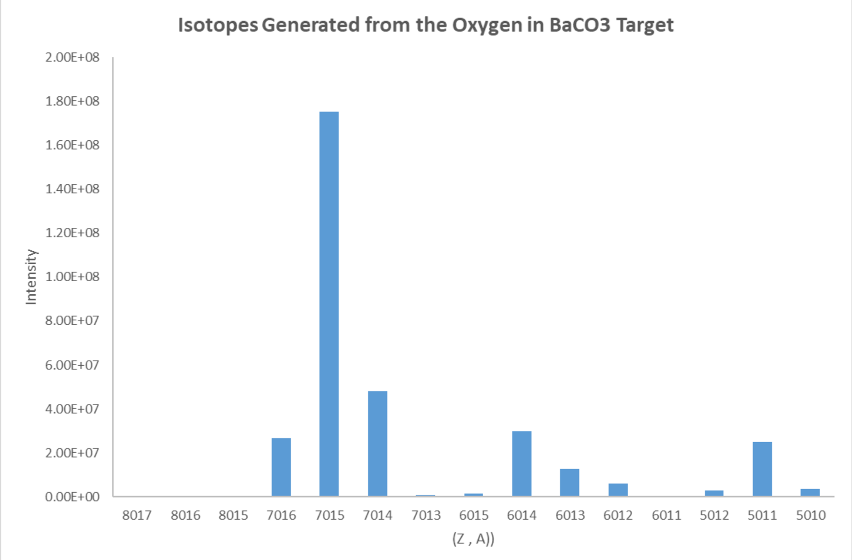

408 keV (not just from Cs-135, but also from other γ from nuclear-reaction like (n, xn') and some from 409.8 keV; Pa-234 and 409.46 keV; AC-228)
MCNP-Bkg
MCNP-Isotopes-Detector
MCNP-Total-without isotopes-Bkg-MuonicXRays(with its components)
MCNP-Muonic X-rays with their components
Exp. Measu
MCNP-Isotopes-Target
434 keV (Ba-M)
441 keV (Ba-M)
1000000
100000
10000
1000
Events
0.400 0.405 0.410 0.415 0.420 0.425 0.430 0.435 0.440 0.445 0.450 0.455 0.460 0.465 0.470 0.475 0.480 0.485 0.490 0.495 0.500
Gamma-Energy, MeV

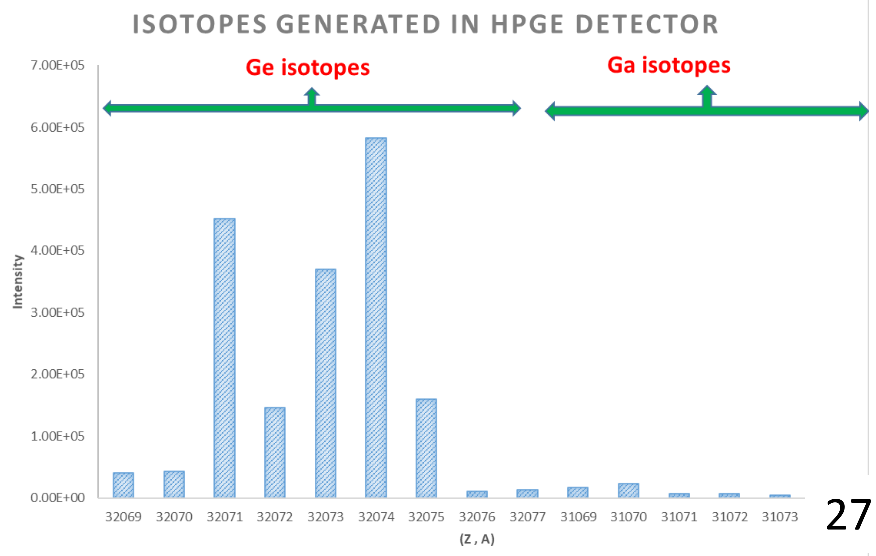
MC simulations of the Isotopes Productions



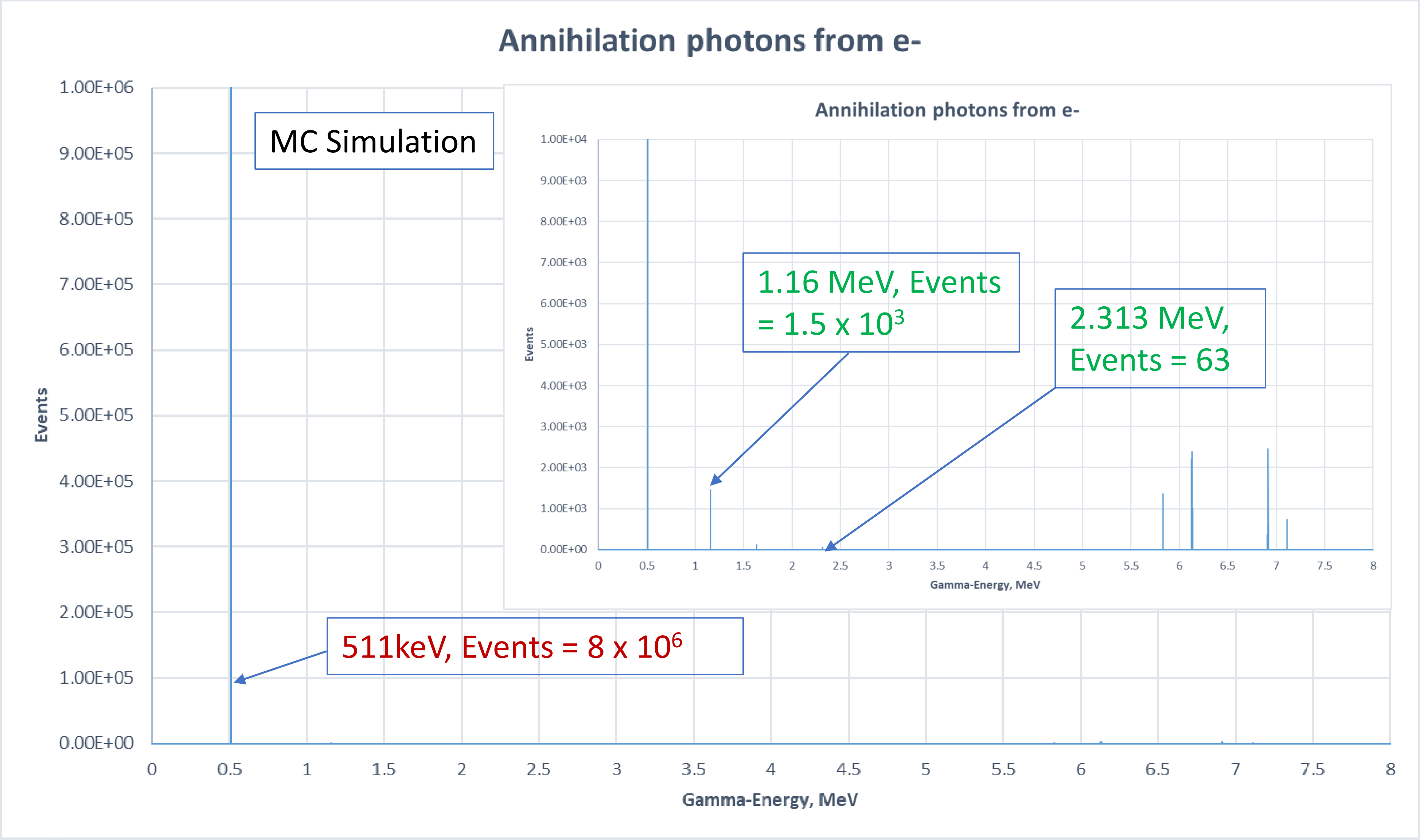








Example of from where some (unexpected !) Gamma-Peaks !



High-energy Michel electrons from muon decay (up to 53 MeV) produce bremsstrahlung photons, some exceeding 11 MeV, leading to pair production.

Positrons with kinetic energies around 5-10 MeV can annihilate, producing photons up to 6-7 MeV.

MCNP6 can simulate this chain:

1- Muon decay to electrons.
2- Bremsstrahlung photon emission.
3- Pair production.
4- Two-photon annihilation with boosted energies.

List of contents

- Short Theoretical introduction.
- Advantages of using Monte-Carlo codes like MCNP6.
- Steps for Monte-Carlo Simulations.
- MONUMENT experiment and Muon-Beam Profile.
- Monte-Carlo Simulation of MONUMENT experiment.
- Simulations of the Calibration Sources.
- Simulations of the Induced Secondary Particles.
- Separating Spectrum into its Components and Isotopes Production.
- **More for Near Future.**

More for Near-Future:

- **Allow more physics and MCNP6 tallies to be incorporated into pulses:**
  - All previous and on-going simulations are Time-independent, and it is very important to do the simulations with **Time-Dependent**, which is available in MCNP6 code: Time binning; Time Triggering.
  - Coincidence/Anti-Coincidence between many detectors.
  - **Coincidence-Summing** Peaks.
  - **Delayed particles** production.
  - Detailed exploring muonic X-ray production – **MUON/RURP codes** included with MCNP6 code.
  - Nuclear resonance fluorescence.
  - Micro/macro beam pulse option – nesting of time distributions provides accurate beam modeling.
  - ROC curve tally option – generates **ROC** (Receiver Operator Characteristic) curves from signal & noise tallies using batches of samples.
  - The possibility of optimizing the **Beam-profile** and **Target** to get the same gamma-intensities with less secondary particles which decrease the background, and maybe also with less Target-material used in the experiments and therefor decreasing the costs !.
- Start doing simulations for other Targets: **Mo-100, Se-76, Ti-48** …

THANK YOU FOR YOUR ATTENTION

Q & A