

ISAPP School 2024 · KIT / Bad Liebenzell

GEANT4 Simulations for Rare Event Searches

Holger Kluck · HEPHY · holger.kluck@oeaw.ac.at

3/3: Radioactive Backgrounds
for Shallow Sites (e.g. reactor based neutrino experiments)
and Deep Underground Experiments (e.g. Dark Matter Searches)

Background Sources

Background sources: sources of primary particles in the MC simulation

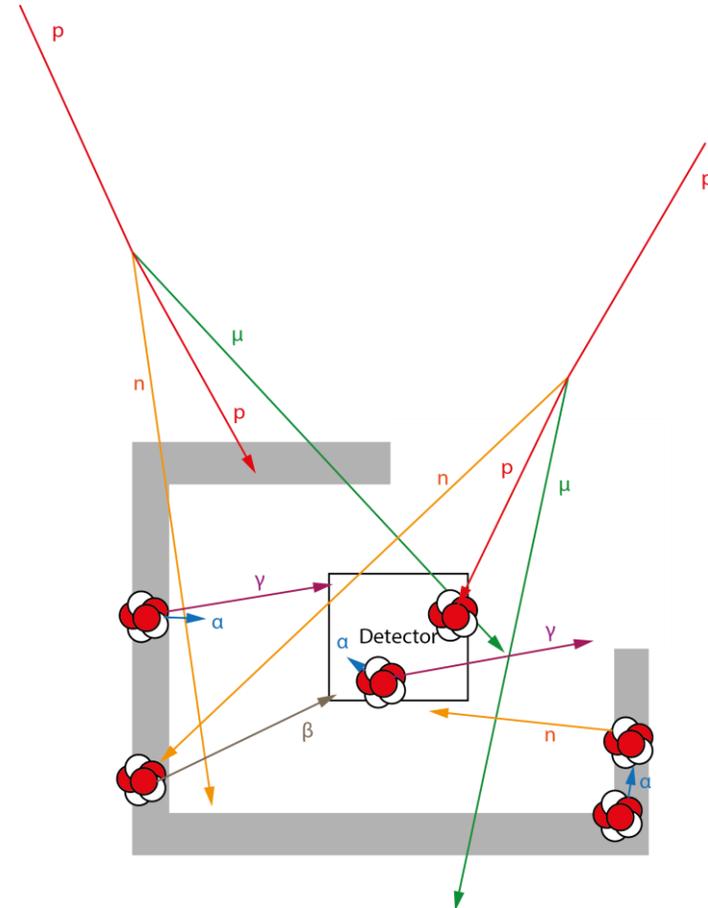
- **Cosmogenic background**

- Primary cosmic rays (p, $^A X$) on surface
- Secondary cosmic rays (n, μ) produced by nuclear spallation in the atmosphere
- Radioactive activation / transmutation of elements by cosmic rays

- **Radiogenic background** caused by natural radioactivity

- EM background (α , β , γ) from
 - Natural radioactive decay chains (^{232}Th , ^{235}U , ^{238}U)
 - Other natural radionuclides, e.g. ^{40}K
 - Anthropogenic radionuclides, e.g. ^{90}Sr , ^{137}Cs
- Neutron background from
 - (α, n) reactions on e.g. ^{14}N
 - Spontaneous fission of e.g. ^{238}U
 - μ -induced spallation of high-Z nuclides*

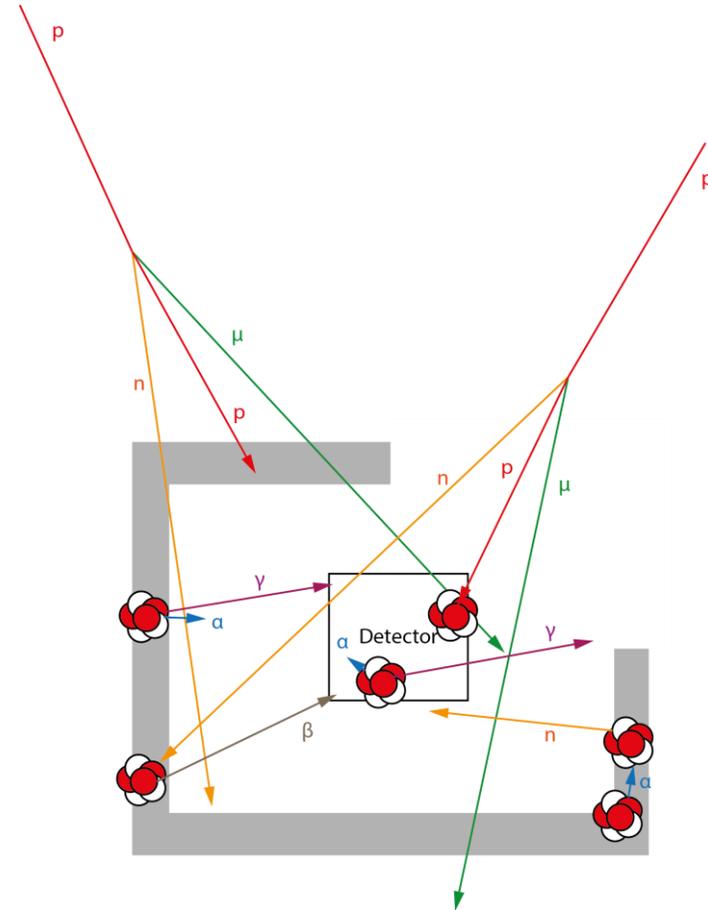
*Nuclide: any type of atomic nucleus $^A_Z X$



Background Sources

Background sources: sources of primary particles in the MC simulation

- **Cosmogenic background**
 - dominant at **shallow sites**,
e.g. neutrino experiments at nuclear reactors
- **Radiogenic background** caused by natural radioactivity
 - dominant at **deep underground sites**
e.g. direct Dark Matter searches



***Nuclide**: any type of atomic nucleus ${}_Z^AX$

Background Mitigation

External (ambient) background

= originate outside of the detector

- Can be **shielded** by placing an absorber between background source and detector
- May be actively rejected by operating an auxiliary detector (= **veto**, tuned to the background) in anti-coincidence with the main detector
- Only **long-range** background radiation is detectable: γ , n , μ , energetic β

Internal background

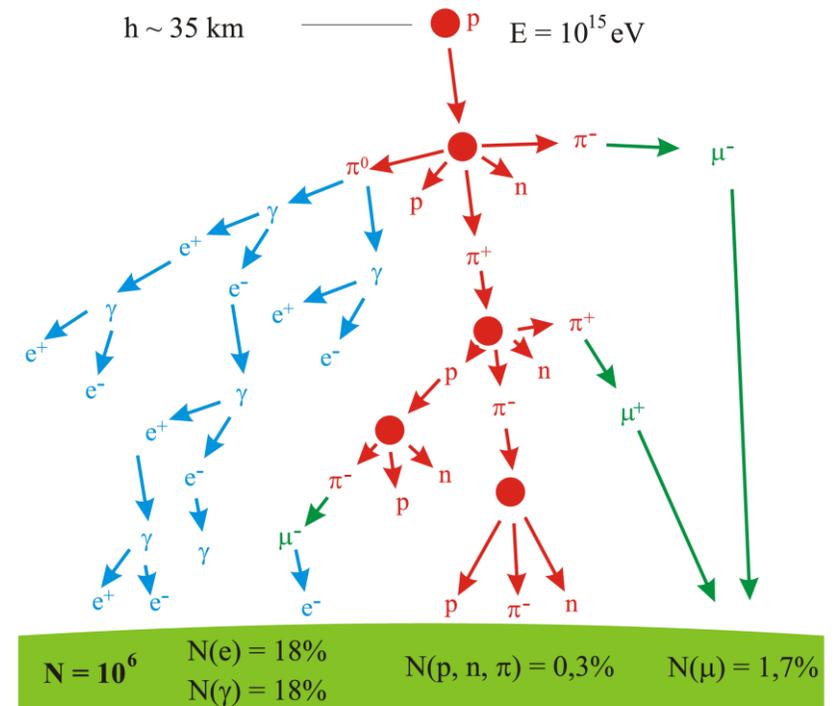
= originate inside the detector

- Can not be shielded
- Select building materials with low radioactive contamination (= high **radiopurity**) during so-called *assay* or *screening* measurement
- Radiochemical purification of the building materials may be needed
- Also **short-range** background radiation is detectable: α , low-energy β

Prompt Cosmogenic Background

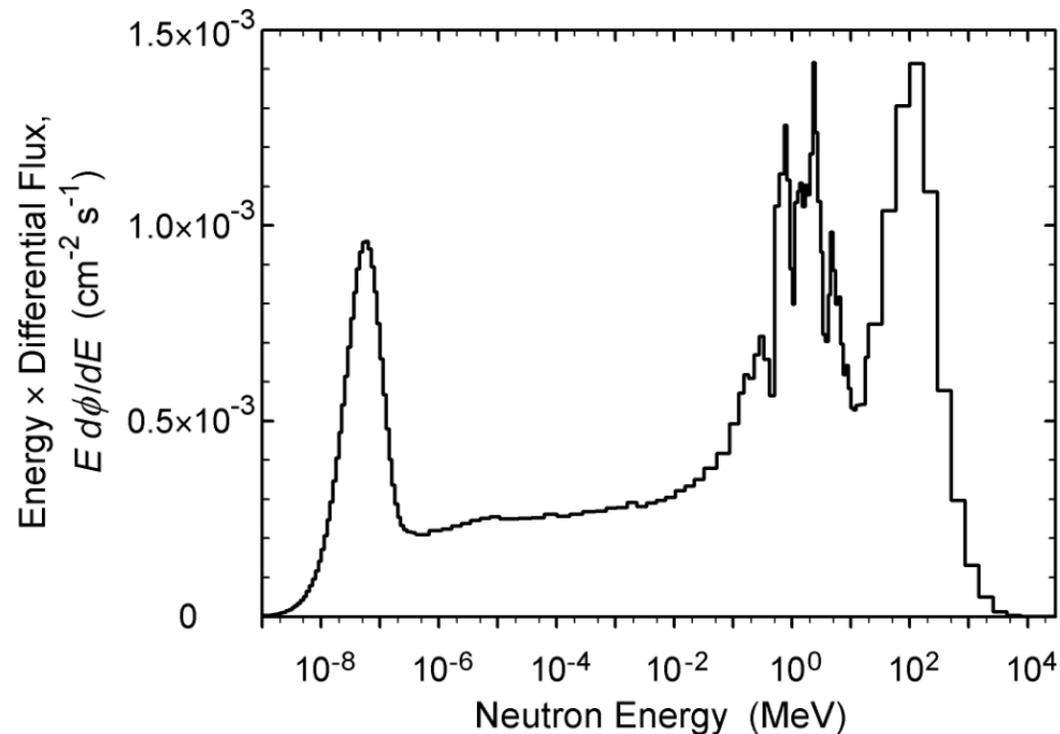
Primary and secondary cosmic rays can be

- Simulated from first principle with dedicated codes, e.g. [CORSIKA](#)
- Sampled from parameterisations of measured fluxes of secondary particles, e.g. [\[T. K. Gaisser, 2016\]](#) for muons
→ **feed into Primary Particle Generators in Geant4**
- Use existing Primary Particle Generators like [CRY](#) or develop your own, e.g. [\[H. Kluck, 2013\]](#).



[Mpfiz via wikipedia]

Atmospheric Neutrons



- At ground, **atmospheric neutrons** can reach up to ~ 10 GeV
- Thermal neutrons at ~ 10 meV
- Actual spectrum depends on atmospheric conditions, and hence on the location:

← IBM T. J. Watson Research Center in Yorktown Heights, NY

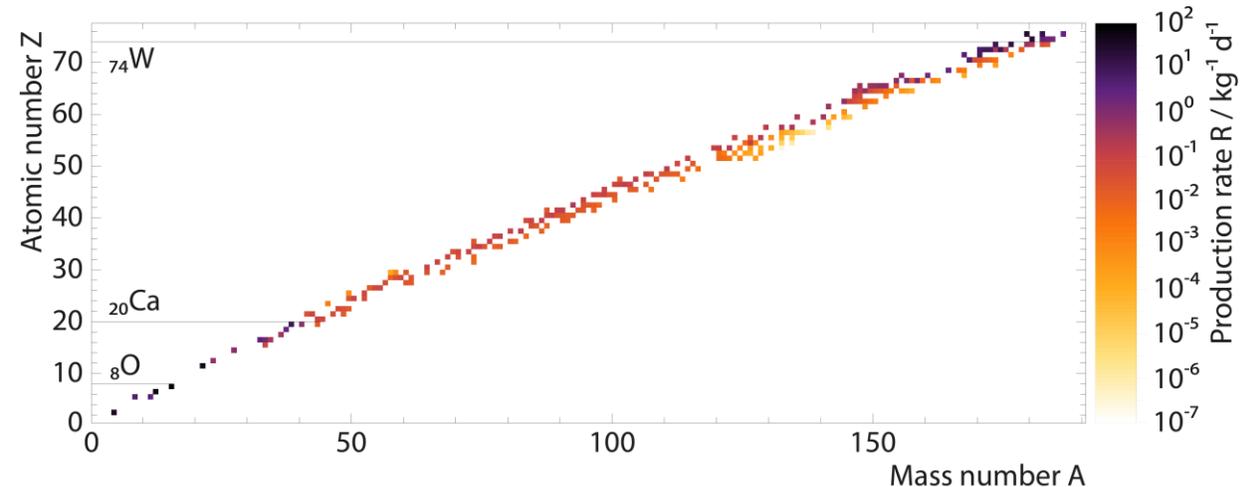
[[M. S. Gordon et al., IEEE Trans. Nucl. Sci., 51.6 \(2004\) 3427-3434](#)]

Cosmogenic Activation

Activation of materials due to **production of radionuclides via atmospheric n** (and to a lesser extent due to μ) can be

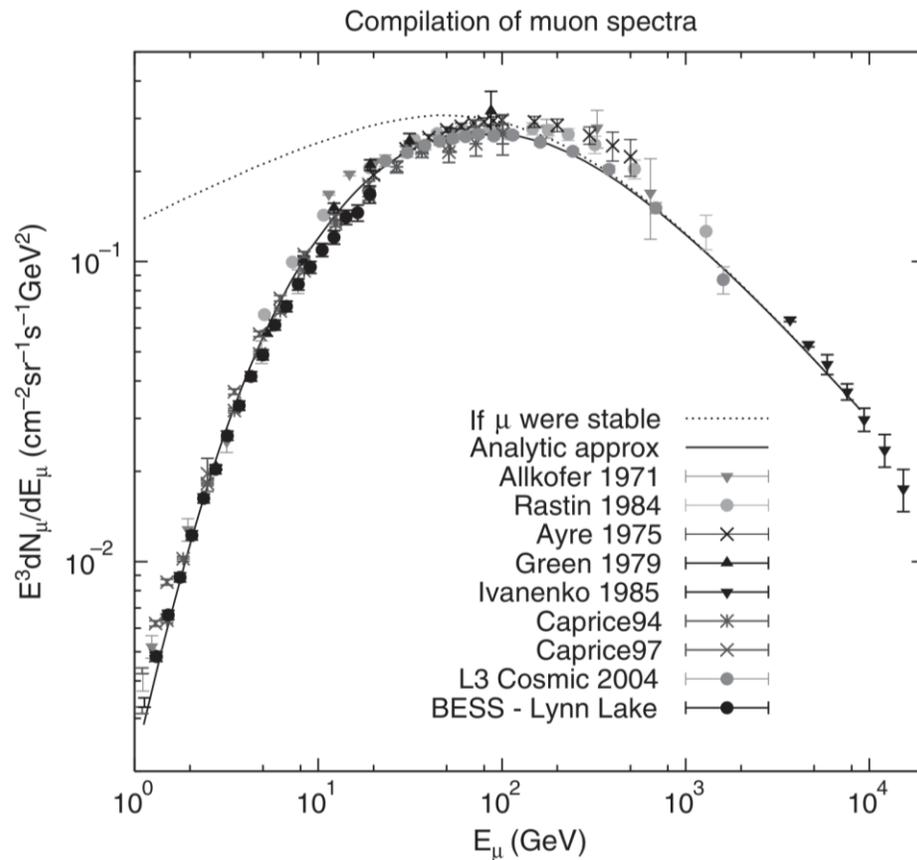
- Directly simulated in Geant4 via [ParticleHP](#) physics
- **Simulate only the decay** of the radionuclides in Geant4; **scale the decay spectra** with the production rates calculated with external, specialized tools ([TALYS](#), [ACTIVIA](#))
- Decay is delayed w.r.t. the prompt cosmic rays

Cosmogenic activation in CaWO_4 calculated with ACTIVIA



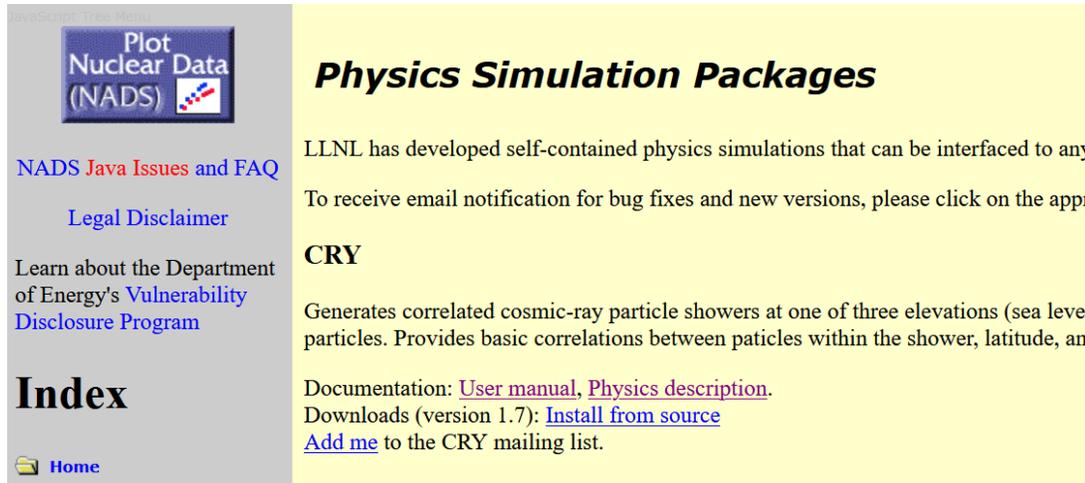
[[H. Kluck et al., J. Phys.: Conf. Ser. 2156 \(2021\) 012227](#)]

Atmospheric Muons



- At ground, **atmospheric muons** can reach up to >10 TeV
- Low energy part $\sim <10$ GeV is affected by:
 - Atmospheric condition
 - Geomagnetism
 - Solar activity
- Spectrum can be described by Gaisser's parametrisation

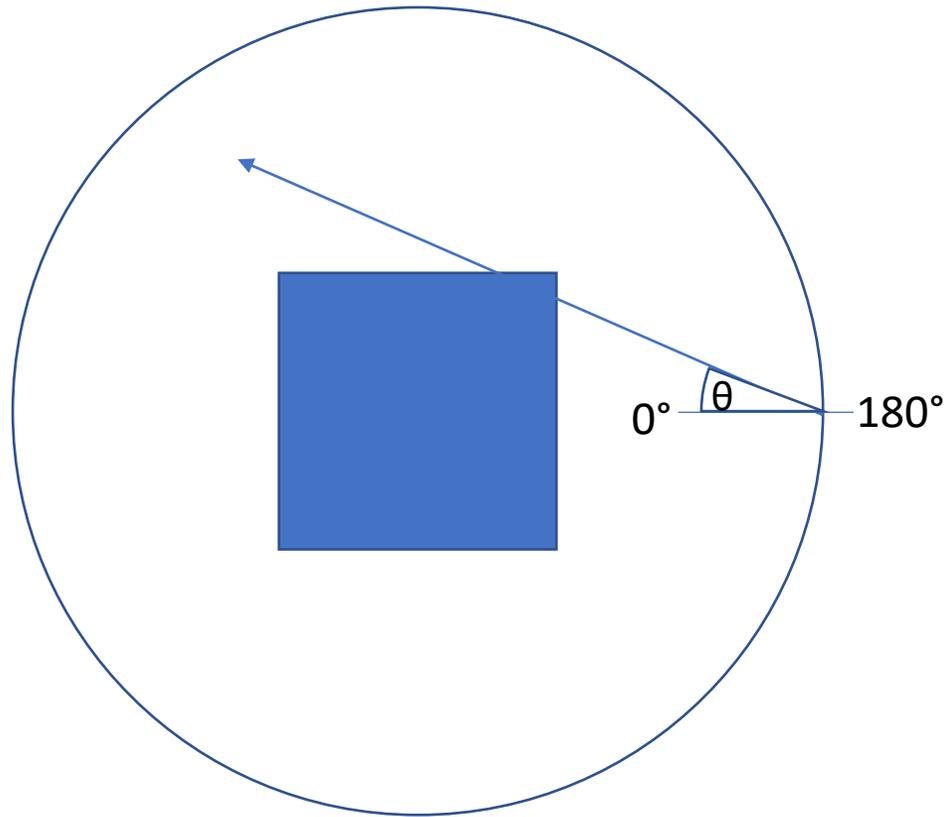
CRY



The screenshot shows the CRY website interface. On the left, there is a sidebar with a logo for 'Plot Nuclear Data (NADS)' and several links: 'NADS Java Issues and FAQ', 'Legal Disclaimer', 'Learn about the Department of Energy's Vulnerability Disclosure Program', 'Index', and 'Home'. The main content area has a yellow background and is titled 'Physics Simulation Packages'. It contains text about LLNL's self-contained physics simulations, a link to 'CRY', and documentation links for the 'User manual' and 'Physics description'. It also provides download instructions for version 1.7 and a link to 'Add me' to the mailing list.

- Geant4 has no built-in particle generator for atmospheric n/μ
- In **this lecture**, we will assume initial spectrum is flat and **use GPS**
- For more realistic spectrum: [CRY](#)
- Advantages:
 - Easy to include (next slide)
 - Full shower, i.e. several primaries per event
 - μ , n , p , e^- , e^+ , pions
- Disadvantages:
 - No overburden
 - Only three altitudes
- Only option for even more details: self-developed code

Using GPS for Atmospheric Particles



- Shooting `<particle>` with `<energy>` from a sphere of `<radius>` inwards on a volume

```
/gps/pos/type Surface
```

```
/gps/pos/shape Sphere
```

```
/gps/pos/radius <radius>
```

```
/gps/pos/centre 0. 0. 0. mm
```

```
/gps/particle <particle>
```

```
/gps/energy <energy>
```

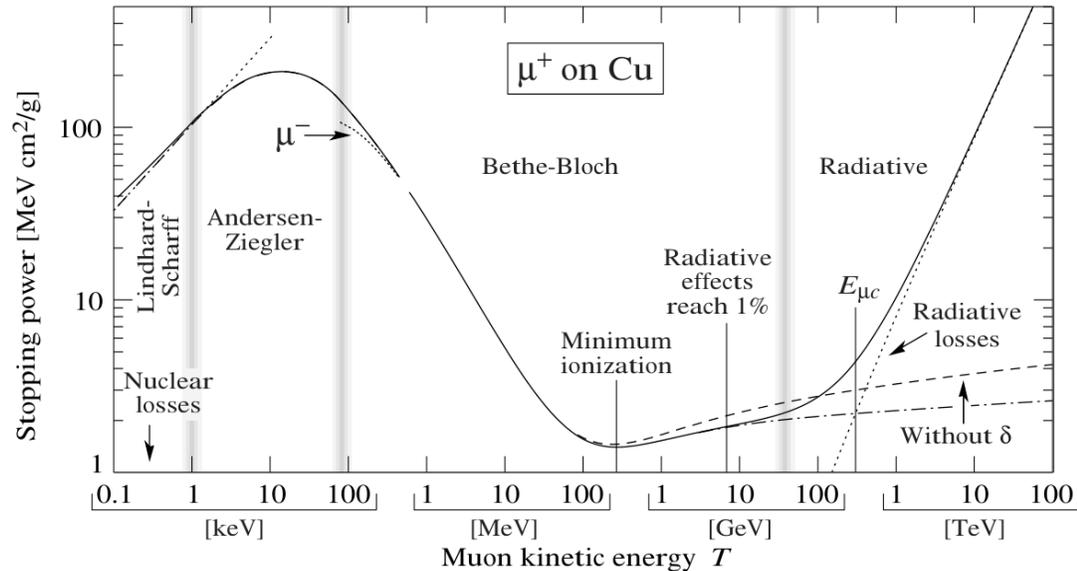
```
/gps/ang/type iso
```

```
/gps/ang/surfnorm false
```

```
/gps/ang/mintheta 0 deg
```

```
/gps/ang/maxtheta 90 deg
```

Average Muon Energy Loss / Stopping Power



[D. E. Groom et al., *Atom. Data Nucl. Data Tab.*, 78.2 (2001) 183-356]

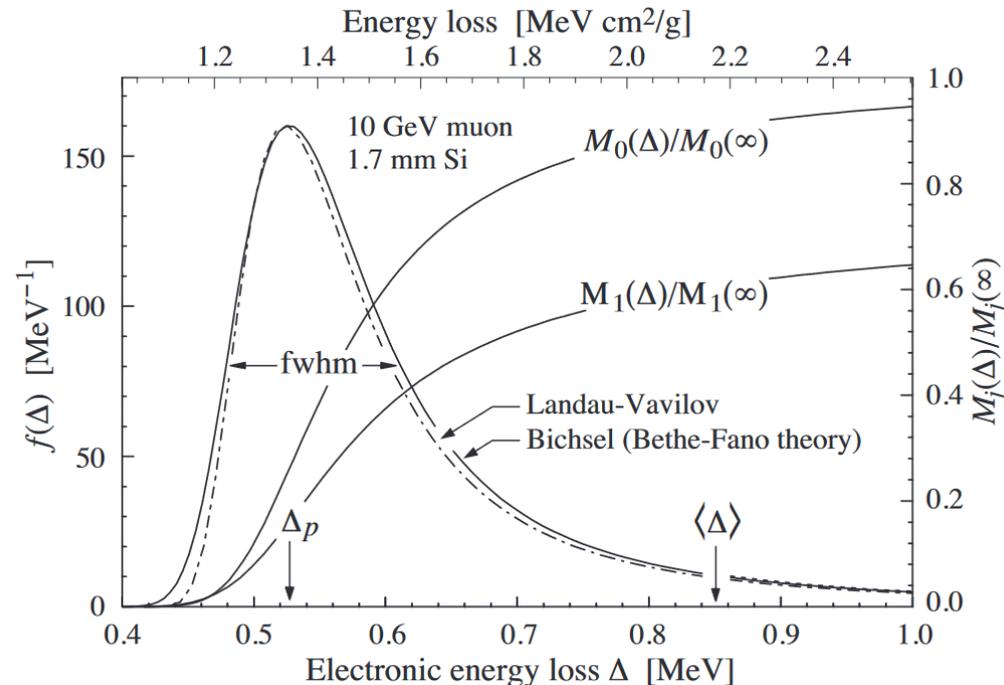
- **Minimum ionising** muons loss
 $\sim 2 \text{ MeV cm}^2 \text{ g}^{-1}$
 e.g. for Ge ($\rho=5.3 \text{ g cm}^{-3}$):
 $\sim 10.6 \text{ MeV cm}^{-1}$

- In general, **stopping power**

$$-\left\langle \frac{dE}{dX} \right\rangle = a(E) + b(E) \cdot E$$

with **material dependent** electronic contribution a and radiative contribution b

Muon Energy Fluctuation



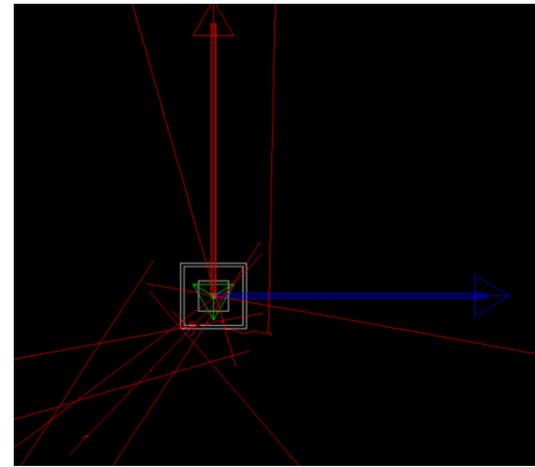
- PDF of muon energy loss is asymmetric with a heavy tail towards higher energies
→ **Average energy loss $\langle \Delta \rangle$ is not the most probable energy loss Δ_p**
- The actual energy loss can be fitted with a Landau function

[R.L. Workman et al. (Particle Data Group), Prog. Theor. Exp. Phys. 2022 (2022) 083C01]

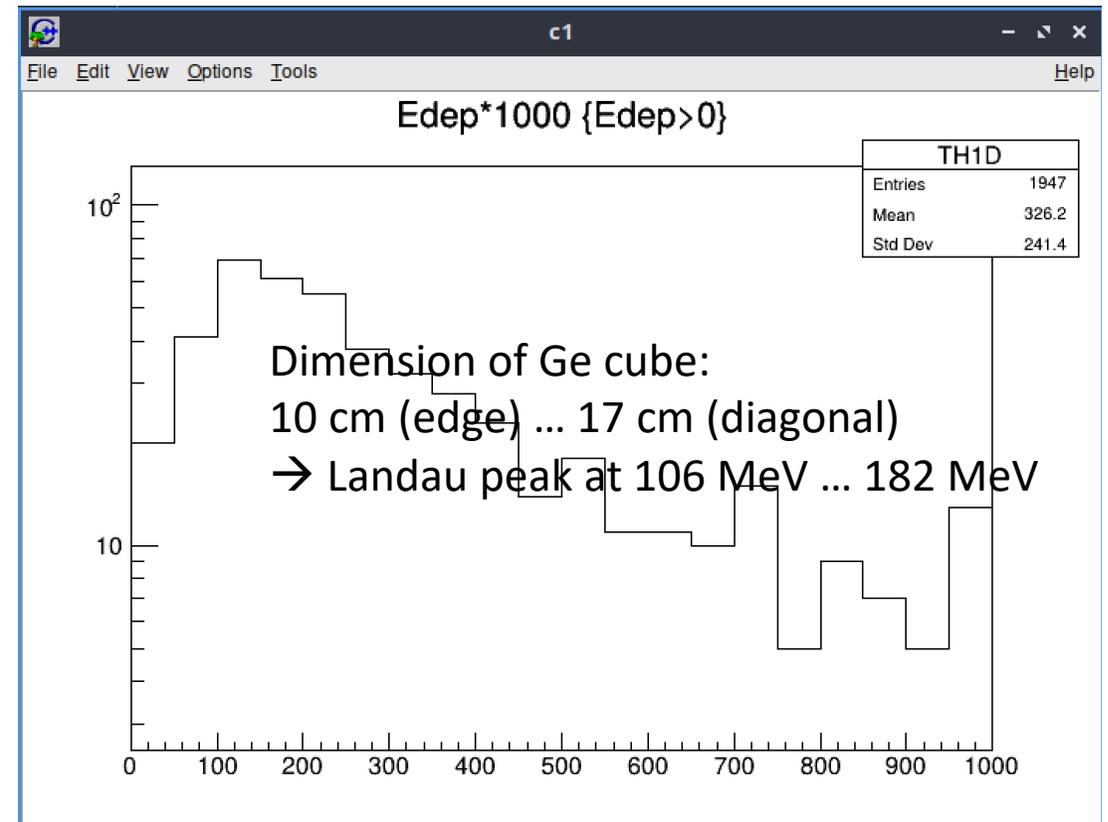
Hands-on

- Copy `./mac/vis_run.mac` to `./mac/vis_run_atm.mac` and modify the GPS commands
 - To use a Sphere as surface source
 - Centred around our geometry
 - With a diameter large enough to enclose the “shell” volume
 - Select mu- of 100 GeV as particle
 - Isotropic distributed between 0° and 90°
 - Simulate 10 events
- Run the simulation, open the produced `scene-0.heprep.zip` to check if the particles are generated as expected
- Copy `./mac/run.mac` to `./mac/run_atm.mac` and replace the GPS commands with the ones from above
- Set “`/event/verbose`” and “`/tracking/verbose`” to 0 and run the simulation for 10000 events
- Open the produced `cube.root` and create a histogram of Edep between 0 and 1GeV
- does the spectrum looks like expected?

Hands-on



```
/gps/pos/type Surface  
/gps/pos/shape Sphere  
/gps/pos/radius 25 cm  
/gps/pos/centre 0. 0. 0. mm  
/gps/particle mu-  
/gps/energy 100. GeV  
/gps/ang/type iso  
/gps/ang/surfnorm false  
/gps/ang/mintheta 0 deg  
/gps/ang/maxtheta 90 deg
```



Deep-underground Laboratories

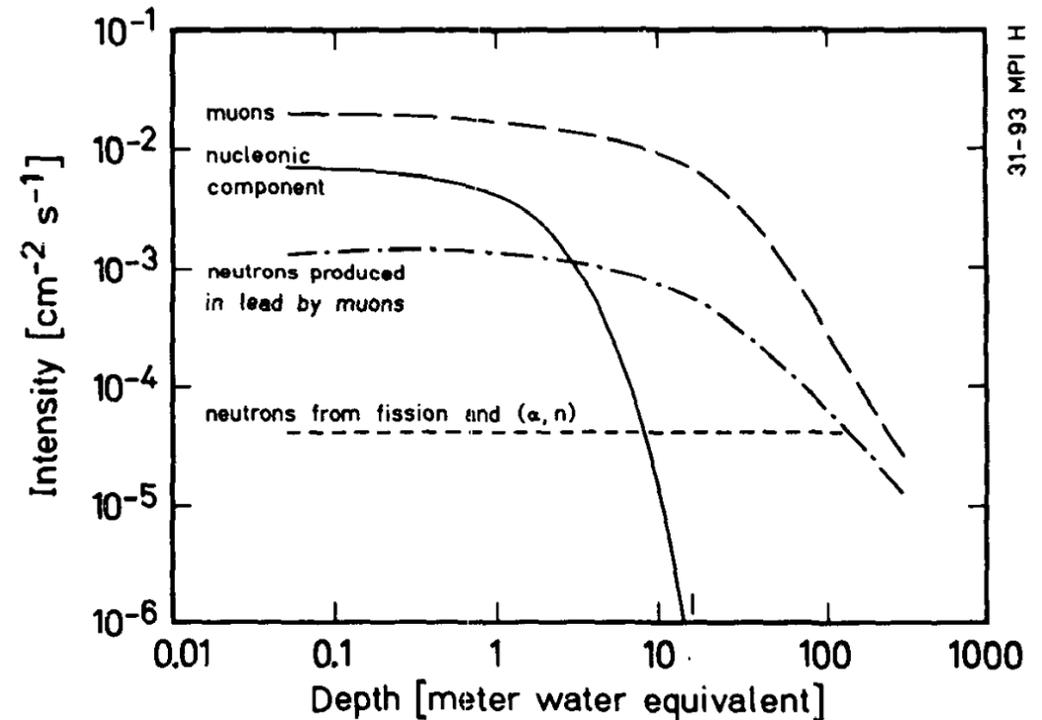
- Rock, concrete etc. above the experiment shields against atmospheric μ (and p, n)
- Shielding power of this **overburden** is given as column density X

$$X = \rho \cdot l$$

along the μ track length l

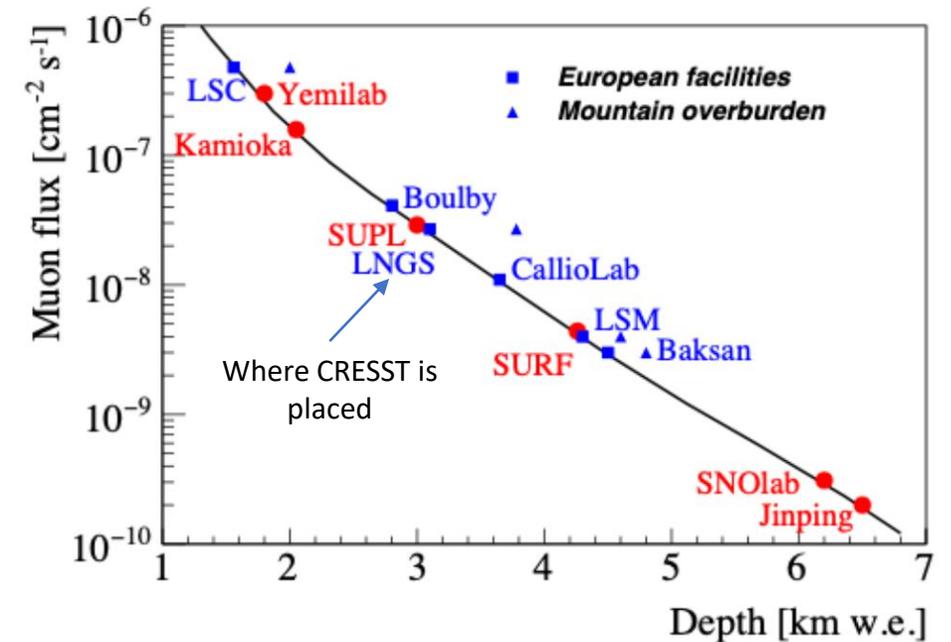
- Given relative to the shielding power of a water column of 1 m height in **meter water equivalent**:

$$1 \text{ m w.e.} = 10^2 \text{ g cm}^{-2}$$



[G. Heusser, Annu. Rev. Nucl. Part. Sci., 45 (1995) 543-590]

Deep-underground Laboratories



[A. Ianni, SciPost Phys. Proc. 12 (2023) 007]

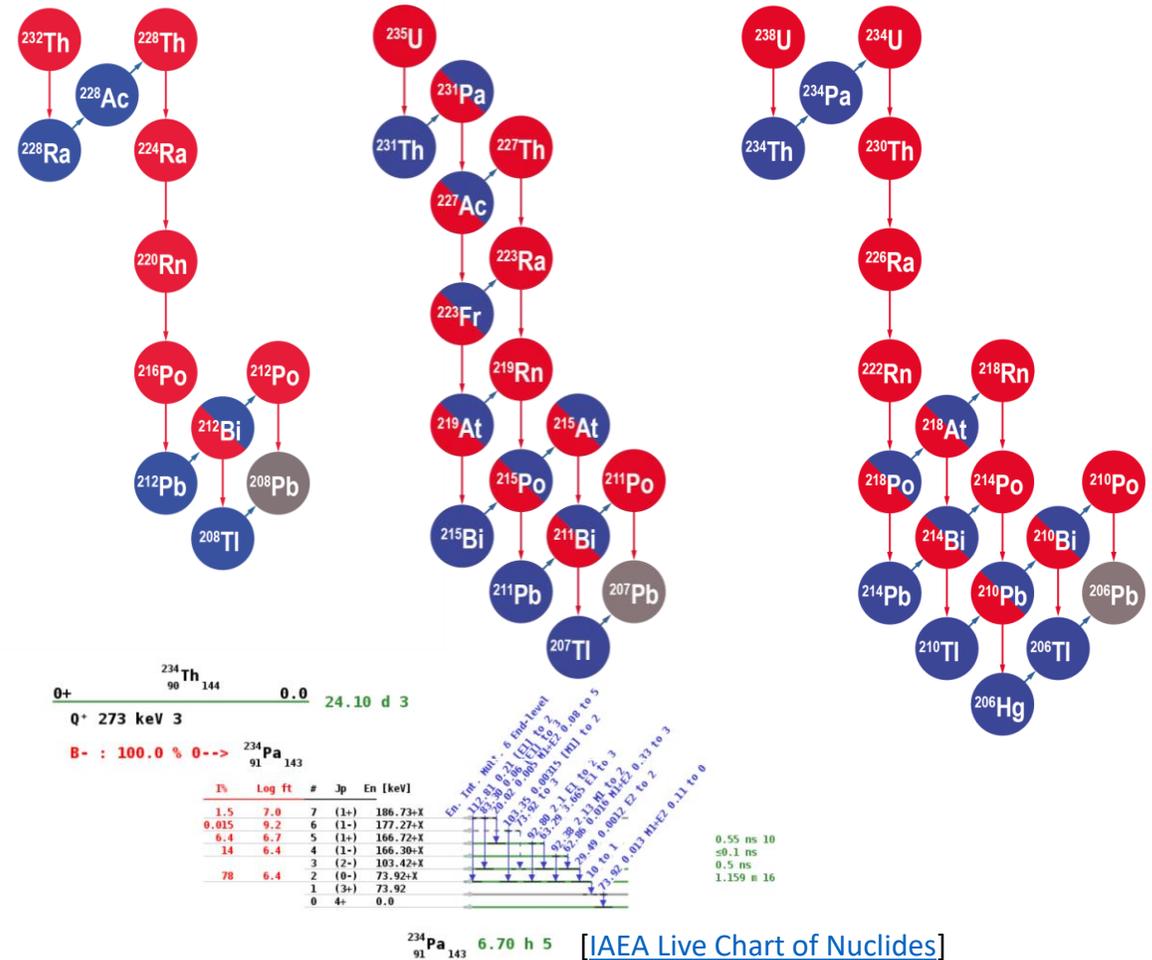
- Reduction of μ -flux by up to $\sim 10^8$ is possible (Jinping lab)
- Deepest lab in Europe: LSM; largest lab in Europe: LNGS
- Simulation of shielding power needs be-spoken primary particle generator that considered the topography of the rock overburden e.g. [H. Kluck, 2013]

Radioactive Decay

- α -, β^- -, β^+ - and Electron Capture (EC)-decay
 → [G4RadioactiveDecay](#)
- If daughter nucleus is in excited state, de-excitation via γ^* -emission or Internal Conversion (IC= e^- emission)
 → [G4PhotoEvaporation](#)
- Subsequent [atomic relaxation](#) (fluorescence, Auger electron-emission)
- Information about decay channels and nuclear level scheme:
 - [IAEA Live Chart of Nuclides](#)
 - R. B. Firestone, *Table of Isotopes*** , 1999, Wiley-VCH

→ Very helpful to check correctness of simulation, e.g. Q-value

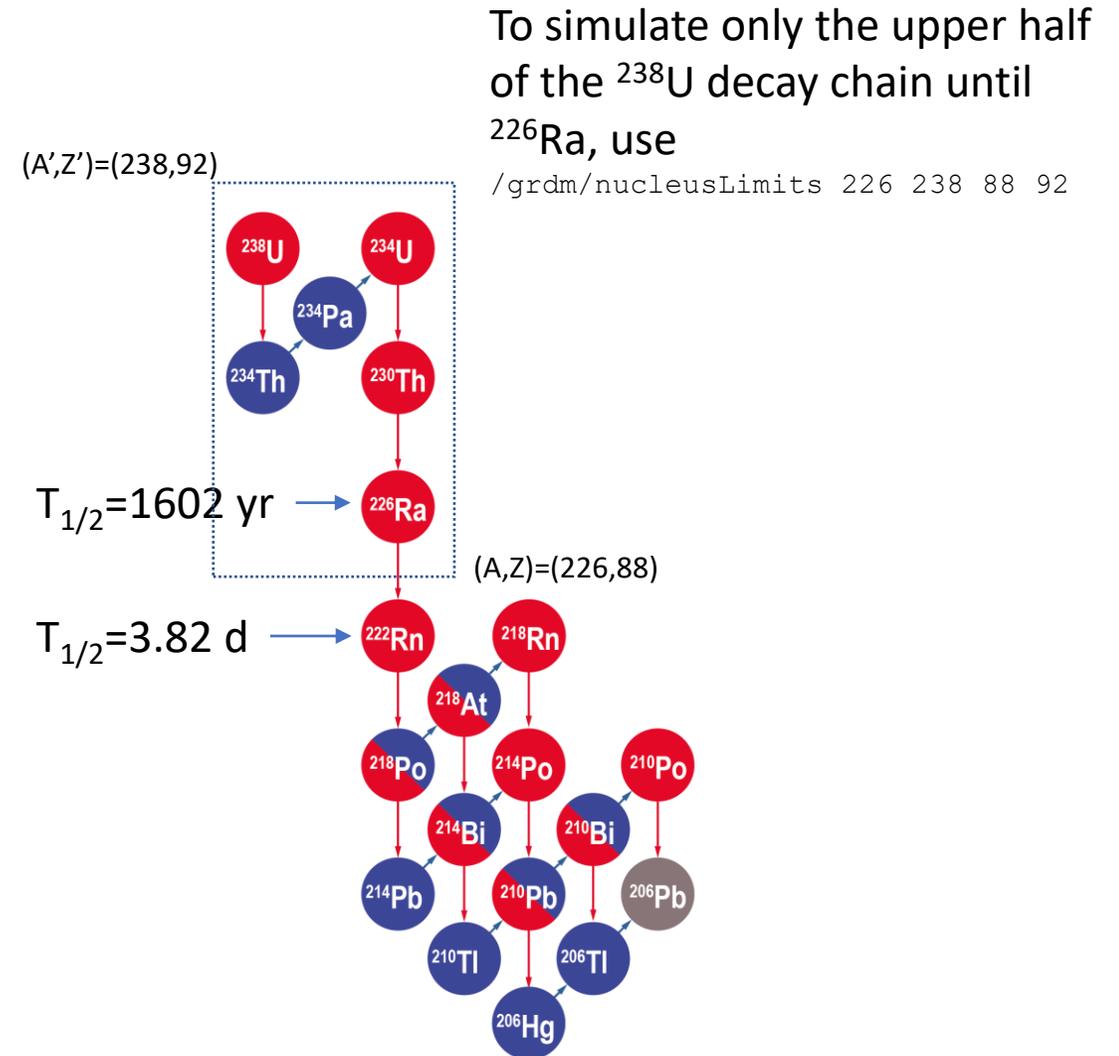
Natural radioactive decay chains of ^{232}Th , ^{235}U , ^{238}U



*Gamma-ray: em radiation emitted through nuclear de-excitation; **Isotope: nuclides belonging to a given element, i.e. same atomic number Z, but different atomic mass A

Secular Equilibrium

- Activity of parent nuclide = activity of daughter nuclide
- If parent nuclide has long half-life and short-lived daughter nuclide is removed (e.g. radiochemical purification) → **Equilibrium is broken**
- Use `/grdm/nucleusLimits A A' Z Z'` command to break decay chain

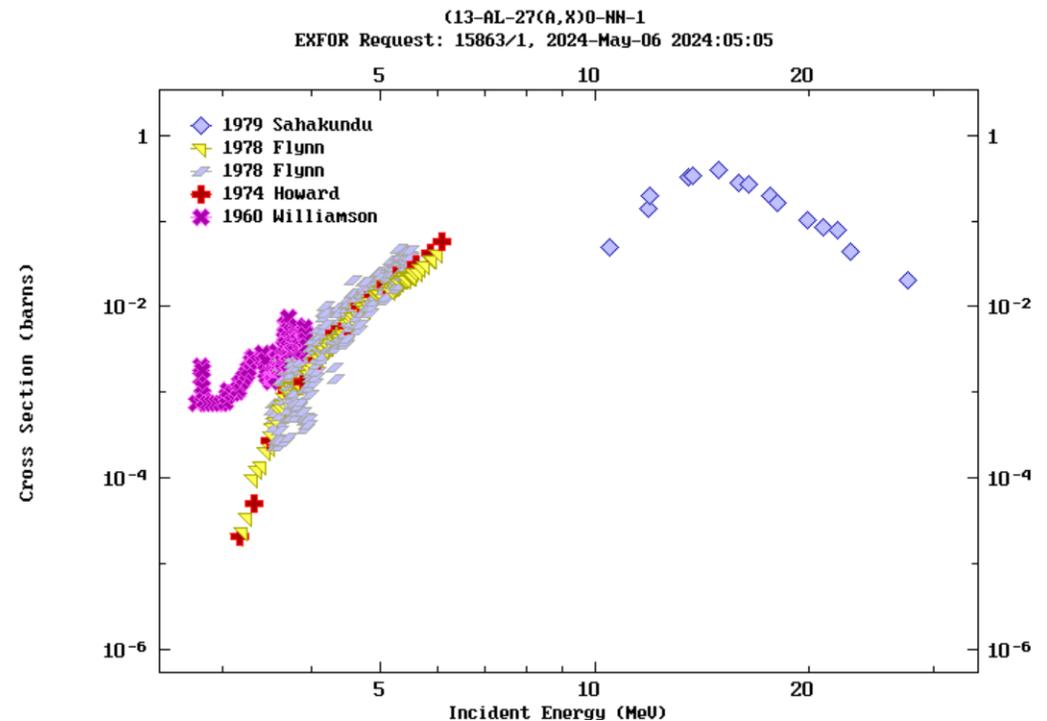


(α, n) reactions

(α, n) reactions can be

- Directly simulated in Geant4 (with input from TALYS via the TENDL data library)
→ [G4ParticleHP](#)
- **Simulate only the neutron propagation in Geant4 and obtain neutron spectra and yield from specialised codes**
 - SOURCES4 (proprietary code)
 - [NeuCBOT](#) (open source)
- Cross sections for (α, n) reactions often inconsistent
→ Simulation is only as good as input data

For example, measured cross sections for $^{27}\text{Al}(\alpha, n)^{30}\text{P}$



[[IAEA, Experimental Nuclear Reaction Data \(EXFOR\)](#)]

Hands-on

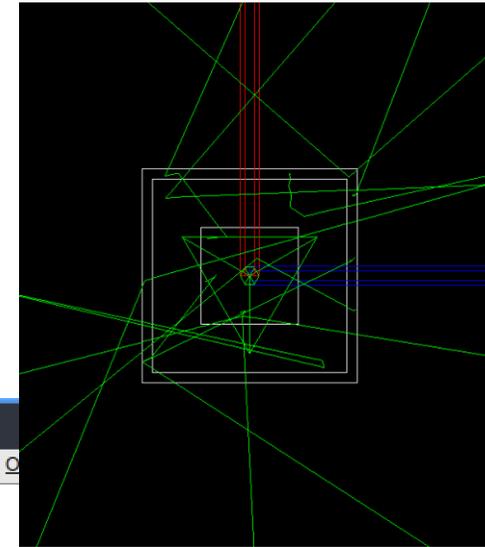
- Assume the Cu of “shell” ($m=23.7$ kg) is contaminated with 500 uBq/kg of ^{58}Co from cosmogenic activation, calculate how many events need to be simulated for 100 d measuring time
- Copy `./mac/vis_run.mac` to `./mac/vis_run_Cu.mac` and adapt the GPS commands by
 - Selecting ^{58}Co as primary particle
 - Placing it inside the “shell” volume by using the `“/gps/pos/confine”` command
- Run the simulation with 10 events, open the produced `scene-0.heprep.zip` to check if the particles are generated as expected
- Copy `./mac/run.mac` to `./mac/run_Cu.mac` and replace the GPS commands with the ones from `vis_run_Cu.mac`
- Set `“/event/verbose”` and `“/tracking/verbose”` to 0 and run the simulation for the number of events equivalent to 100 d measuring time
- Open the produced `cube.root` and create a histogram of Edep between 0 and 2 MeV
- does the spectrum looks like expected?

Hands-on

```

/run/initialize
#Place 58Co ions
/gps/pos/type Volume
/gps/pos/shape Para
/gps/pos/halfx 12 cm
/gps/pos/halfy 12 cm
/gps/pos/halfz 12 cm
/gps/pos/paralp 0
/gps/pos/parthe 0
/gps/pos/parphi 0
/gps/pos/centre 0. 0. 0. mm
/gps/pos/confine shell
/gps/particle ion
/gps/ion 27 58
/gps/energy 0 MeV
/gps/ang/type iso
#500 uBq/kg * 23.7 kg * 3600 s/h * 24 h/d * 100 d
/run/beamOn 102384

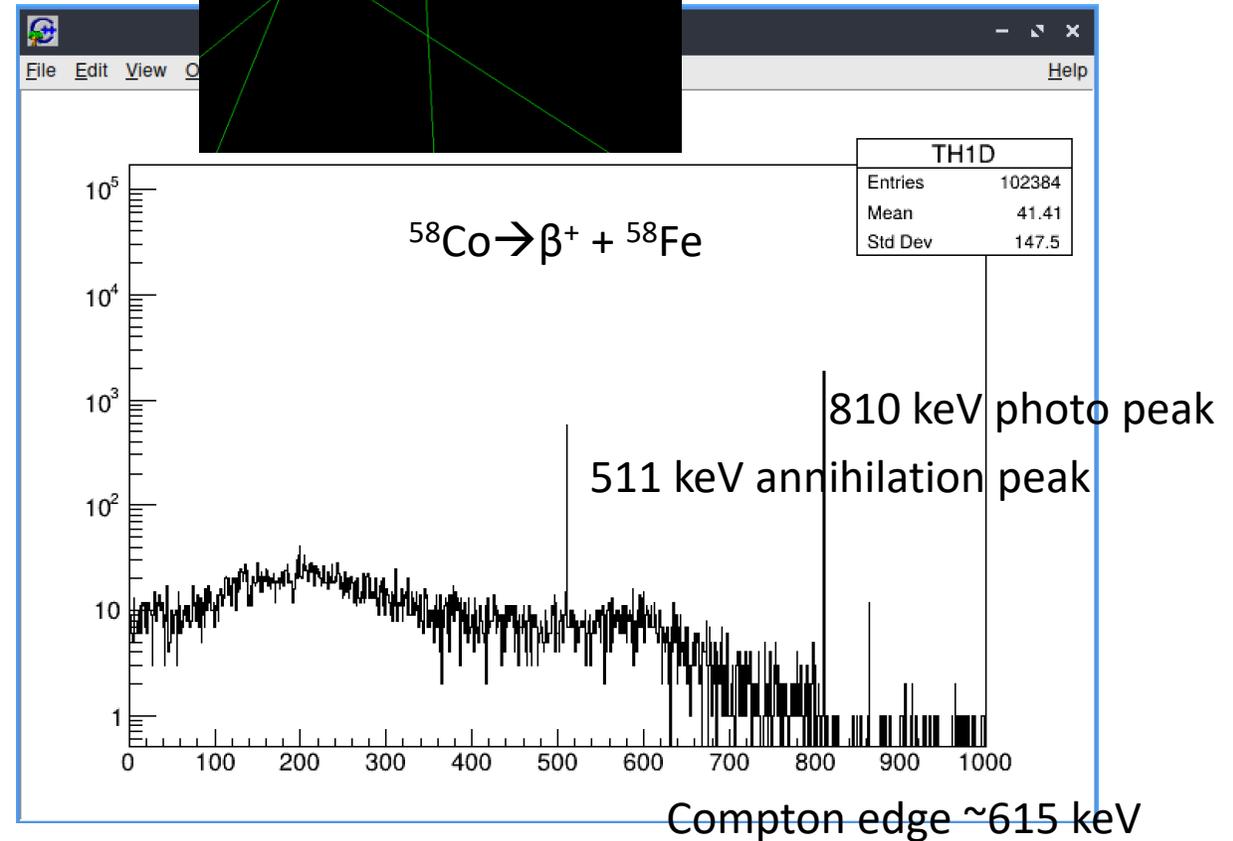
```



Gamma 

#	E_γ [keV]	$I_\gamma(\text{abs})$ [%]
1	810.7593 20	99.45 7
2	863.951 6	0.686 10
3	1674.725 7	0.517 10

[[IAEA Live Chart of Nuclides](#)]



Questions, Comments, Feedback

Additional Information

Gaisser Parameterisation

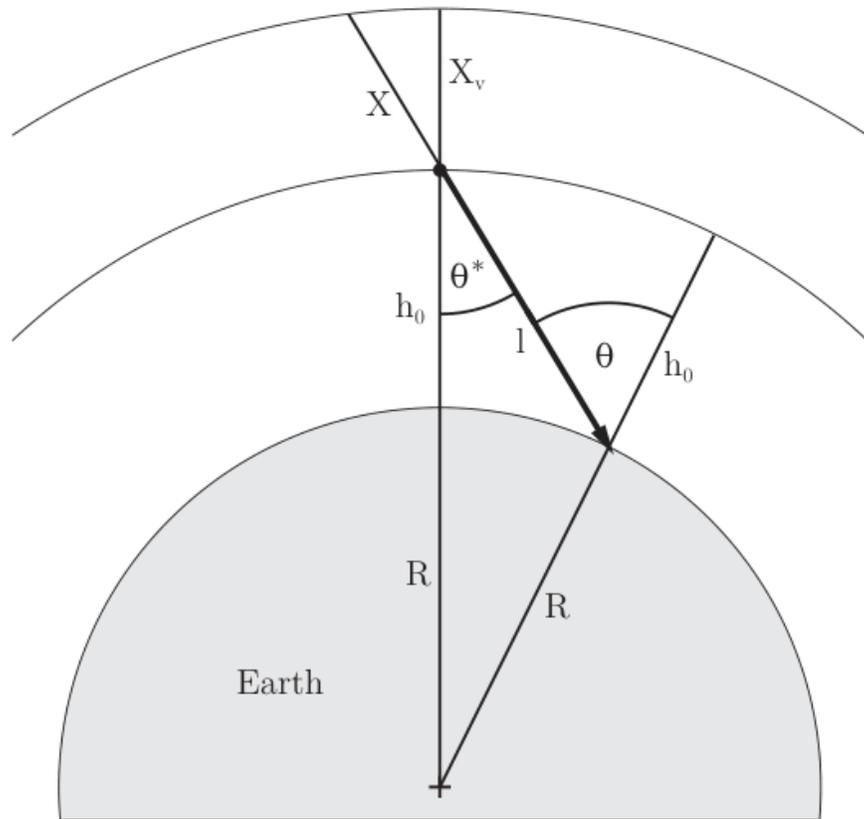
$$\frac{dN_i(E_i, X)}{dX} = -\frac{N_i(E_i, X)}{\lambda_i} - \frac{N_i(E_i, X)}{d_i} + \sum_{j=i}^J \int_E^\infty \frac{F_{ji}(E_i, E_j)}{E_i} \frac{N_j(E_j, X)}{\lambda_j} dE_j.$$

$$\begin{aligned} \pi^\pm &\rightarrow \mu^\pm + \nu_\mu(\bar{\nu}_\mu) \quad (\sim 100\%) \\ K^\pm &\rightarrow \mu^\pm + \nu_\mu(\bar{\nu}_\mu) \quad (\sim 63.5\%). \end{aligned}$$

$$\begin{aligned} \frac{dN_\mu}{dE_\mu} \simeq S_\mu(E_\mu) \frac{N_0(E_\mu)}{1 - Z_{NN}} &\left\{ \mathcal{A}_{\pi\mu} \frac{1}{1 + \mathcal{B}_{\pi\mu} \cos\theta E_\mu/\epsilon_\pi} \right. \\ &\left. + 0.635 \mathcal{A}_{K\mu} \frac{1}{1 + \mathcal{B}_{K\mu} \cos\theta E_\mu/\epsilon_K} \right\}. \end{aligned}$$

- The **Gaisser parameterisation** describes the development of particle cascades with a set of coupled equations
- For muons, mainly the decay of pions and kaons are feeding the cascade
- Given as function of E_μ at *ground level* and zenith angle

Zenith Angles



- Due to Earth's curvature, the **zenith angle** at *ground* θ is different from the zenith angle at the *production vertex* θ^*
- Production height is $h_0 \sim 17$ km
- In general, track length also depends on altitude of experiment

Gaisser Parameterisation II

$$\frac{dN_\mu}{dE_\mu} \simeq S_\mu(E_\mu) \frac{N_0(E_\mu)}{1 - Z_{NN}} \left\{ \mathcal{A}_{\pi\mu} \frac{1}{1 + \mathcal{B}_{\pi\mu} \cos\theta E_\mu/\epsilon_\pi} + 0.635 \mathcal{A}_{K\mu} \frac{1}{1 + \mathcal{B}_{K\mu} \cos\theta E_\mu/\epsilon_K} \right\}.$$

- Below ~ 200 GeV, the suppression S_μ due to **muon decay** and **energy loss** in the atmosphere has to be considered
 - Above, it can be neglected
 - Relativistic time dilation
 - Small energy loss relative to initial energy
- Gaisser's Parameterisation**

$$\frac{dN_\mu}{dE_\mu} \approx \frac{0.14 E_\mu^{-2.7}}{\text{cm}^2 \text{ sec sr GeV}} \left\{ \frac{1}{1 + \frac{1.11 E_\mu \cos\theta}{115\text{GeV}}} + \frac{0.054}{1 + \frac{1.11 E_\mu \cos\theta}{850\text{GeV}}} \right\}.$$

Muon Range

- To stop a 1 TeV-muon in concrete*:

- $\rho = 2.3 \text{ g cm}^{-3}$
- $a = 2.605 \text{ MeV cm}^2 \text{ g}^{-1}$
- $b = 3.752 \cdot 10^{-6} \text{ cm}^2 \text{ g}^{-1}$
- $\rightarrow X = 1.5 \cdot 10^5 \text{ g cm}^{-2}$
- $\rightarrow d = \frac{X}{\rho} = 65 \text{ km}$

- Energy loss in 10 m w.e.

$$E = \frac{dE}{dX} \cdot X = 6.6 \text{ GeV}$$

i.e. <1% of initial energy

- Get the **muon range** via the *Continuous Slowing Down Approximation (CSDA)*: assume a and b are constant in energy:

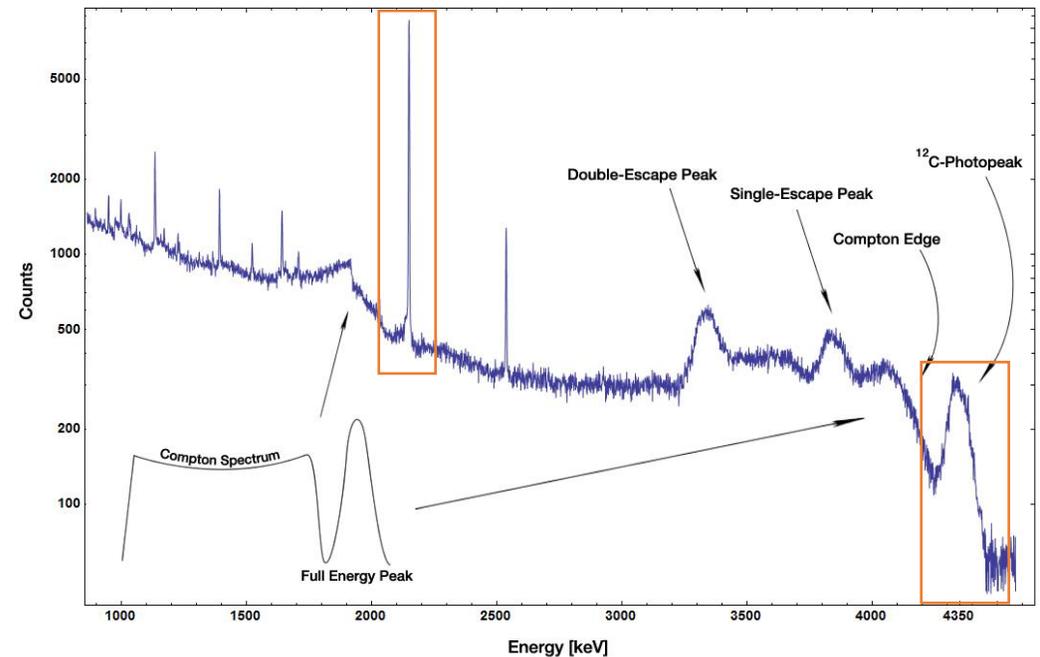
$$X(E) = \int_{E_0}^E \left(\frac{dE'}{dX} \right)^{-1} dE'$$

- CSDA overestimate the muon range for $E > 1 \text{ TeV}$ as it ignores discrete but high energetic scatterings
- **No significant shielding** against muons at **shallow sites**

* From table IV-2 of [\[D. E. Groom et al., Atom. Data Nucl. Data Tab., 78.2 \(2001\) 183-356\]](#); caution: a ="Ionization", b =($\text{"Brems"} + \text{"Pair prod"} + \text{"Photonucl"}$)/ T

Photopeak

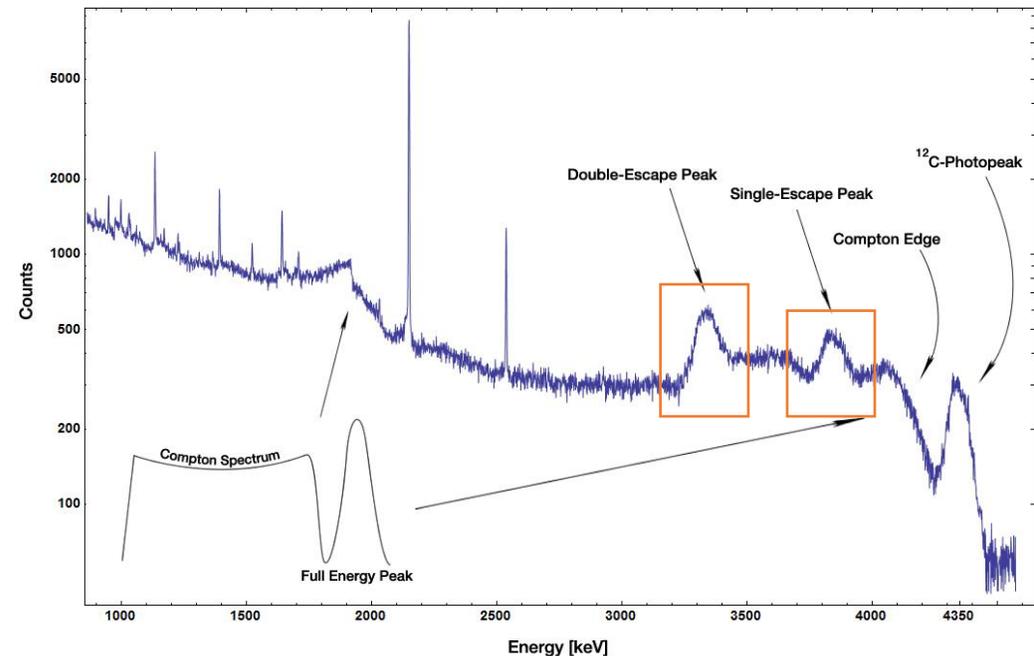
- If the **full energy** E_γ of a γ -ray is absorbed in the detector via the photoelectric effect
→ **photopeak** at E_γ
- Similar if an α is absorbed



[Allen McC via Wikipedia]

Escape Peak

- If $E_\gamma > 2 \cdot 511 \text{ keV}$
 - Pair creations of e^+e^-
 - Creation of positronium
 - Annihilation, 2 γ -rays of 511 keV each
- If both γ -rays get absorbed
 - photopeak at E_γ
- If only one γ -ray gets absorbed
 - **Single-escape peak** at $E_\gamma - 511 \text{ keV}$
- If no γ -ray gets absorbed
 - **Double-escape peak** at $E_\gamma - 1022 \text{ keV}$
- Similar, if after photo absorption, a fluorescence X-ray E_x escape
 - Peak at $E_\gamma - E_x$



[Allen McC via Wikipedia]

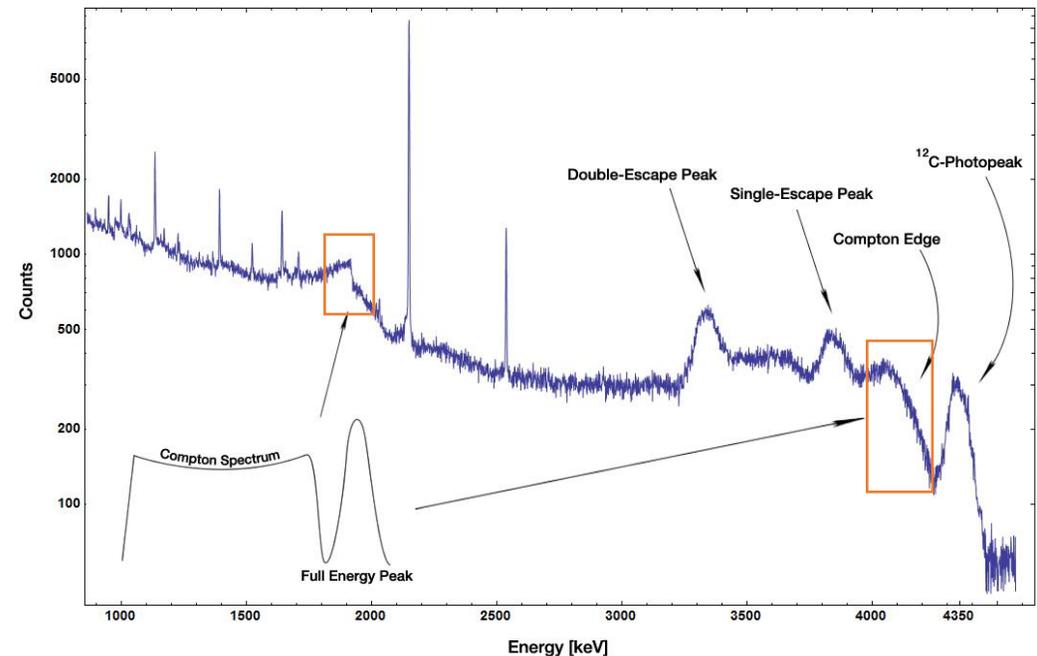
Compton

- Compton scattering: incoherent scattering of a γ -ray with an atomic electron, transferring some energy to the electron
- If scattered γ -ray leaves the detector, only the transferred energy is visible
- Maximum transferred energy for backscattering

$$E_{\max} = E_{\gamma} \left(1 - \frac{1}{1 + \frac{2E_{\gamma}}{m_e c^2}} \right)$$

→ **Compton edge** at E_{\max}

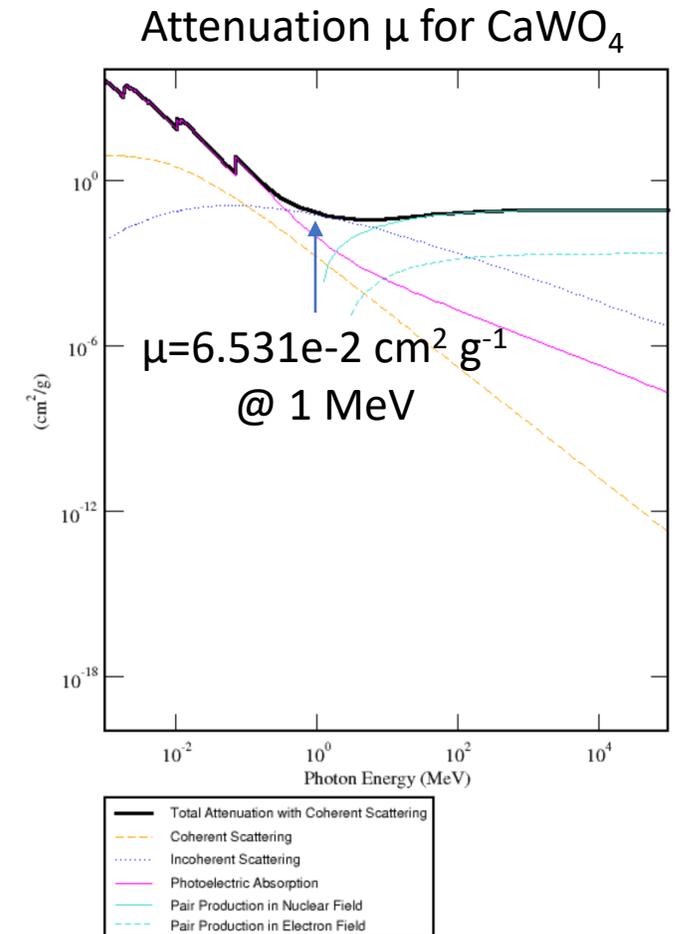
→ **Compton continuum** between 0 and E_{\max}



[[Allen McC via Wikipedia](#)]

Leakage

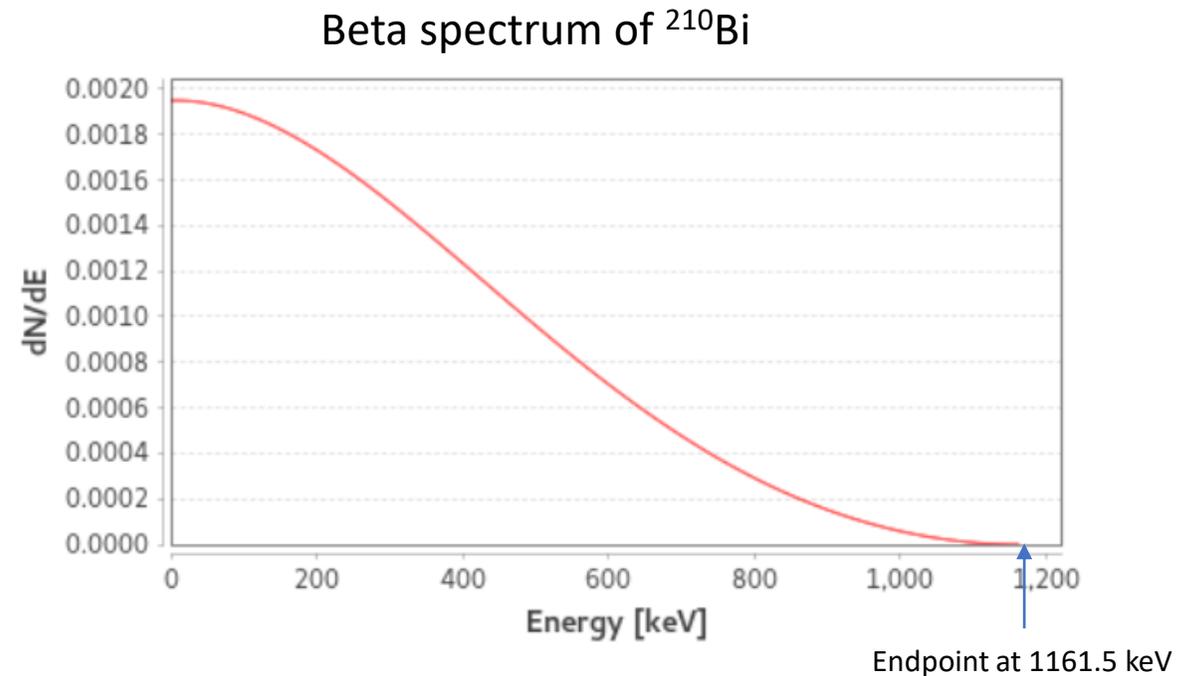
- If the detector dimensions are smaller than the absorption length, the incident particle may deposit only a part of its energy and escape the detector with the remaining energy (~ energy may **leak out of the detector**)
- For example, to contain a 1 MeV- γ -ray in a CaWO_4 detector:
$$\begin{aligned}\lambda^{-1} &= \mu \cdot \rho \\ &= 6.531 \cdot 10^{-2} \text{ cm}^2 \text{ g}^{-1} \cdot 6.06 \text{ g cm}^{-3} \\ &= 0.396 \text{ cm}^{-1} \\ &\rightarrow \lambda = 2.53 \text{ cm}\end{aligned}$$
- Set Geant4's range cut to a value smaller than the detector dimension, so that the leakage can be properly simulated



[XCOM]

Beta spectrum

- Beta decay
$${}^A_Z X \rightarrow {}^A_{Z+1} Y + \bar{\nu}_e + e^-$$
- Continuous spectrum
- Endpoint of the spectrum =
Q-value – neutrino mass



[[IAEA Live Chart of Nuclides](#)]

Include CRY

```
• MyPGA::MyPGA() {  
    Setup=new CRYSetup(...);  
    GenPrimaries = new CRYGenerator(Setup);  
}  
• MyPGA::GeneratePrimaries(G4Event *evt) {  
    std::vector<CRYParticle*> primaries;  
    GenPrimaries->genEvent(&primaries);  
    for(auto* p : primaries){  
        //Get pos, energy, etc. from p and fill  
        //it into vertex and particle  
  
        ...  
        auto* vertex = new G4PrimaryVertex (...)  
        auto* particle = new G4PrimaryParticle(...)  
        vertex->SetPrimary(particle);  
        evt->AddPrimaryVertex(vertex);  
    }  
}
```

- Call it from ParticleGeneratorAction (PGA) (similar to Geant4's GPS)
- Multiple primaries per event possible → loop over it
- Need to “translate” CRY data types to Geant4 data types