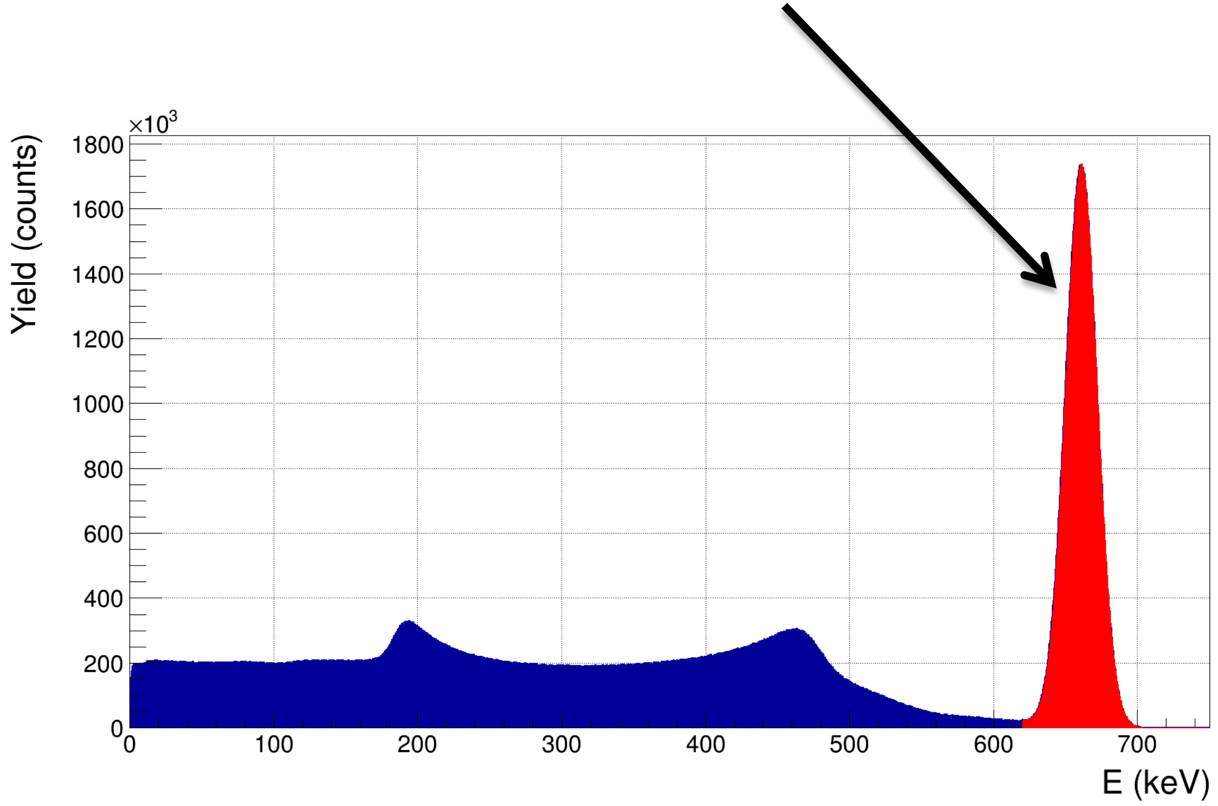
Full Energy Peak efficiency
using Monte Carlo simulations: principles

NKS GammaSkill 2023, 28/09/2023, STUK

Guillaume Lutter

Definition: Full Energy Peak Efficiency (Ɛ)

"*ratio of the number of counts detected in a peak to the number emitted by the source*"



(Total efficiency: ratio of the total number of counts [blue+red] detected to the number emitted by the source)

Why using Monte Carlo simulations ?

Gammay-ray spectrometry is a none destructive method
→ Can measure samples which should not be destroyed



→ '*None standard*' geometries, composition,…

How to get the FEP efficiencies ??

→ Monte Carlo modelling !

Get the Absolute Full Energy Peak efficiencies for any type/composition/shape of sample

→ No calibration sample/source needed

How To

Software:

- General purpose packages

  - Wide range of applications (gamma-ray spectrometry, particle physics, nuclear physics, medical physics, criticality calculations, radiation protection, dosimetry,…)
  - Programming skills may be required
  - Can handle arbitrary/complex geometries

  MCNP, Geant4, Penelope, EGSnrc,…

- Specialised software

  - Limited to gamma-ray spectrometry
  - User friendly
  - No programming required
  - Limited number of geometries

  GESPECOR, DETEFF,…

Principle

User:

- Create a model (geometries) of your measurement setup
- Define all your materials (composition, density)

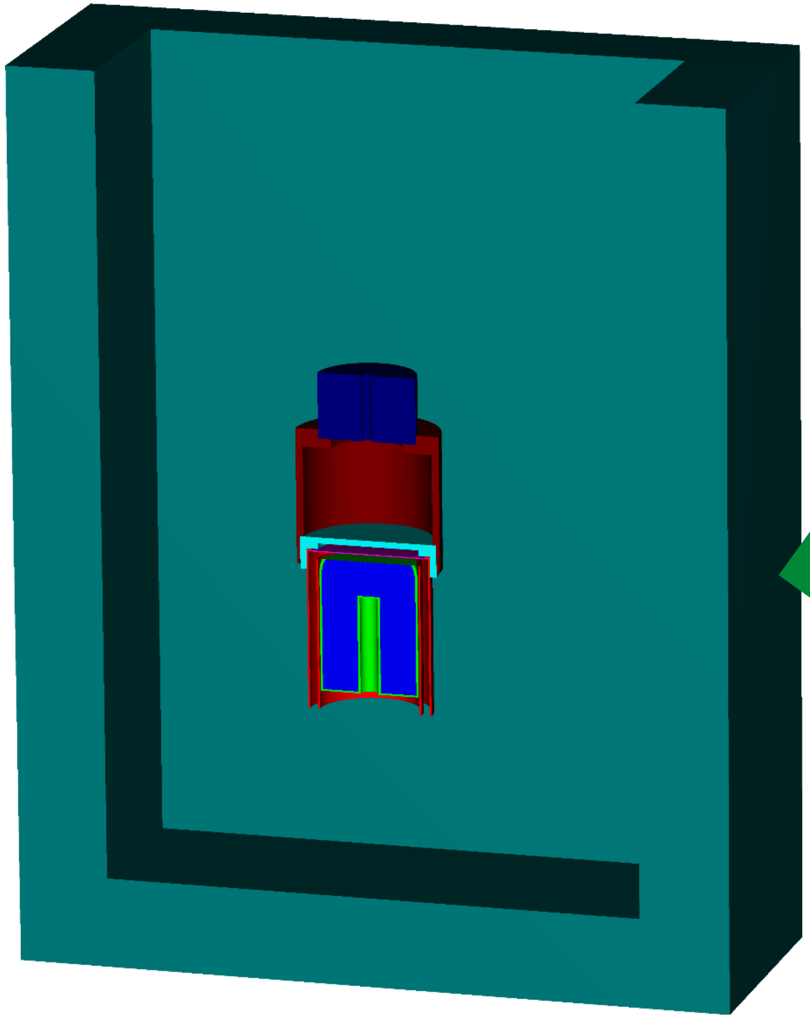
- Define your sample
(composition, density, particle and energy or radionuclide)

- (Define the possible particle interactions)

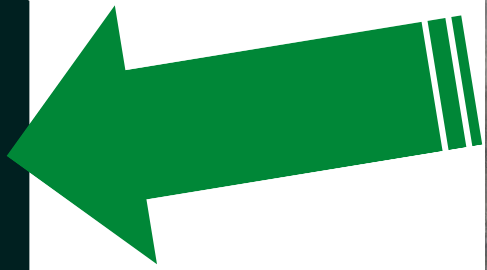
Software will provide the necessary tools to make all this

→ Each software is different !
→ It can be a graphical interface, predefined syntax or pure code (C++, Fortran)

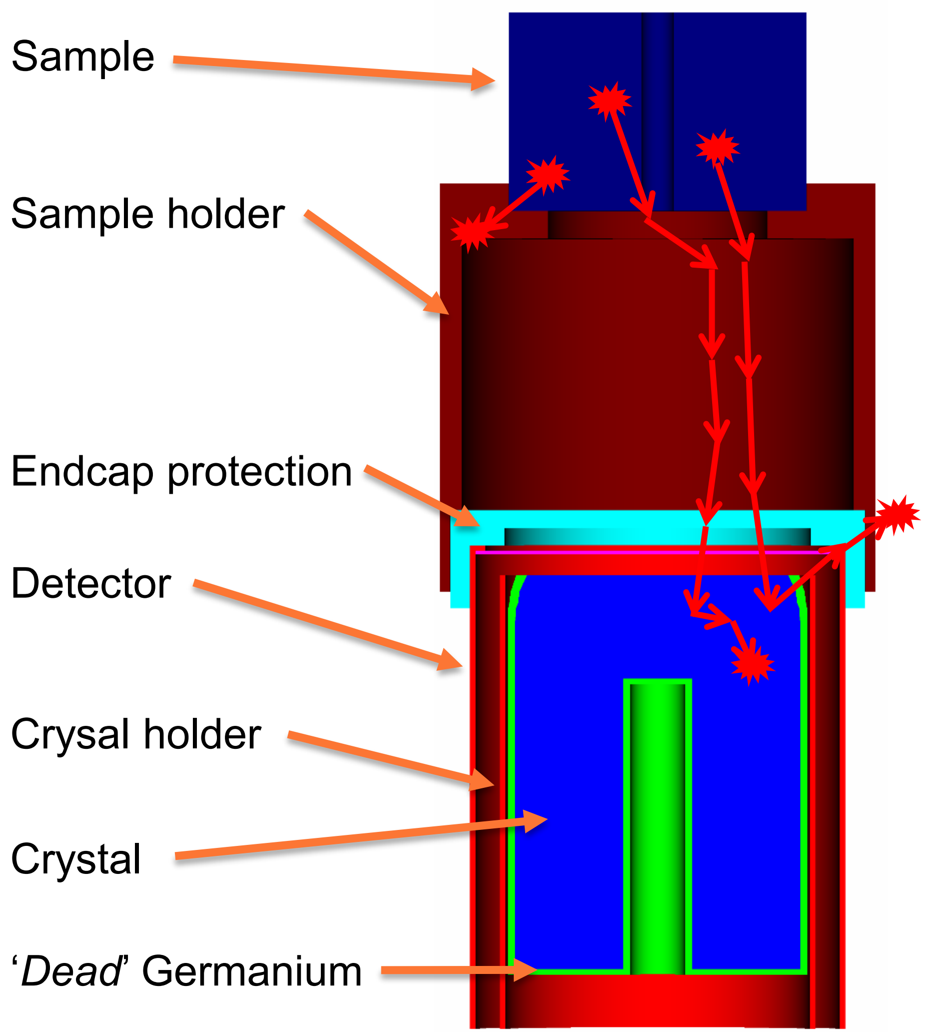
Principle



(EGSnrc)



Principle



i. Create particle in your sample

ii. Propagate particle *step* by *step* using Monte Carlo method until all energy is lost

At each step, physical processes, interactions are selected randomly depending on the type, the energy of the particle and the material

iii. Store and add all the energy deposited in the Ge crystal (not the dead-layer) if the particle reaches the crystal

Steps i to iii = 1 event or history

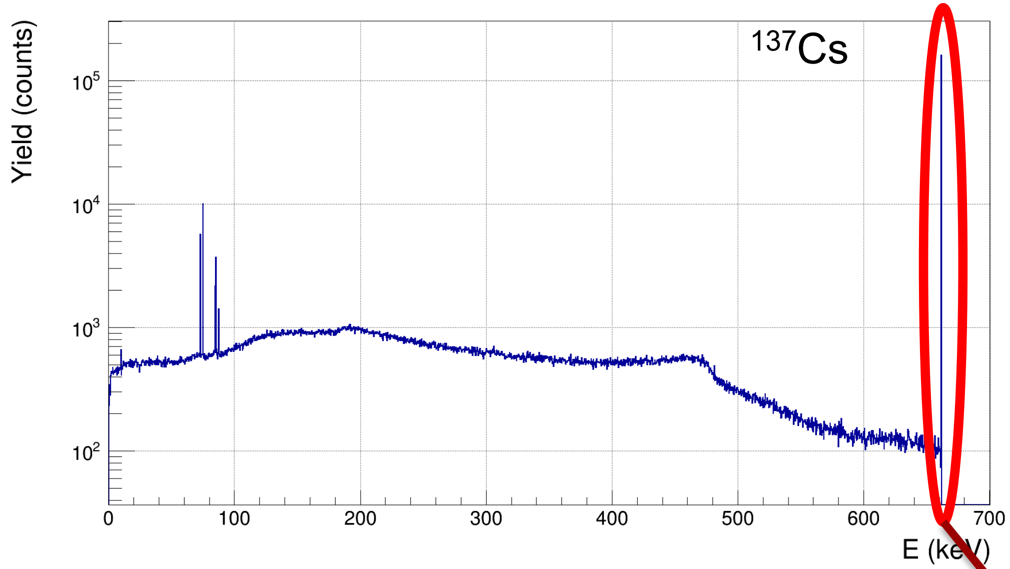
Statistical process → need several events (>$10^{5\text{-}6}$)

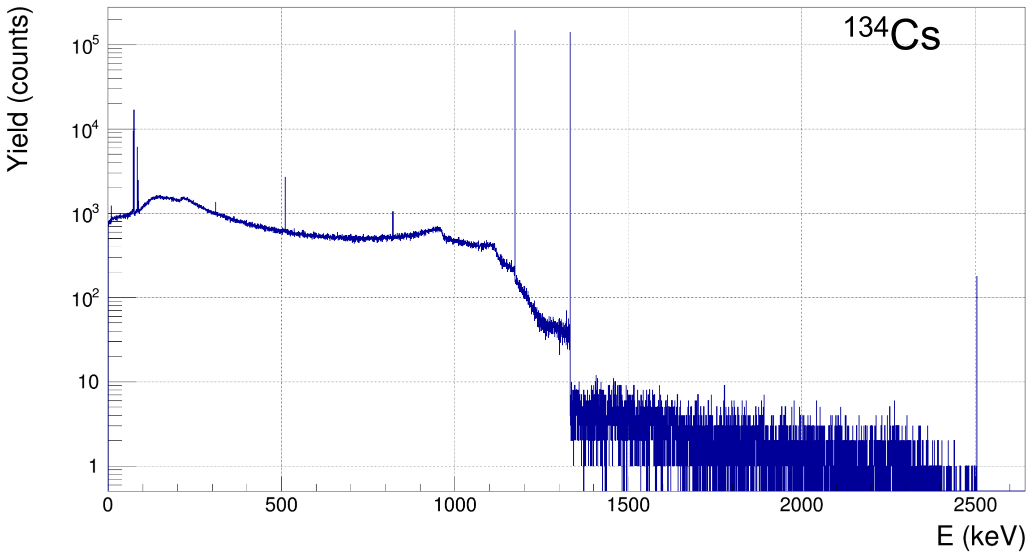
Output of simulations

Ask the software for the total energy deposited in the Ge crystal for each simulated event

→ Histogram

→ Number of *counts* in the region of interest





$$\varepsilon = \frac{\textit{number of counts in region of interest}}{\textit{total number of events/histories}}$$

= 0.2×10^6 counts

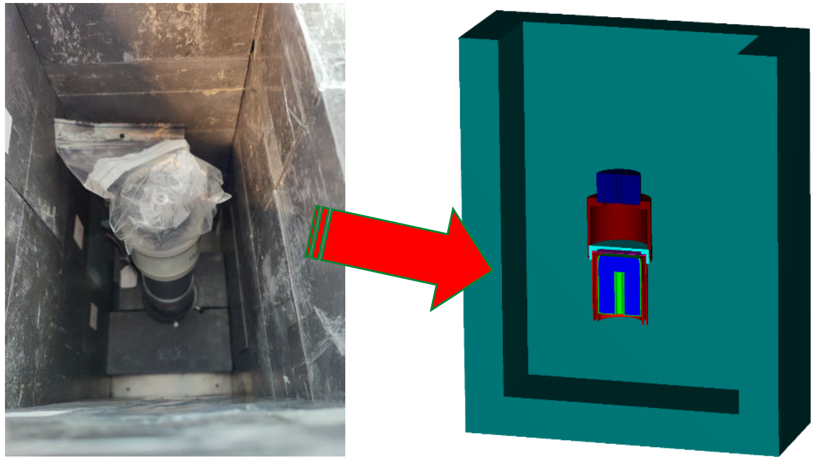
= 0.02 ?

= 10×10^6 events

How to create a "good" model of a detector ?

Model = your experimental setup in your Monte Carlo code

"Good" model → efficiency you can trust (within some limits)



- ❑ Models are always a simplification of the reality
- ❑ Not all parameters can be known exactly, even by the producer
- ❑ Model of detector is a compromise between (accuracy & precision) & flexibility
- ❑ It can be time consuming

Input parameters

CANBERRA

Basic characteristics

Type

Dimensions

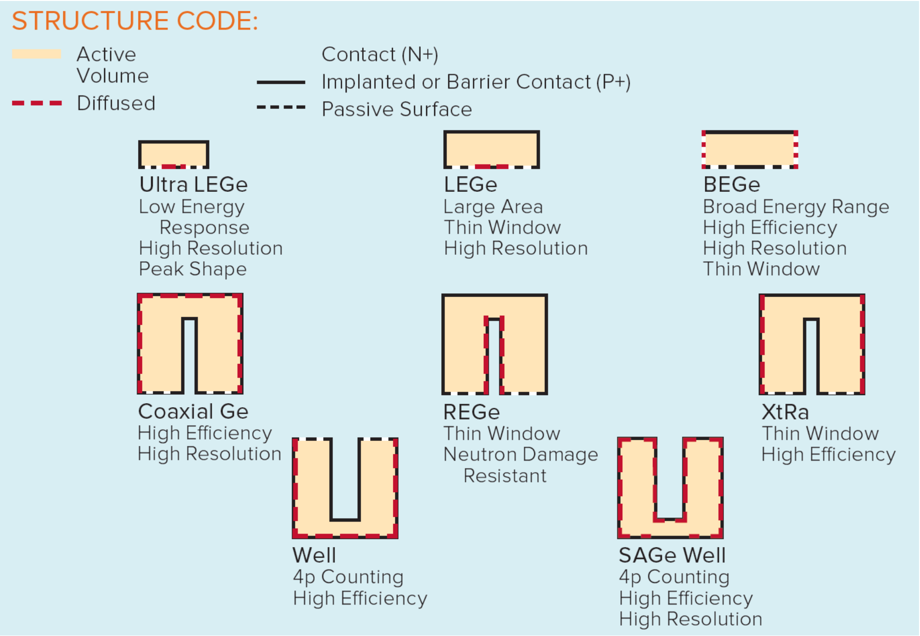
Dead-layer ?

thin (~0.5 µm)

thick (~0.7 mm)

Expected performance of the Monte Carlo model

20% to 30%



Mirion brochure: Germanium Detector Overview

DETECTOR SPECIFICATION AND PERFORMANCE DATA
CERTIFICATE OF CONFORMITY

Specifications

Detector Model BE5030P — **Serial number** b 23049
Cryostat Model 7500SL-RDC-6-ULB — Order number GOR7317
Preamplifier Model iPA-SL

The purchase specifications and therefore the warranted performance of this detector are as follows :

Energy	5.9 keV	122 keV	1332.5 keV
Resolution eV(FWHM)	425	675	1800

Cryostat description or Drawing Number if special 7500SL-RDC-6-ULB

Physical Characteristics

Active Diameter	80.6	mm	Distance from window (outside)	5	mm
Active Area	5000	mm^2	Window thickness	0.6	mm
Thickness	32	mm	Window material	Carbon Epoxy	

Characteristics

ltage (+) 2500 Vdc
ed bias voltage Vdc (+) 3500 Vdc
recommended bias / sec (PO preamp only)
test point voltage at recommended bias - 0.8 Vdc (RC preamp only)
output polarity Neg.

Resolution and Efficiency

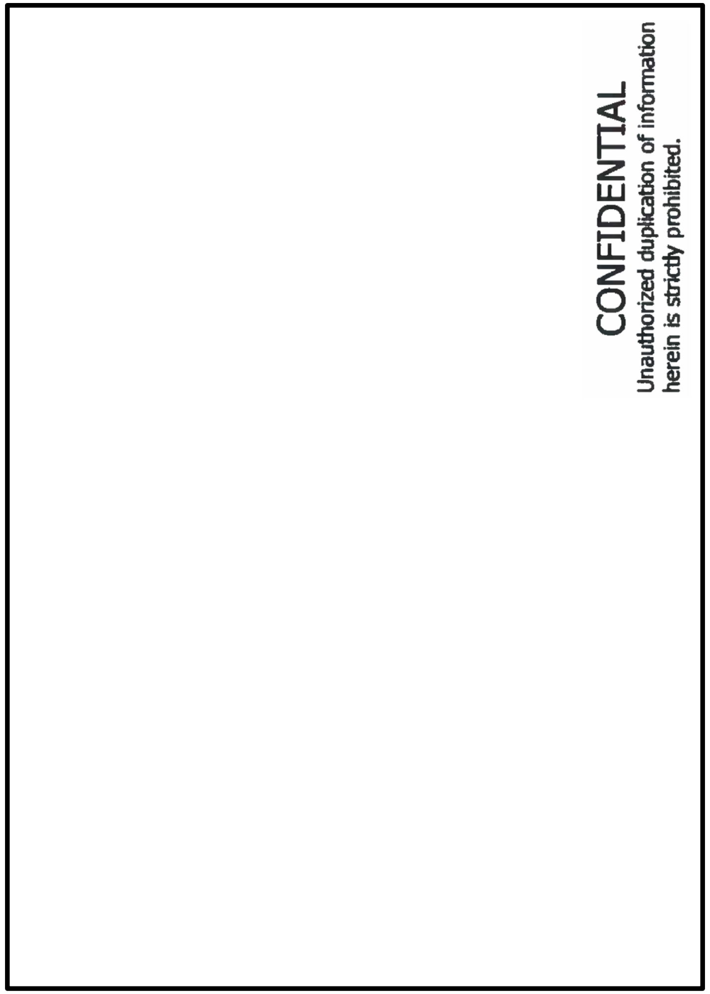
With amp time constant of 4 us - 7.2 us Rise Time , 0.8 µs Flat Top

^{57}Co	^{60}Co
122	1332.5
610	1745
1119	3220

Cooldown time 14 h
Coldtip setpoint (if CP5 config) : _____°C
- Tests are performed following IEEE standard test ANSI/IEEE std325-1996
- Standard Canberra electronics used - See Germanium detector manual Section 7

Advanced characteristics

Ex: Mirion BEGe BE5030P



Request it to the manufacturer

May be not free or available for old detectors

Additional information (≈ technical drawing)

- On the crystal size
- Dead-layers
- Crystal holder
- Distance endcap-crystal
- Endcap (materials & dimensions)

Expected performance of the Monte Carlo model

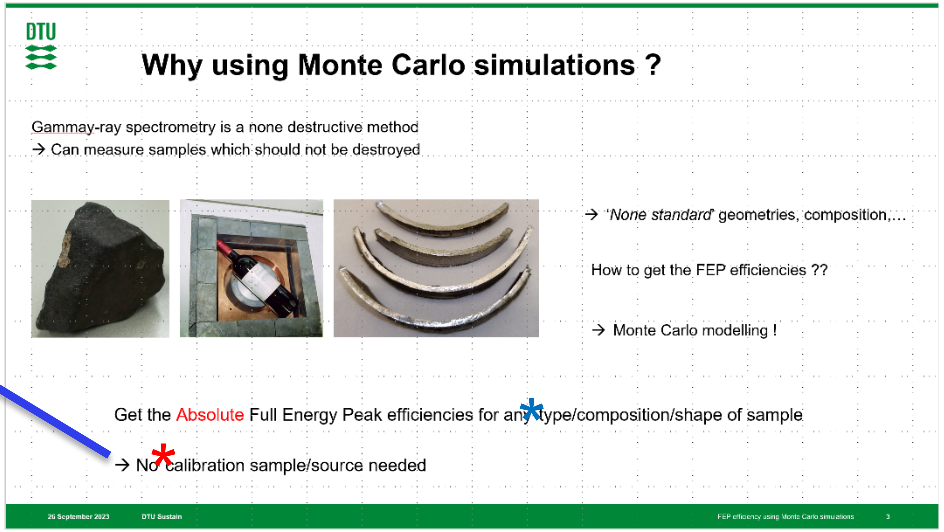
≤ 5-15%

Sufficient for most of the cases

Monte Carlo model validation

→ No calibration sample/source needed

* = AFTER validation of the Monte Carlo model !



Validation:

Compare Monte Carlo efficiencies and experimental efficiencies using:

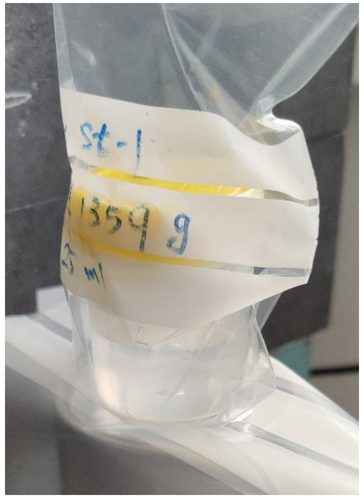
* depends on the software

- Calibration source/sample
- Reference samples
- Samples from previous proficiency tests

→ Limitation/performance of your model

Validation/Improvement of the model

How to validate/improve the model ?



- ❑ Use reference/calibration sources with low uncertainty on the activity(ies)

- ❑ Use a simple geometry source/container & composition

Simple experimental setup:

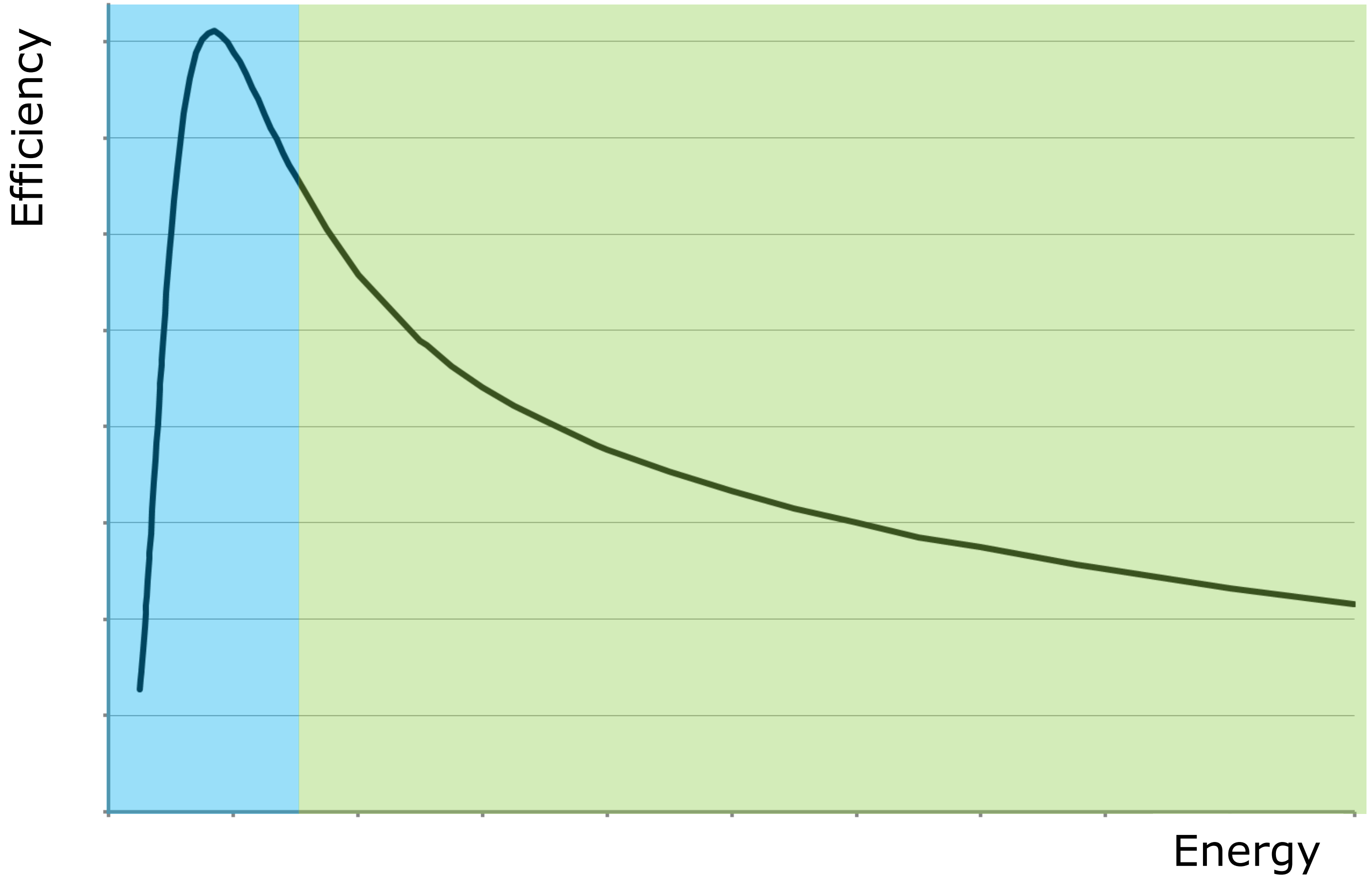
- ➢ Volume source on top and centre of the endcap
- ➢ Focus first on single gamma-ray emitters (= no coincidence summing effect)

- ➢ Volume source at different distance from the endcap (less coincidence summing effect)

→ **Check the relative difference between the experimental FEP & Monte Carlo efficiency**

Adjust the model to get *reasonable* agreement with the experimental measurements

How to validate/improve the model ?



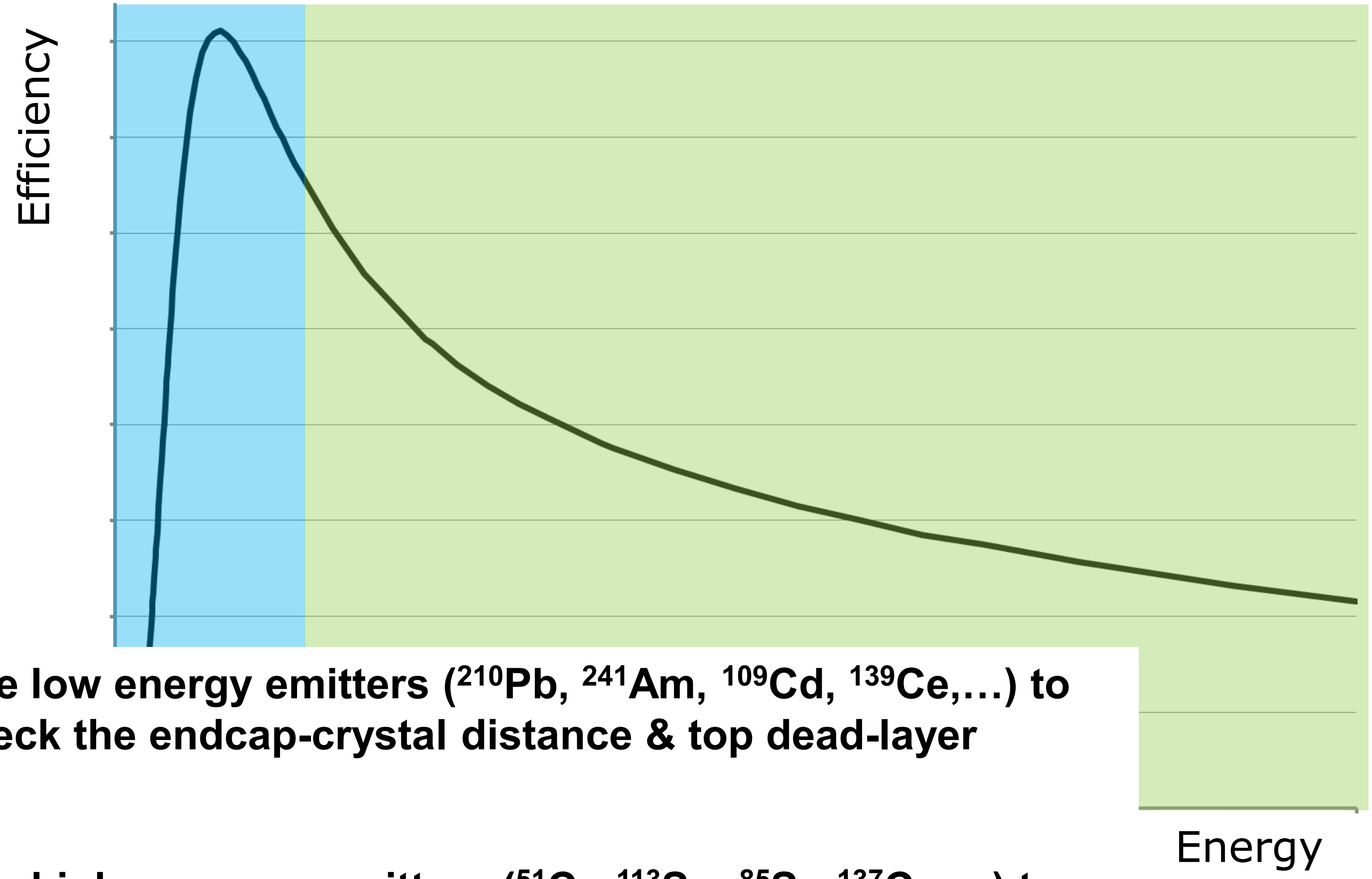
‘Low’ energy:

- ➢ Endcap thickness ?
- ➢ Distance endcap-crystal ?
- ➢ Top dead-layer ?
- ➢ Rounding edge ?

‘High’ energy:

- ➢ Crystal size ?
- ➢ Top & side dead-layer ?
- ➢ Inner dead-layer (coaxial) ?
- ➢ Bottom dead-layer ?

How to validate/improve the model ?



'Low' energy:

- Endcap thickness ?
- Distance endcap-crystal ?
- Top dead-layer ?
- Rounding edge ?

'High' energy:

- Crystal size ?
- Top & side dead-layer ?
- Inner dead-layer (coaxial) ?
- Bottom dead-layer ?

- **Use low energy emitters (^{210}Pb, ^{241}Am, ^{109}Cd, ^{139}Ce,…) to check the endcap-crystal distance & top dead-layer**

- **Use higher energy emitters (^{51}Cr, ^{113}Sn, ^{85}Sr, ^{137}Cs,…) to check detector size & inner dead-layer (coaxial)**

How to validate/improve the model ?

- ❑ Use reference/calibration sources with low uncertainty on the activity

- ❑ Use point sources

→ Check '*locally*' your model

→ Check the crystal size, round edges by moving the sources around the endcap

→ Check the relative difference between the experimental FEP & Monte Carlo efficiency

Adjust the model to get *reasonable* agreement with the experimental measurements

Check that your model still works fine with previous measurement(s) !!

How to validate/improve the model ?

- ❑ Use reference/calibration sources with low uncertainty on the activity
- ❑ Use other volume sources/calibration sample with different geometries, composition,…

Real experimental setup:

- ➢ Position: like your samples

- ➢ For Marinelli : do not forget the side dead-layers !

Adjust the model to get *reasonable* agreement with the experimental measurements

Check that your model still works fine with previous measurement(s) !!

Remarks

- Trial & error procedure
- Multi-gamma emitters: check activity agreement between the gamma-rays
- Plot the Monte Carlo FEP efficiencies curves
- Test at different distances sample-endcap
- Use holder(s) to get well-defined positions & make pictures of the different setups
- Monte Carlo is a statistical process, try to get enough statistics in your simulated peak(s)

(by experience ≈ 1000 counts for a check)

Remarks

- Keep in mind to make a realistic model !

(dead-layer of 10 cm is not realistic even if you get good results, try to increase the distance endcap-crystal instead)

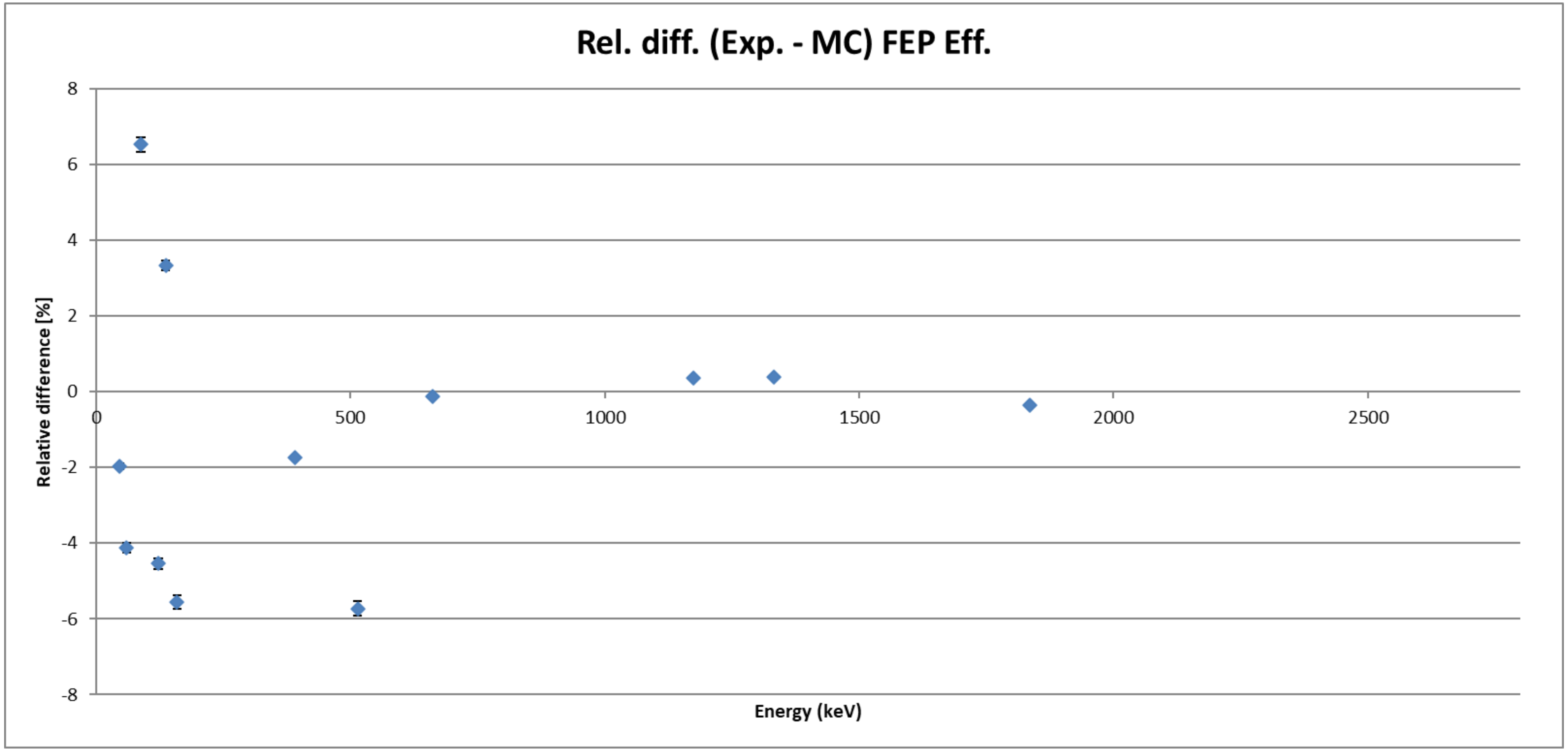
- Model will never be perfect !

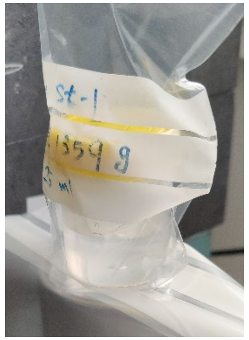
Make many measurements to know the 'limits' of your model → Uncertainty

Energy range (keV)		Rel. Diff. MC-Exp
0	50	15%
50	120	10%
120	1460	5%
1460	3000	10%

Example

Relative difference between experimental full energy peak efficiency and Monte Carlo efficiency





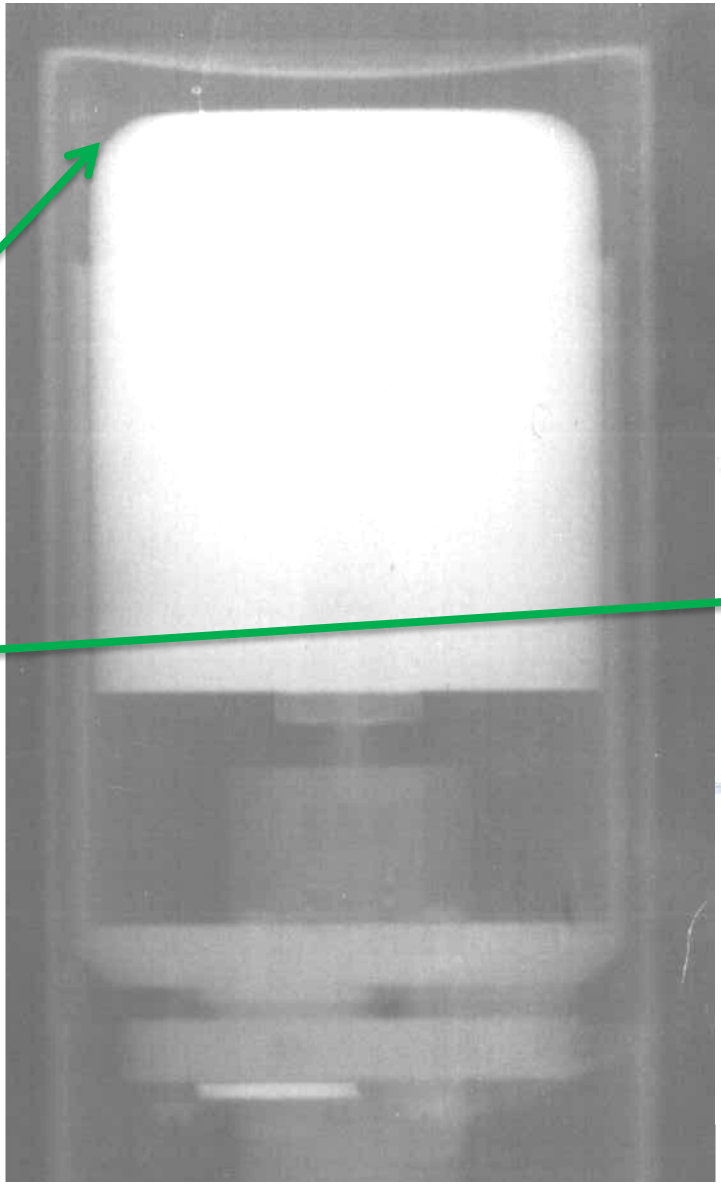
Exp. Eff vs MC			
	low	high	
Mean dev.	-1.0	-1.3	[%]
Stdev of dev.	5.2	3.3	[%]
Median	-3.0	-0.1	[%]
Median (ABS)	4.3	1.7	[%]
MAD	4.5		[%]
MC eff. is	**high**	**high**	
(based on Median value)			

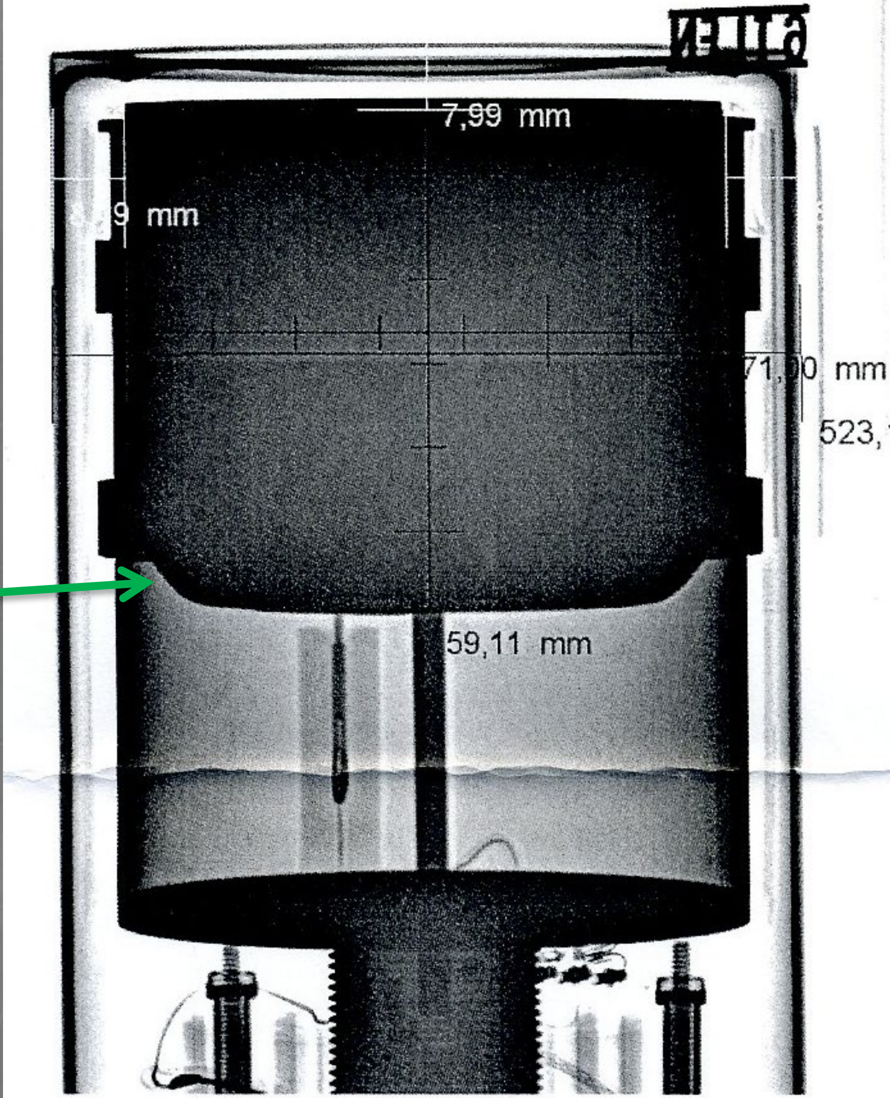
Additional checks for improvement

Radiography

- Get dimensions
- "See" the crystal shape

Rounded edges !



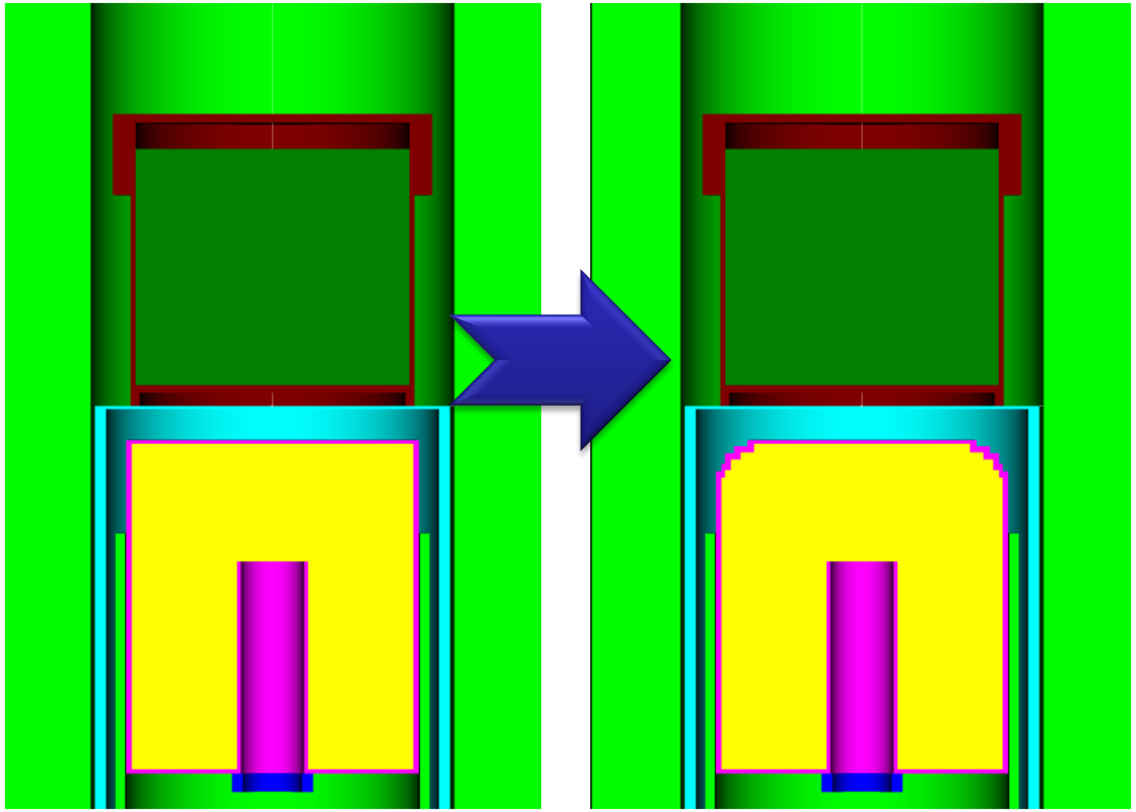


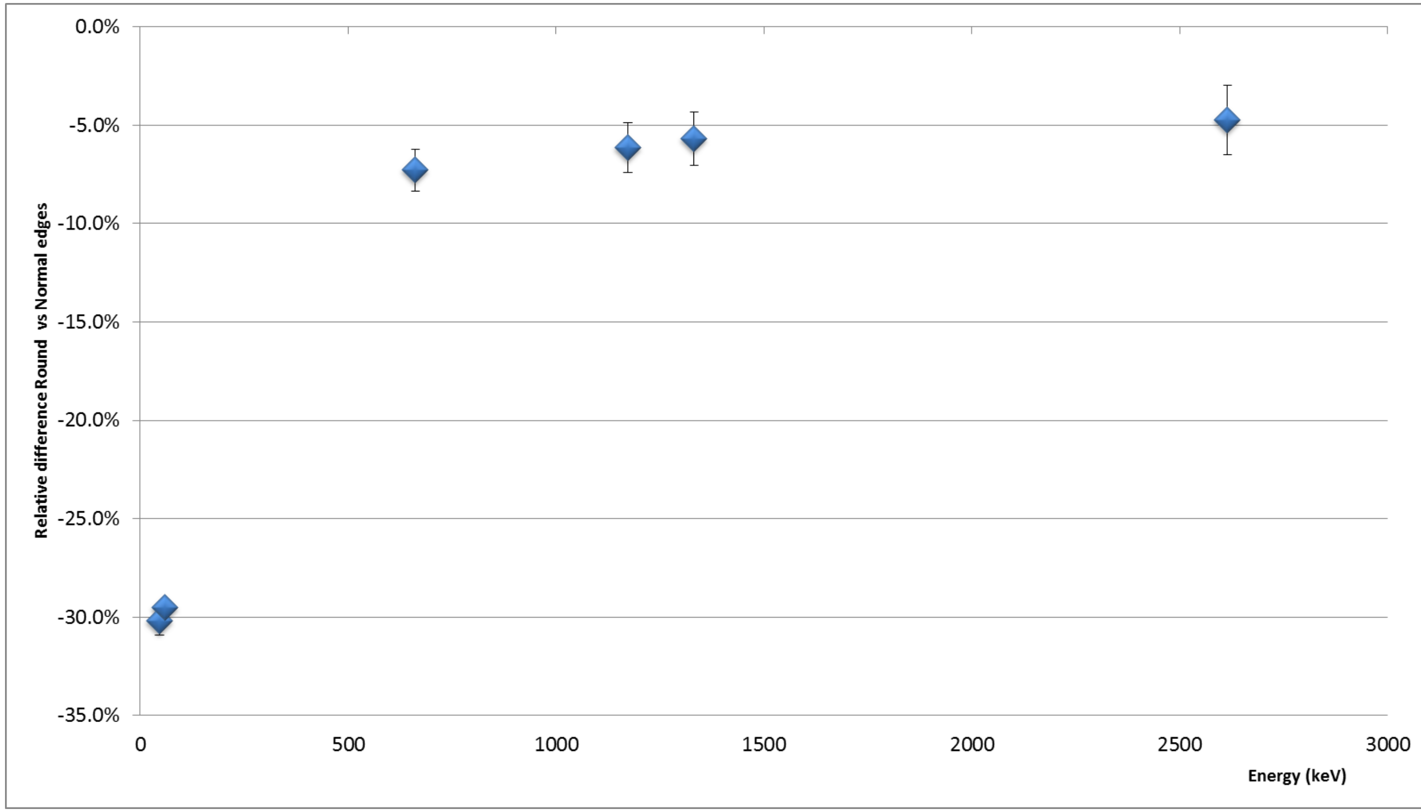
European Commission

Rounded edge effect: top

Monte Carlo FEP efficiency

Relative difference

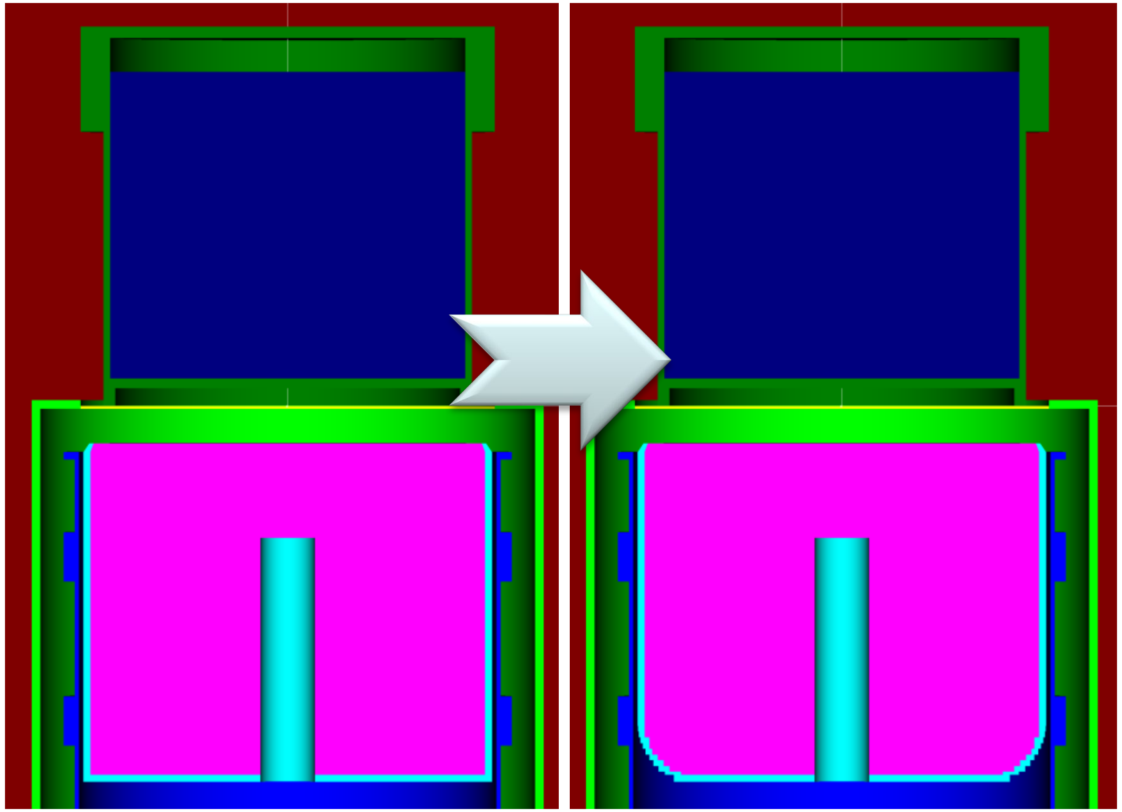




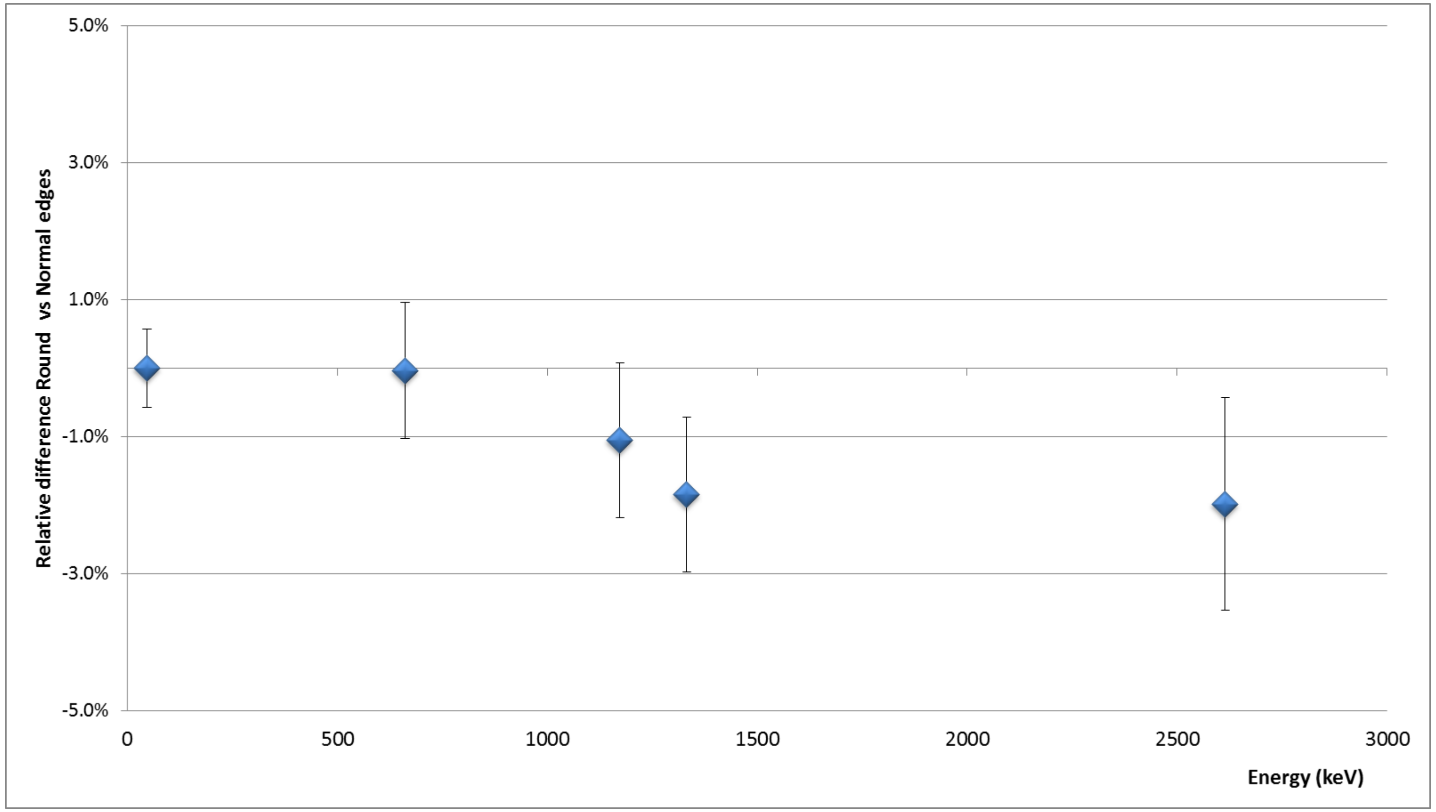
Coaxial P-type, 60% rel. eff., Al endcap, top dead-layer: 0.85 mm

Rounded edge effect: bottom

Monte Carlo FEP efficiency



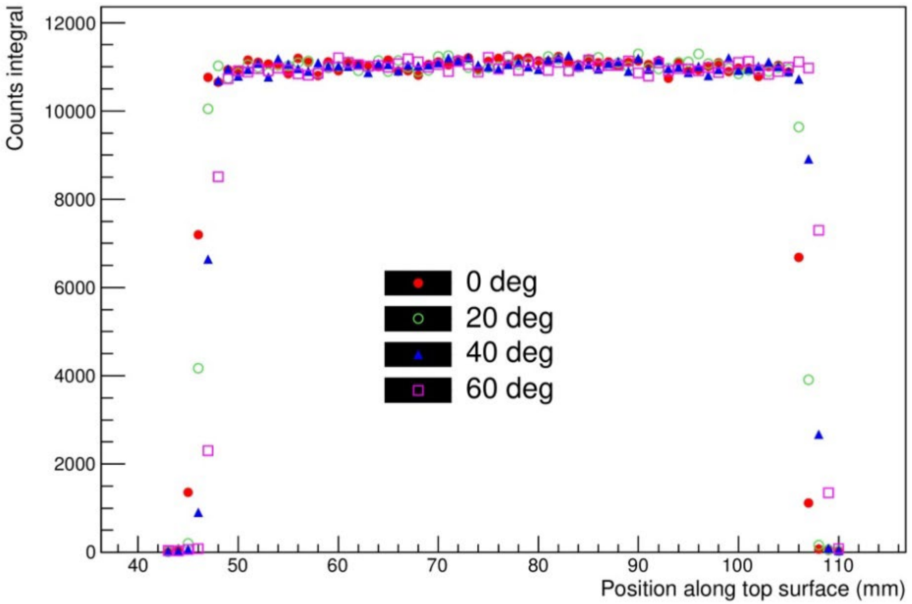
Relative difference



Coaxial P-type, 60% rel. eff., CarbonEpoxy window, top dead-layer: 0.3 µm

Dead-layer scanning

- Collimated ^{241}Am source



- Planar detector
- Produced in 2006
- Top dead-layer: ~0.3 μm
- **Kept at 77° K**

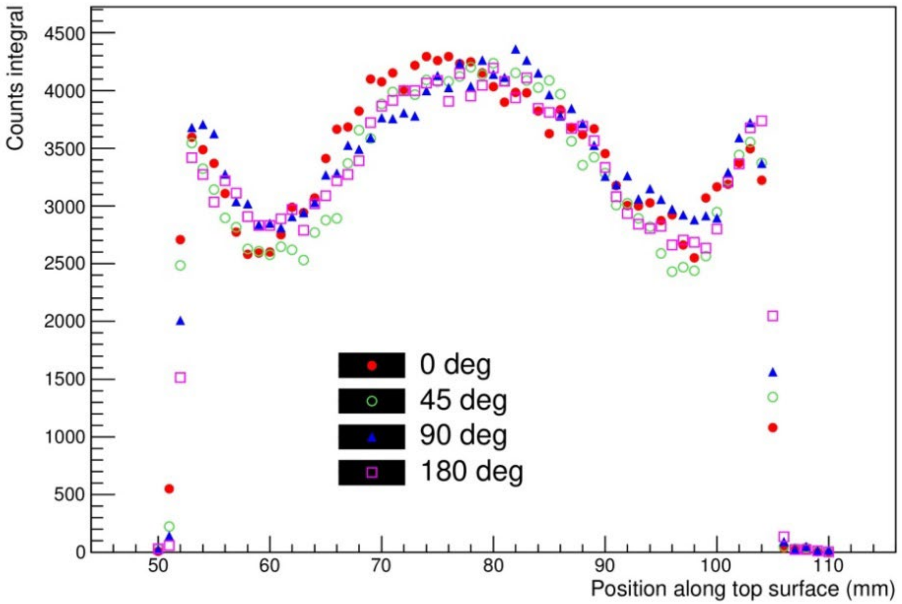
Facility from Gerda neutrino experiment

Determination of dead-layer variation in HPGe detectors,

E. Andreotti, Applied Radiation and Isotopes 87, pp 331-335, May 2014

Dead-layer scanning

➢ Collimated ^{241}Am source



➢ Coaxial detector

➢ Produced in 1984

➢ Top dead-layer: ~1 mm

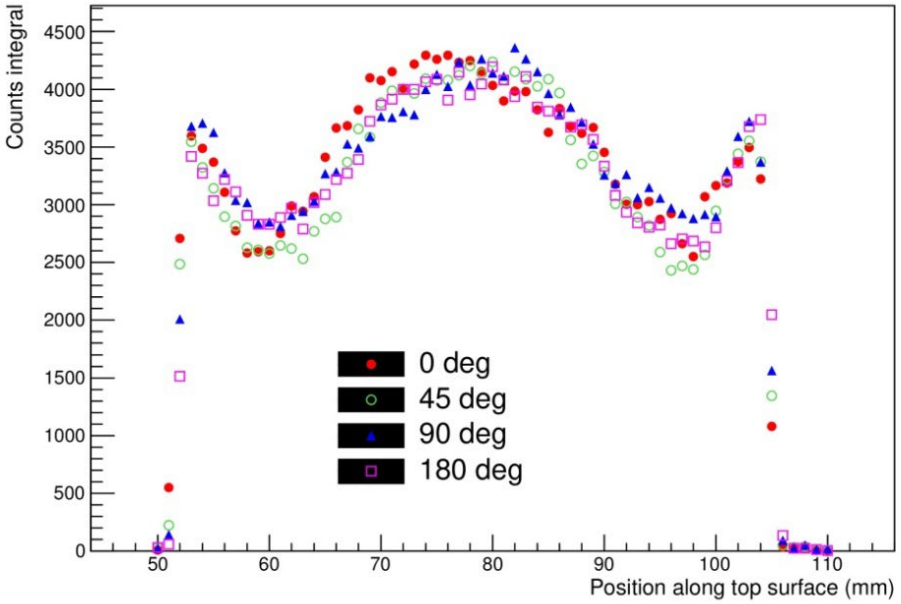
➢ **Several thermal cycles (total 4.4 y at room temperature)**

Facility from Gerda neutrino experiment

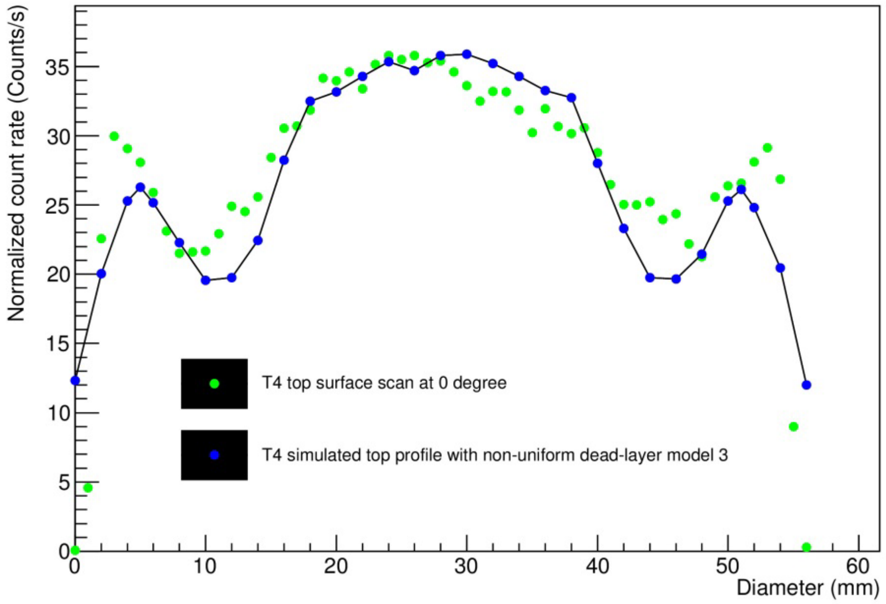
Determination of dead-layer variation in HPGe detectors,

E. Andreotti, Applied Radiation and Isotopes 87, pp 331-335, May 2014

Dead-layer scanning



Monte Carlo model



Energy (keV)	Δε (%)
46.5	32
59.5	22
609	6
1460	3

Relative difference of the simulated efficiency Δε between uniform and non-uniform dead-layer

Determination of dead-layer variation in HPGe detectors,

E. Andreotti, Applied Radiation and Isotopes 87, pp 331-335, May 2014

Sample modelling

Sample modelling

- Elemental composition

Container → Manufacturer

Sample → XRF analysis,…

- Density

Container → Manufacturer

Sample → Calculated

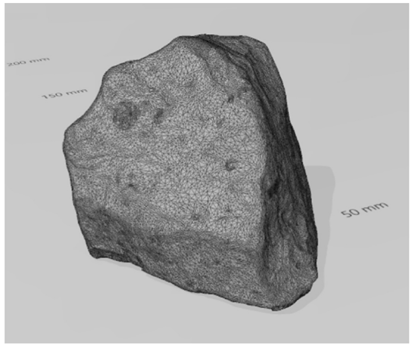
Important for low energy emitters

Sample modelling

- Shape

For complex geometries:

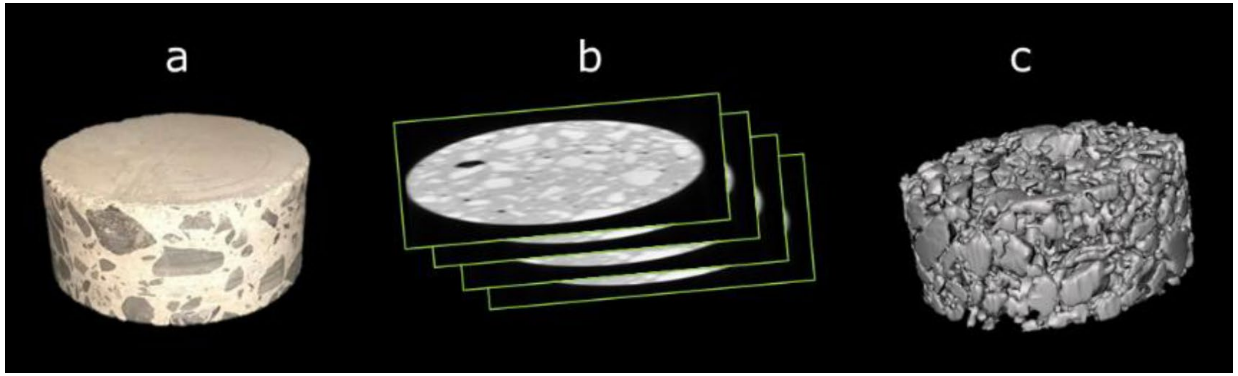
3D scanning



Underground radioactivity measurements of meteorites: Development of methods suitable to determine precise terrestrial age of recent falls,

Z. Tyminski et al, Appl. Rad. and Isotopes 195 (2023) 110733

CT scan



Modelling supported non-destructive in situ depth profiling of 137Cs contaminated concrete,

L. Brabant, PhD thesis, University of Hasselt, Belgium (2023)

Geant4, MCNP, EGSnrc can handle 3D/CT scan data

Key parameters

- Crystal size
- Crystal dead-layers (top, side, bottom)
- Distance endcap-crystal
- Endcap (thickness & composition)
- *Decay data*
- Crystal holder
- Shielding: distance shield-detector
  thickness ≈3-5 cm is enough in model
- Distance sample-detector
- Sample density
- Sample composition
- Sample height
- Sample geometry

Comments

- ✓ Monte Carlo technique is a well-established method
- ✓ Allows to measure a wide range of sample type/shapes
- ✓ It can give ‘good’ results
- ✓ Very good results for Efficiency Transfer method

- ❖ Time consuming at the beginning (especially for old detectors)
- ❖ Easy to make mistakes in the modelling (distance detector-sample, sample size,…)
- ❖ Calculation time is no more a real issue for most of the case (still longer than efficiency transfer)