Estimating measurement uncertainties when the traditional GUM approach «fails»

Alexander Mauring

Contents

Any measurement that you make without the knowledge of its uncertainty is ***completely meaningless***

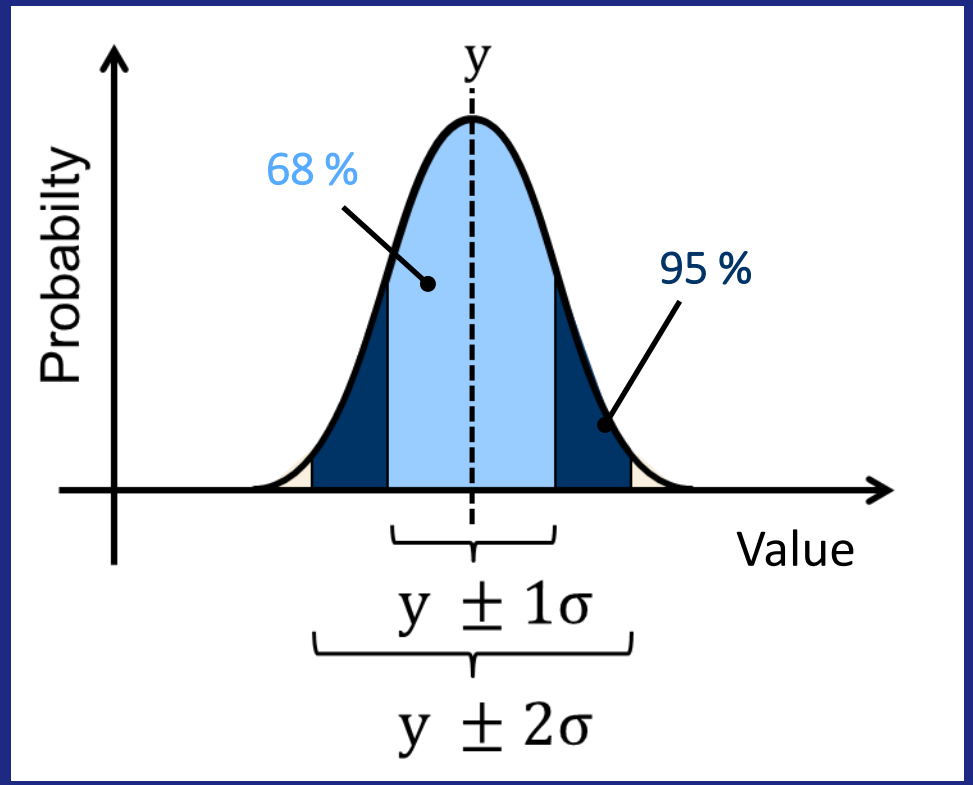
- Walter Lewin

What is uncertainty?

- The number after the "±" sign of a measurement result
- Tells something about how certain we are about our measured value

It’s more than just a number!

- The uncertainty actually tells you something about the likelihood of the “true value” of the measurand being within a certain **interval**
- We define a **probability distribution** together with the measurement result & uncertainty, to state exactly how sure we are about it
- This probability distribution usually has a known shape such as Gaussian/normal, rectangular or triangular distribution



84 ± 12 Bq/kg (k=2)

«I am 95 % certain that the true activity is somewhere between 72 Bq/kg and 96 Bq/kg»

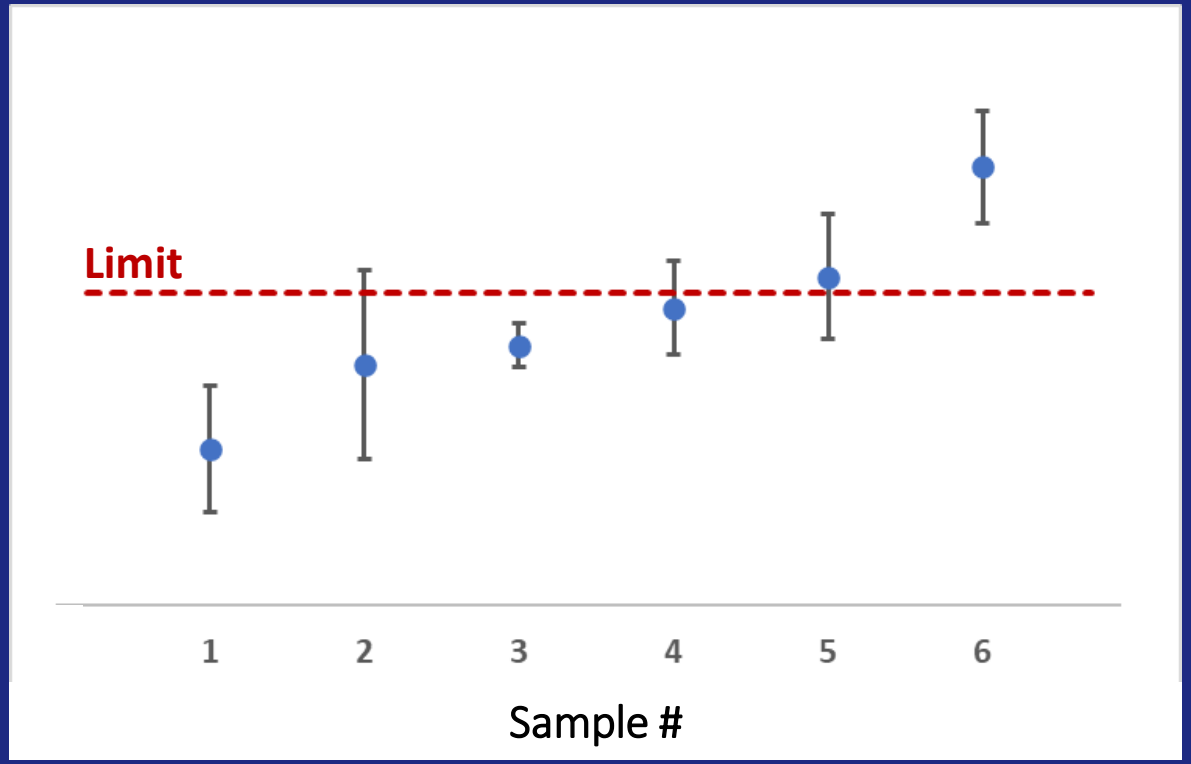
Why do we need to care?

- Imagine that you are measuring samples to compare against some regulatory limit

  Which of the results can you with confidence say are definitely below the limit?

- Good uncertainty estimations can help us to **optimize risks** and **minimize costs**.
  It's worthwhile to do them correctly!

- But if you do not use the correct input, or do the calculations incorrectly, the output will also be inaccurate…



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The «GUM»
Guide to the expression of uncertainty in measurement

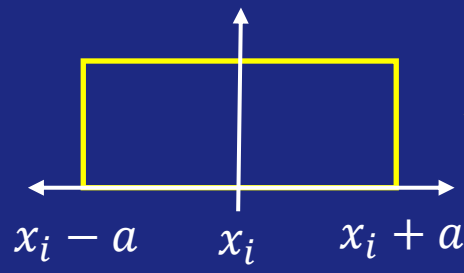
The «bible» for uncertainty calculations since more than 25 years!

https://www.bipm.org/en/committees/jc/jcgm/publications

GUM basics (quick and dirty):

- The quantity you would like to measure $\boldsymbol{y}$ is calculated from measurement function $\boldsymbol{f}$, which consists of several input quantities $\boldsymbol{x_i}$
- Each input quantity has an uncertainty associated with it, with a specific distribution of its **probability density function** (pdf)
- Input quantity uncertainties are all converted into "standard uncertainties" by considering the assumed distributions of their pdf's
- Standard uncertainties are combined through propagation using "sensitivity coefficients" to indicate how variation in each input quantity influences measurand $\boldsymbol{y}$
- This calculation gives the **combined standard uncertainty** of the measurand

$$y = f(x_1, x_2, \dots, x_n)$$



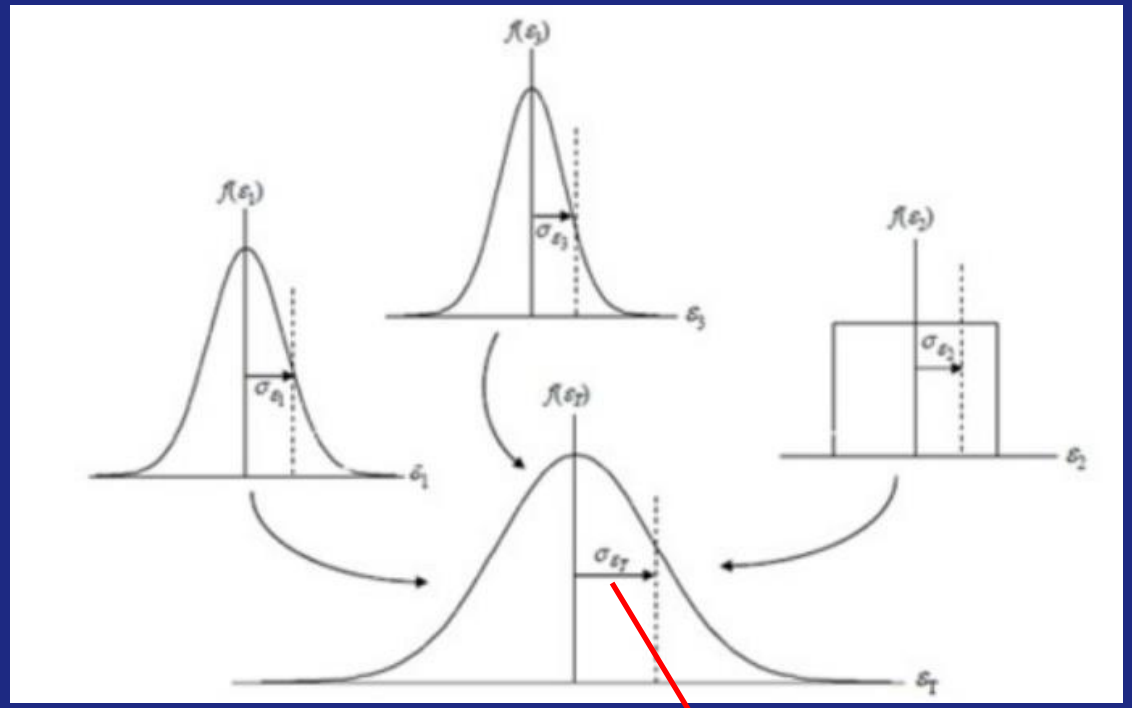
$$\begin{matrix} x_1 \pm u(x_1) \\ \vdots \\ x_n \pm u(x_n) \end{matrix}$$

$$u_c^2(y) = \sum_{i=1}^{n} c_i^2 \cdot u^2(x_i) \quad \text{where} \quad c_i = \frac{\partial y}{\partial x_i}$$

(assumes uncorrelated input quantities)

GUM basics (quick and dirty):

- After combination of individual input quantity uncertainties, the measurand is generally assumed to follow an approximately normal distribution
- Due to the central limit theorem this can also be the case even if the input quantities have other distributions… But not always!
- The normal distribution is very nice to work with, and for expressing uncertainties at a certain confidence level (e.g. ~95 % for k=2)



$$y \pm U(y) = y \pm k \cdot u_c(y)$$

Applied to gamma spec.

- Net peak area $n_{\mathrm{net},E}$
  - Peaked background subtraction
- Measurement live time t
- Efficiency curve fitting
- Gamma emission probability P_E
- Full energy peak efficiency ε_E
  - Efficiency curve fitting
- Correction factors f_E
  - Geometry / self-attenuation correction
  - True Coincidence Summing correction
  - Decay
- Sample quantity q
- … others?

Useful article:
Uncertainties in gamma-ray spectrometry - IOPscience

Measurement equation:

$$a = \frac{n_{\mathrm{net},E}/t}{P_E \cdot \varepsilon_E \cdot q \cdot f_E}$$

Special case of the uncertainty propagation formula when all input quantities are multiplied or divided:

$$\left(\frac{u_c(a)}{a}\right)^2 = \left(\frac{u(n_{\mathrm{net},E})}{n_{\mathrm{net},E}}\right)^2 + \left(\frac{u(P_E)}{P_E}\right)^2 + \left(\frac{u(\varepsilon_E)}{\varepsilon_E}\right)^2 + \left(\frac{u(q)}{q}\right)^2 + \left(\frac{u(f_E)}{f_E}\right)^2$$

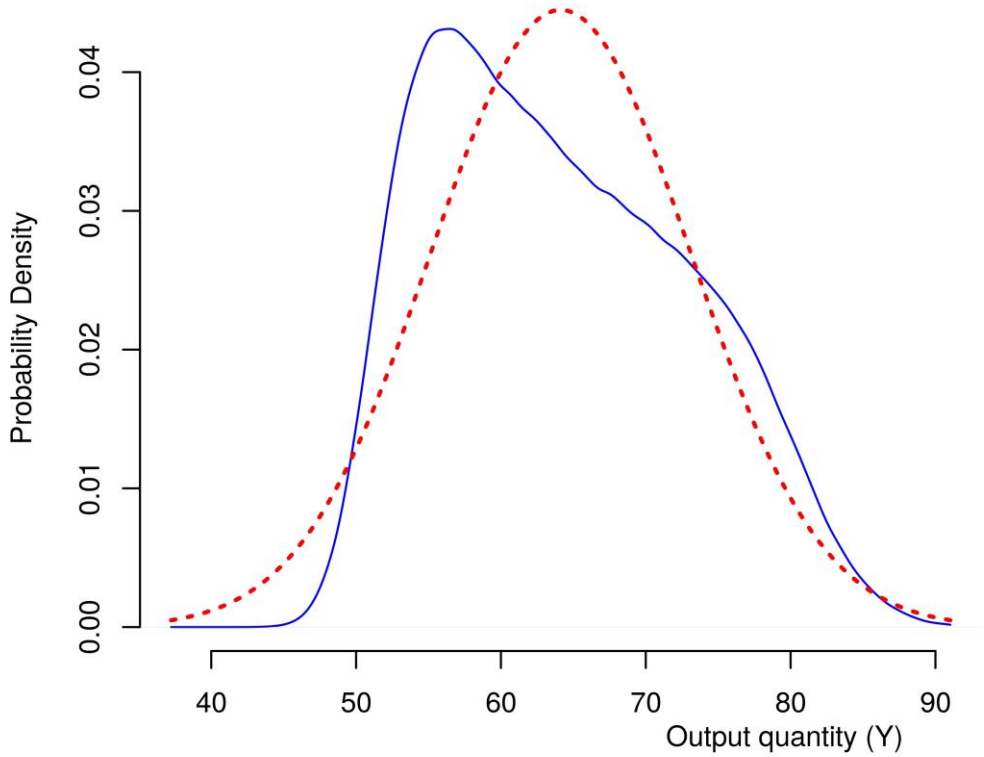
(assuming that the measurement time does not contribute significantly to the overall uncertainty)

So when can this tried and true approach “fail”?

- When a dominant uncertainty component has a pdf with non-normal distribution
- When one or more significant input quantities have a pdf distribution which cannot easily be expressed by a single number ± uncertainty
- When there is no clear “model equation” to propagate the uncertainty through

Example

Dominant uncertainty component with rectangular distribution in the denominator of a fraction

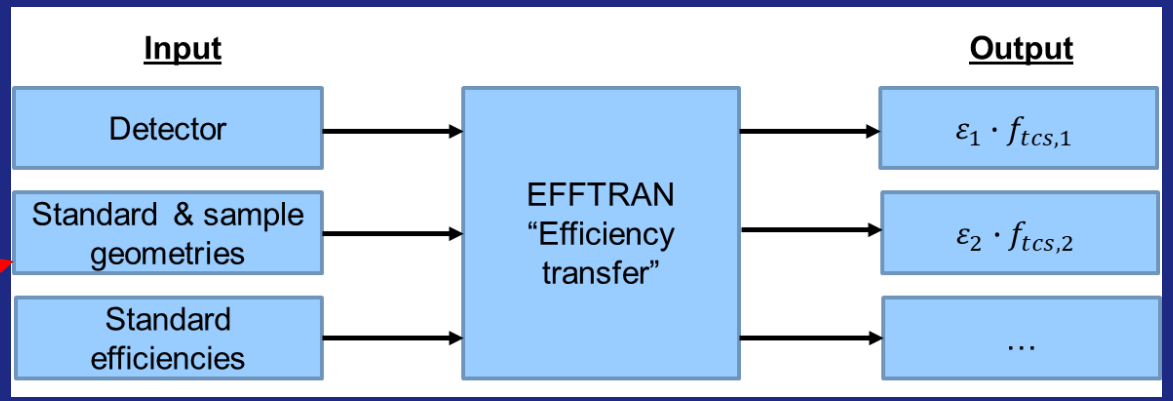


Gaussian output distribution assumed by GUMUF

Actual output distribution

Some relevant examples where the normal GUM approach does not properly apply

- Calculation of full energy peak efficiencies or certain correction factors by software codes
- Certain correction factors in *in situ* gamma-ray spectrometry are calculated from complex expressions involving (numerical) integration
- **In both cases there is no straightforward equation to take partial derivatives of. How can we then deal with the propagation of uncertainties?**



$$\left(\frac{\Delta\Phi_m}{\Phi}\right)_{E,V} = \frac{\int_{\theta_{int}}^{\theta_{ext}} \exp\left(-\mu_{air}\cdot\frac{h}{\cos\theta}\right)\cdot\left[1-\exp\left(-\mu_s\cdot\frac{y}{\cos\theta}\right)\right]\cdot\sin\theta\cdot d\theta}{\int_{0}^{\pi/2} \exp\left(-\mu_{air}\cdot\frac{h}{\cos\theta}\right)\cdot\left[1-\exp\left(-\mu_s\cdot\frac{y}{\cos\theta}\right)\right]\cdot\sin\theta\cdot d\theta}$$

(relative angular fluence for one (!) polar angle segment of «uniform slab» source model)

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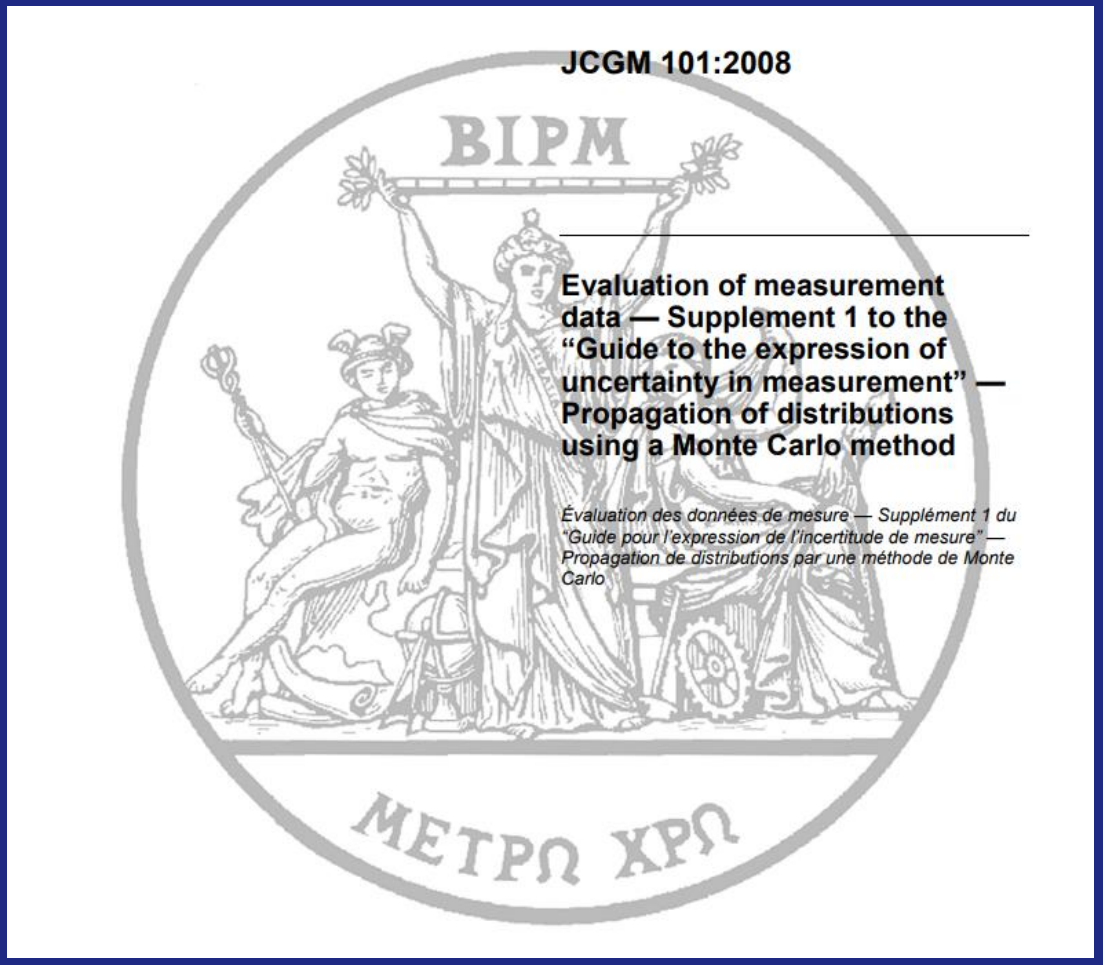
Supplement 1 to GUM deals with Monte Carlo uncertainty propagation, and seems to be getting more and more attention in recent years.



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How does it work?

- Normal GUM approach (GUMUF)
- GUM supplement 1 (MC propagation)

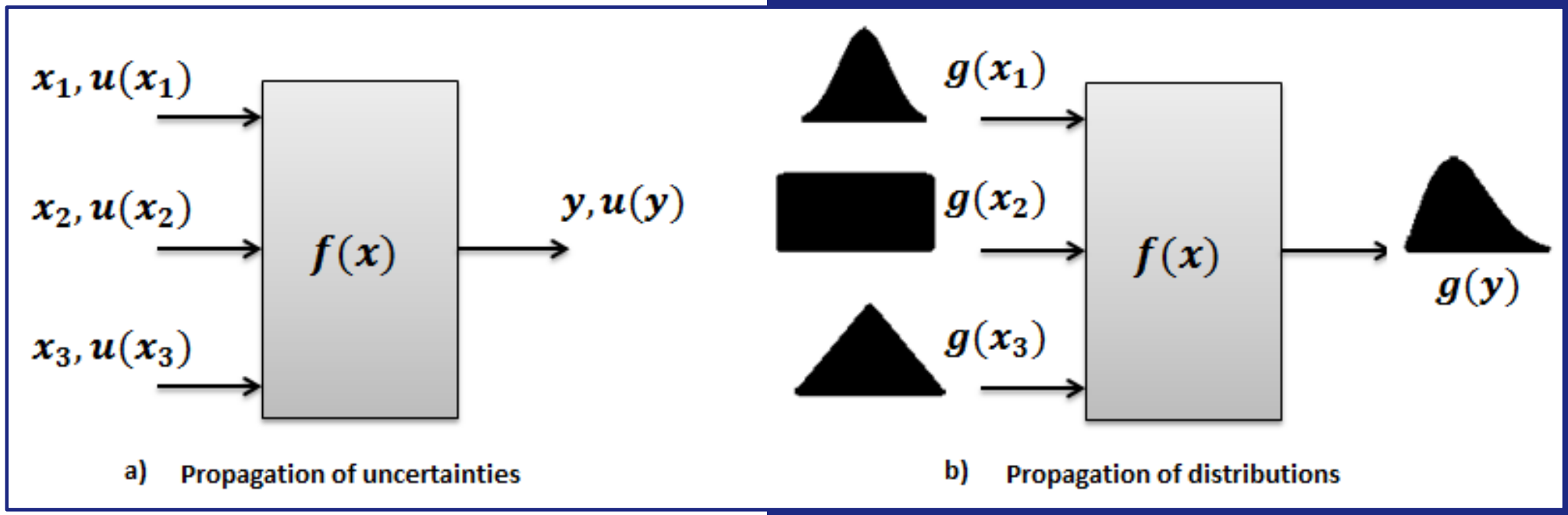
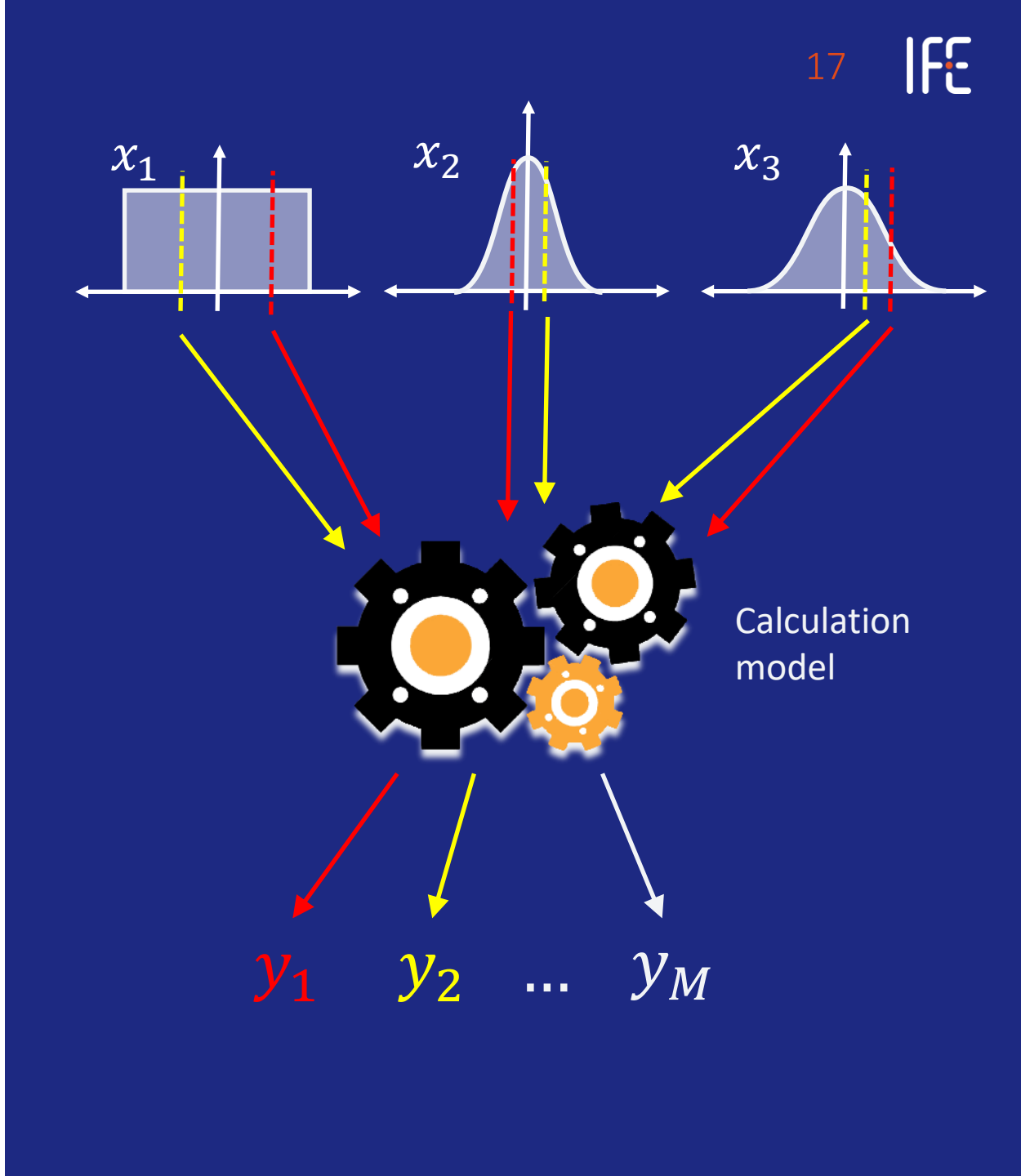


Figure source: Monte Carlo Simulations Applied to Uncertainty in Measurement | IntechOpen

How does it work?

- Each input parameter involved in the computation of the measurand is defined by its pdf with corresponding distribution
- A value is sampled **at random** from each input parameter's pdf distribution
- The computation of the measurand is carried out deterministically using the sampled input values. It could include software computation, numerical integration, strongly non-normal pdf distributions, etc.
- The final output is one possible value of the measurand
- The process is repeated *M* times, so that in the end we get *M* values of the measurand



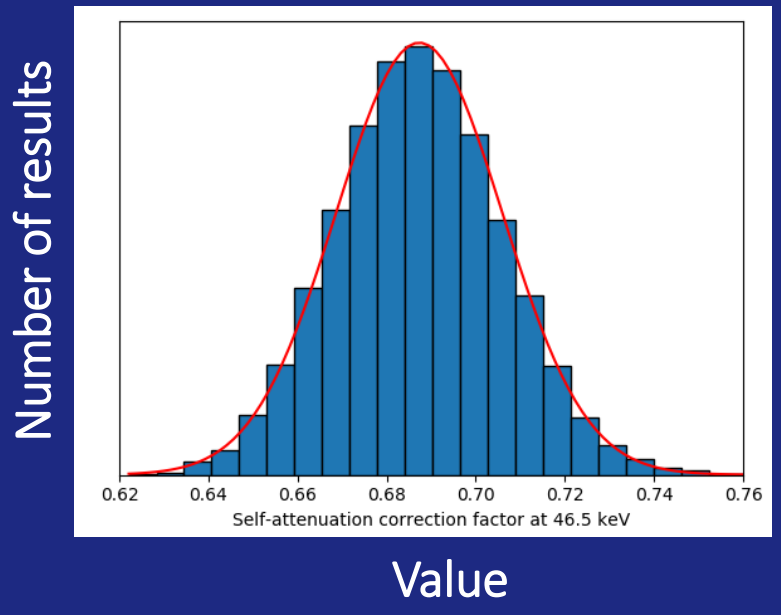
How does it work?

- From the large number of values of the measurand we can then calculate the mean, standard deviation, confidence interval, etc.

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \end{pmatrix} \rightarrow$$

Mean
Standard deviation
Confidence interval
…

- For high numbers of data we can also make a histogram plot to see the actual shape of the distribution of y, even comparing it to a Gaussian distribution



How many runs are needed?

- **How many runs are needed?** Two options:
  1. *M* is chosen a priori
  2. *M* is chosen by adaptive method

- Typically, many thousand runs are carried out. Sometimes even several million!

- There are some clever ways to reduce this number, by using structured sampling schemes such as Latin Hypercube Sampling

1. A priori selection of number of runs

$$M \geq \frac{10^4}{1-p}$$

where p is the chosen coverage probability (e.g. 95% or 0.95)

2. Adaptive method considers the numerical tolerance

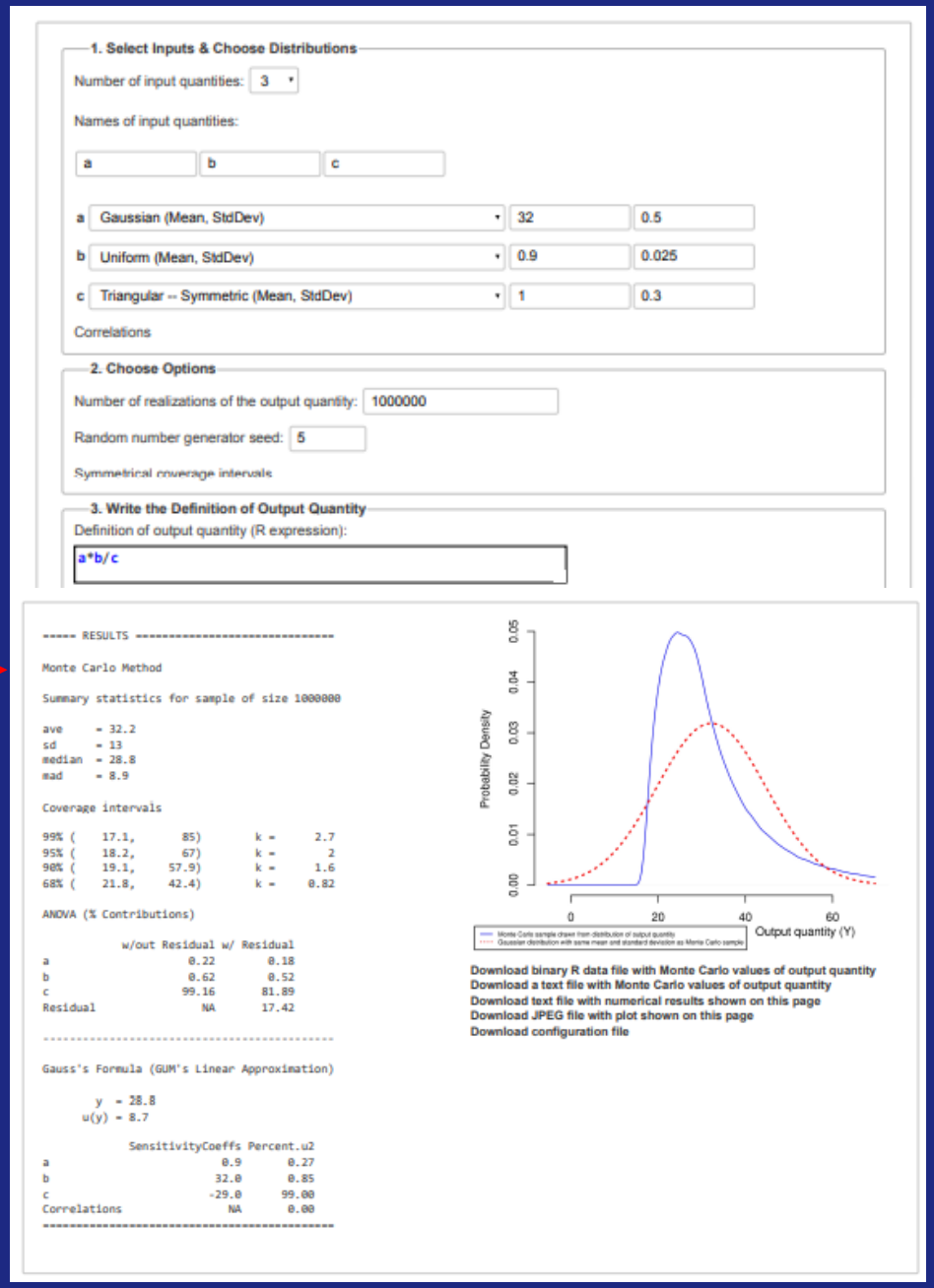
$$\delta \leq 0.5 \cdot 10^{\ell}$$

Result is considered to be stabilized if twice the standard deviation associated with it is less than the numerical tolerance

How can we do it?

- Specialized software
- Programming languages (e.g. Python)
- MS Excel
- NIST Uncertainty Machine (https://uncertainty.nist.gov/)

- **Random number generation is important!**



Simple MC example in Python

- Consider the measurement function

$$y = x_1 + x_2$$

with independent input quantities

$$x_1 = 12 \pm 4 \quad \text{and} \quad x_2 = 8 \pm 3$$

- Using the GUMUF approach:

$$y = 12 + 8 = \underline{20}$$

$$u_c(y) = \sqrt{\left(\frac{\partial y}{\partial x_1}\right)^2 u^2(x_1) + \left(\frac{\partial y}{\partial x_2}\right)^2 u^2(x_2)}$$
$$= \sqrt{4^2 + 3^2} = \underline{5}$$

```python
from numpy import random
from statistics import mean, stdev

x1, u_x1 = 12, 4
x2, u_x2 = 8, 3

M=1000000
y=[]

for i in range(1,M):
    x1_gen = x1 + u_x1*random.randn()
    x2_gen = x2 + u_x2*random.randn()
    y.append(x1_gen + x2_gen)

print("Mean = ", mean(y))
print("Stdev= ", stdev(y))
```

```
Mean =  19.99600148695952
Stdev=  4.999021231763567
```

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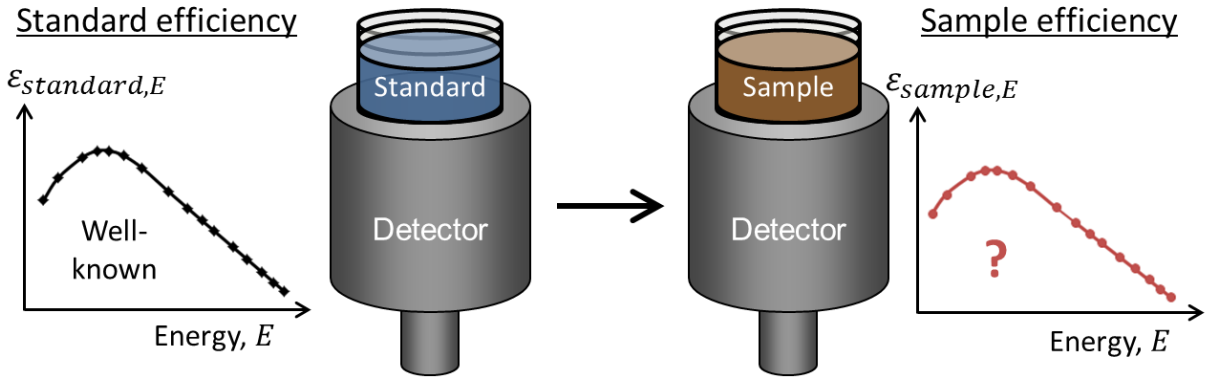
Self-attenuation corrections - theory

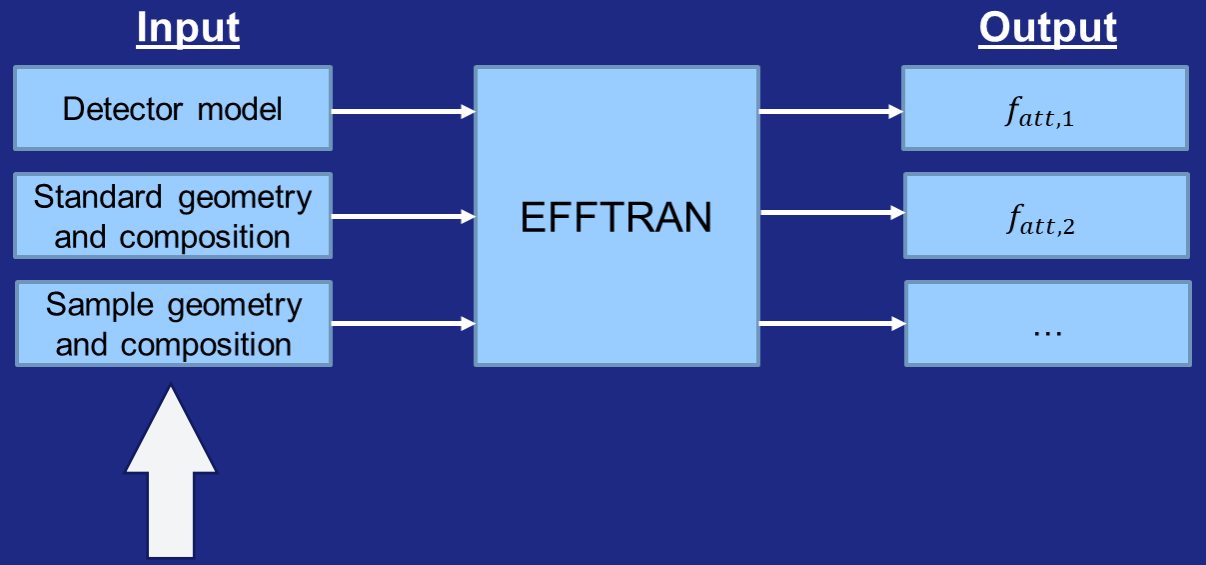


- We measure a sample which is different from the standard used for efficiency calibration in terms of its composition and geometry.
- The FEP efficiency of the sample is given by

$$\varepsilon_{sample,E} = f_{att,E} \cdot \varepsilon_{standard,E}$$

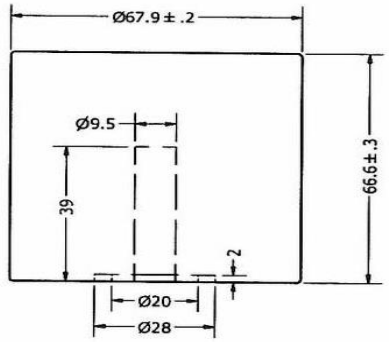
$f_{att,E}$ is the **self-attenuation correction factor**

Calculation of $f_{att,E}$ was done using the free EFFTRAN software tool:

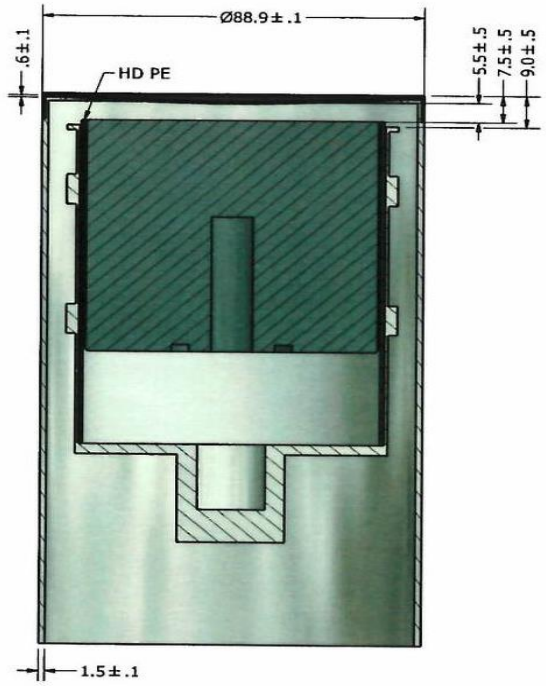


These inputs consist of many parameters, most of which are associated with some kind of uncertainty.

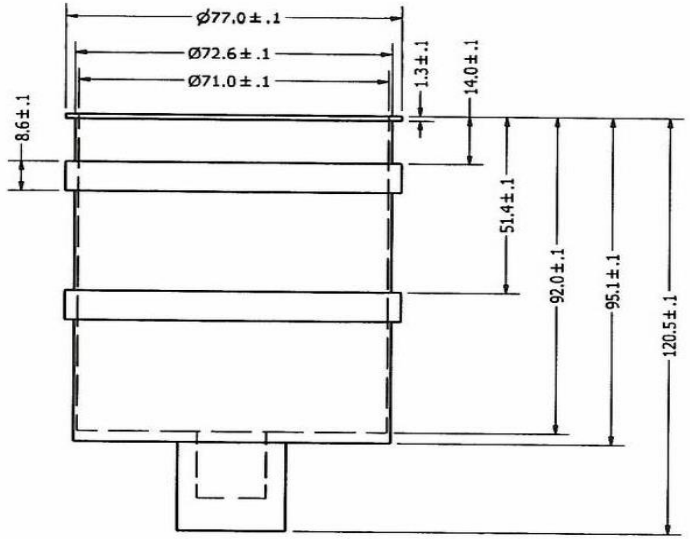
CRYSTAL



ASSEMBLY



HOLDER



S/N: 17013

Front Dead Layer: 0.4µm
Outer Electrode Thickness: 0.5mm
Inner Electrode Thickness: 0.3µm eq. Ge

Ge front to center endcap outside: 5.5mm
Window Material: Carbon Epoxy
Endcap Material: Al
Holder Material: Al

Canberra Semiconductor NV
Lammerdries-Oost 25
2250 Olen
Belgium
Tel. +32-(0)14-221975
CANBERRA

Title: MCNP - DATA

Drawn	mverreydt	6/03/2015	Calculated Weight:
Checked			Project
Approved			CAGE Code 24114
Scale			Size A2
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Other inputs to the computation

- Measurement container parameters
  - Container outer diameter: 45.8 ± 0.2 mm
  - Container side wall thickness: 1.8 ± 0.2 mm
  - Container bottom thickness: 1.25 ± 0.2 mm
  - Container material: C_8H_8, density 1.05 g/cm^3

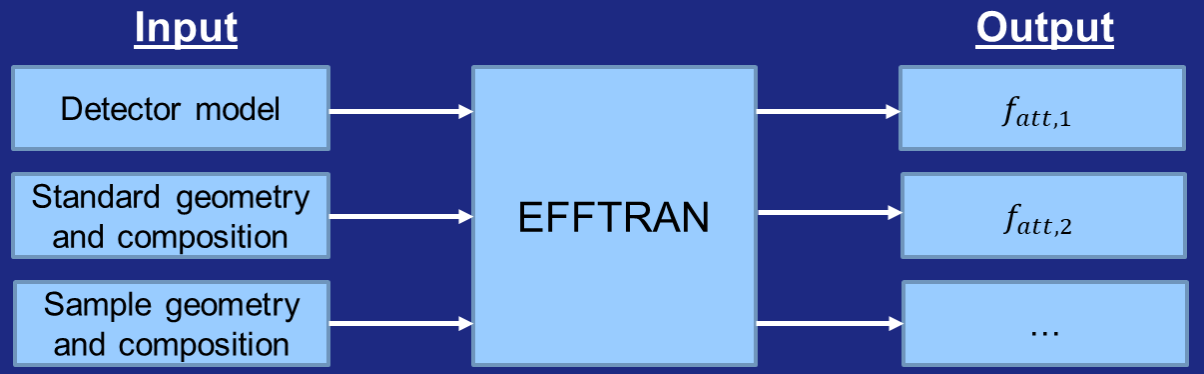
- Standard material: Water (H_2O) with density 1.00 g/cm^3 and filling height 20.0 ± 0.5 mm

- Sample material: Generic material determined by collimated beam transmission measurements resulting in the mass attenuation coefficient

$$\left(\frac{\mu}{\rho}\right)_{46.54\ \mathrm{keV}} = 0.300 \pm 0.016\ \mathrm{cm^2\ g^{-1}}$$

with density 1.54 ± 0.04 g/cm^3 and filling height 26.0 ± 0.5 mm

Calculation methodology



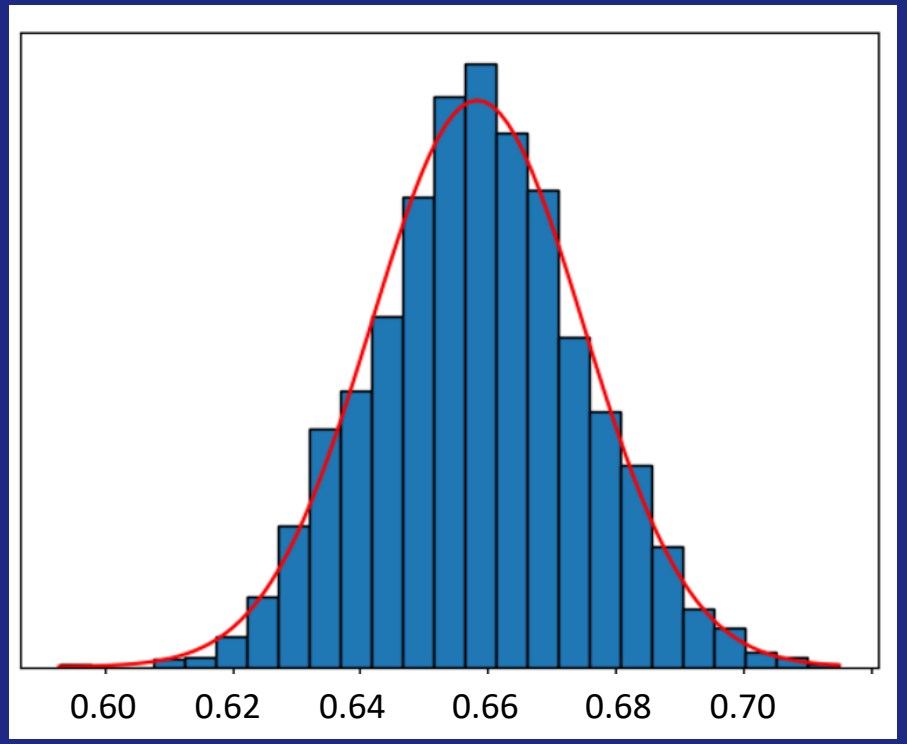
A Python script was set up to run EFFTRAN thousands of times, each time varying each input parameter according to its uncertainty.

The calculated self-attenuation correction factors for each gamma-ray energy was stored to an array after each run.

Results from the Monte Carlo uncertainty propagation

Energy	Relative standard deviation of $f_{\mathrm{att}.E}$	
[keV]	**Case #1**	**Case #2**
46.54	2.41 %	2.37 %
59.54	1.32 %	1.29 %
88.03	0.77 %	0.63 %
122.06	0.67 %	0.49 %
158.97	0.63 %	0.44 %
320.08	0.55 %	0.34 %
391.7	0.53 %	0.32 %
661.66	0.49 %	0.26 %
834.85	0.47 %	0.23 %
898.04	0.46 %	0.22 %
1173.2	0.44 %	0.20 %
1332.5	0.43 %	0.18 %
1836.0	0.41 %	0.16 %

Case #1: All parameters varied during MC computation.
Case #2: Only sample composition and density varied.



Histogram plot of the self-attenuation correction factor at 46.5 keV

Contents

What is sensitivity analysis?

- Also known as "**what-if**" analysis
- **What** happens to my output parameter **if** there is a change in one of the inputs?
- Allowed according to GUM!
- Not as comprehensive as Monte Carlo uncertainty propagation, but often "good enough" for many applications

5.1.3 The partial derivatives $\partial f/\partial x_i$ are equal to $\partial f/\partial X_i$ evaluated at $X_i = x_i$ (see Note 1 below). These derivatives, often called sensitivity coefficients, describe how the output estimate y varies with changes in the values of the input estimates $x_1, x_2, \ldots, x_N$. In particular, the change in y produced by a small change Δx_i in input estimate x_i is given by $(\Delta y)_i = (\partial f/\partial x_i)(\Delta x_i)$. If this change is generated by the standard uncertainty of the estimate x_i, the corresponding variation in y is $(\partial f/\partial x_i)u(x_i)$. The combined variance $u_c^2(y)$ can therefore be viewed as a sum of terms, each of which represents the estimated variance associated with the output estimate y generated by the estimated variance associated with each input estimate x_i. This suggests writing Equation (10) as

$$u_c^2(y) = \sum_{i=1}^{N} \left[c_i u(x_i)\right]^2 \equiv \sum_{i=1}^{N} u_i^2(y) \qquad (11a)$$

where

$$c_i \equiv \partial f/\partial x_i, \quad u_i(y) \equiv |c_i| u(x_i) \qquad (11b)$$

NOTE 1 Strictly speaking, the partial derivatives are $\partial f/\partial x_i = \partial f/\partial X_i$ evaluated at the expectations of the X_i. However, in practice, the partial derivatives are estimated by

$$\frac{\partial f}{\partial x_i} = \left.\frac{\partial f}{\partial X_i}\right|_{x_1, x_2, \ldots, x_N}$$

NOTE 2 The combined standard uncertainty $u_c(y)$ may be calculated numerically by replacing $c_i u(x_i)$ in Equation (11a) with

$$Z_i = \frac{1}{2}\left\{f\left[x_1, \ldots, x_i + u(x_i), \ldots, x_N\right] - f\left[x_1, \ldots, x_i - u(x_i), \ldots, x_N\right]\right\}$$

That is, $u_i(y)$ is evaluated numerically by calculating the change in y due to a change in x_i of $+u(x_i)$ and of $-u(x_i)$. The value of $u_i(y)$ may then be taken as $|Z_i|$ and the value of the corresponding sensitivity coefficient c_i as $Z_i/u(x_i)$.

How to do the calculations?

- Vary input quantity x_i by an amount $\pm u(x_i)$, and look at how the output y changes

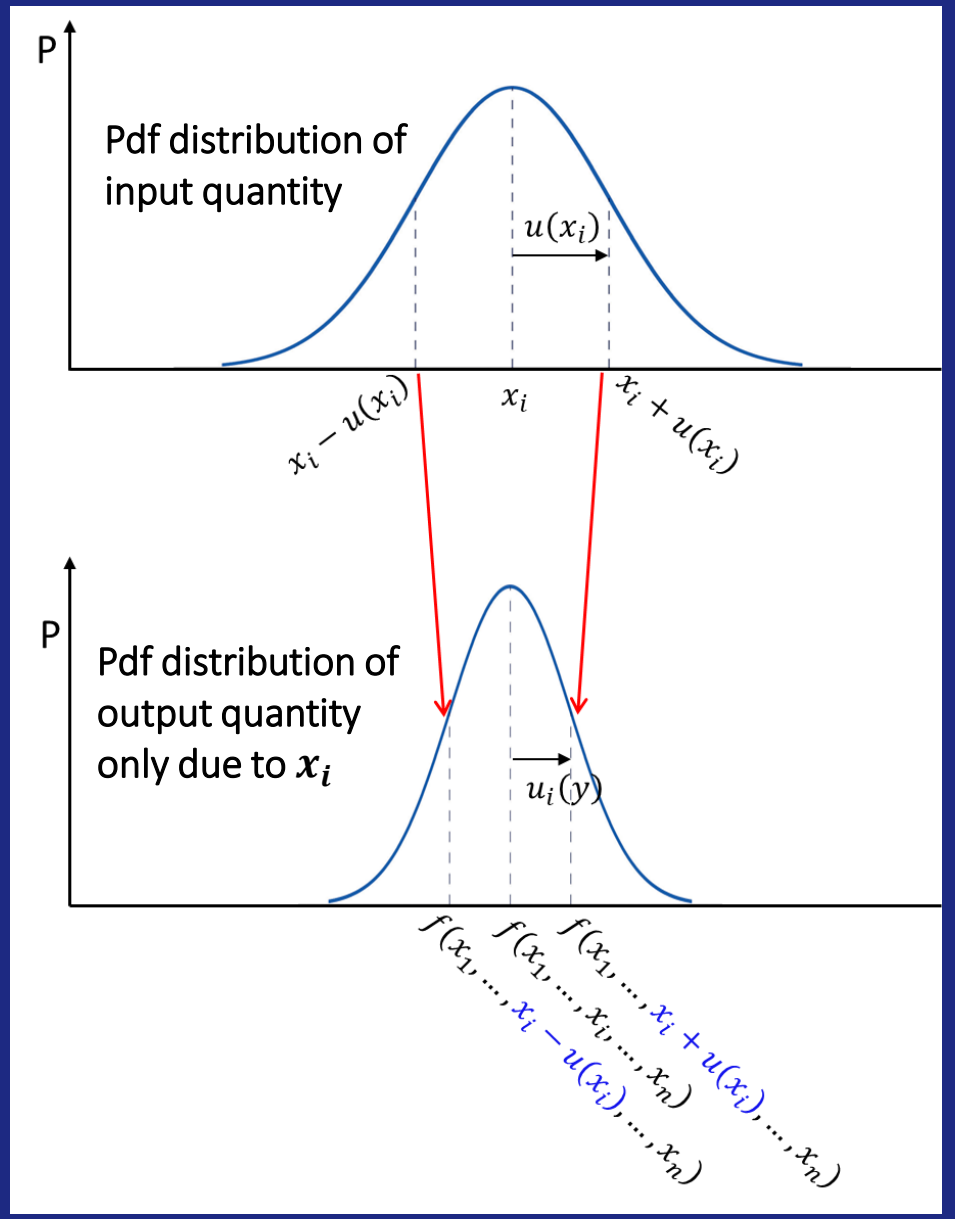
- The standard uncertainty contribution to y from input x_i is formally calculated as

$$u_i(y) = \left| \frac{f(x_1, \ldots, \boldsymbol{x_i + u(x_i)}, \ldots, x_n) - f(x_1, \ldots, \boldsymbol{x_i - u(x_i)}, \ldots, x_n)}{2} \right|$$

- Is then repeated for other input quantities, and the total combined standard uncertainty of y can be calculated from the equation

$$u_c^2(y) = \sum_{i=1}^{n} u_i^2(y)$$

- **There's no need for a definite "measurement equation" or any partial derivatives!**

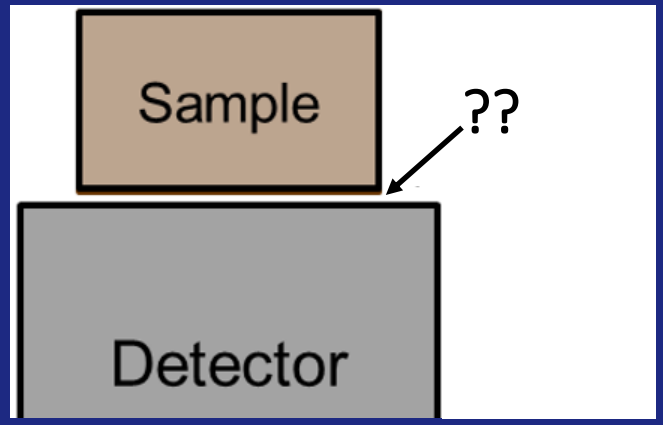


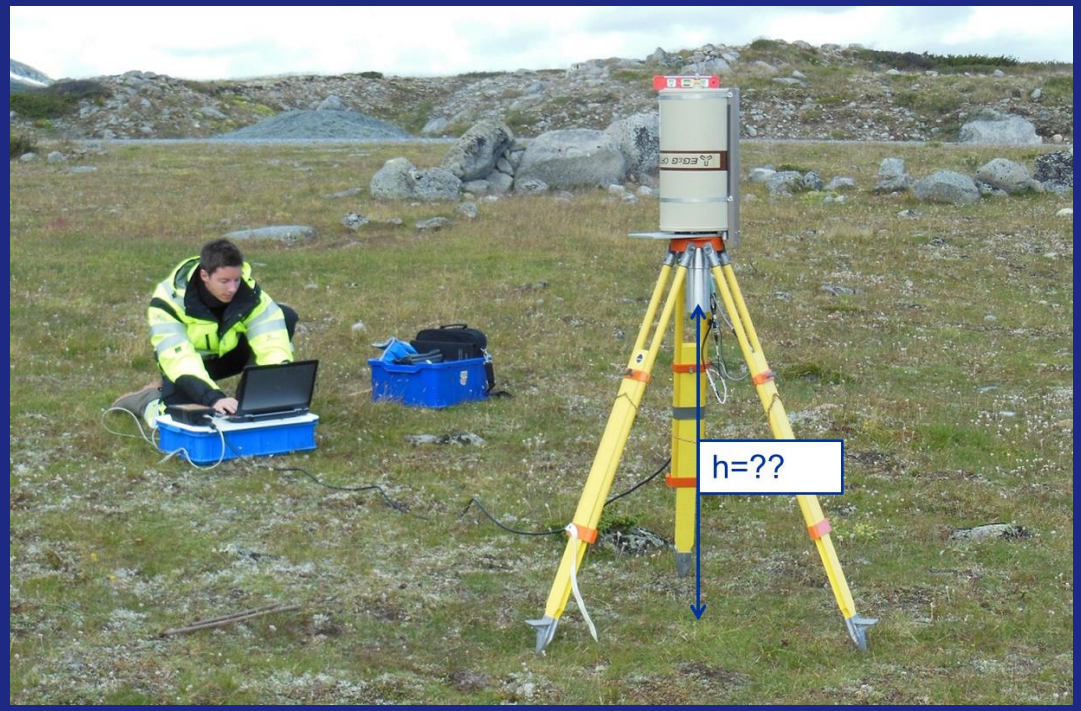
Some relevant cases

- How much does the TCS correction factor vary if the distance between the container and the detector changes by 1 mm? 2 mm? 5 mm?

- What is the change in the self-attenuation correction factor if the sample composition is varied in the calculation?

- When making *in situ* gamma-ray spectrometry measurements, the height of the detector above the ground was not properly recorded. How can this influence the final result (and its associated uncertainty?)





Example: Impact of filling height on the TCS correction for Co-60

- You measure a water sample containing Co-60
- The sample is in a cylindrical container with inner diameter 50 mm, directly on top of the "standard" p-type detector defined in EFFTRAN
- The filling height of the sample is estimated to 5 ± 1 mm (Gaussian distribution, k=1)
- What is the uncertainty in the TCS correction factor for the 1173 keV gamma peak due to the uncertainty in the filling height?

Using EFFTRAN

Sample filling height	TCS correction factor for 1173 keV peak
4 mm	1.161 $f(\dots, x_i - u(x_i), \dots)$
5 mm	1.157
6 mm	1.153 $f(\dots, x_i + u(x_i), \dots)$

Uncertainty in TCS correction factor due to uncertainty in filling height:

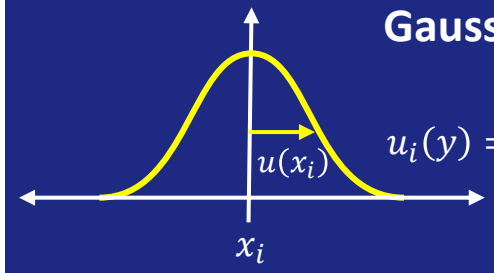
$$\left|\frac{f(\dots, x_i + u(x_i), \dots) - f(\dots, x_i - u(x_i), \dots)}{2}\right|$$

$$= \left|\frac{1.153 - 1.161}{2}\right| = \underline{0.004}$$

(or around 0.34 % relative to 1.157…)

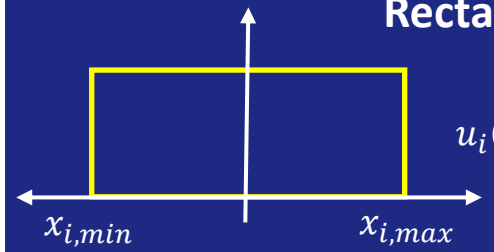
A “worst case” approach for more tricky cases

- It is possible to extend the sensitivity analysis to other types of input distributions
- This could be useful when you only know what the maximum and minimum possible values of a certain input parameter are, and you’re not sure if it has a Gaussian distribution
- **Example from *in situ* gamma spectrometry:** *“I know that the Cs-137 deposition in the ground is a uniform layer with thickness between 5 cm and 15 cm. What is the uncertainty due to this variation?”*



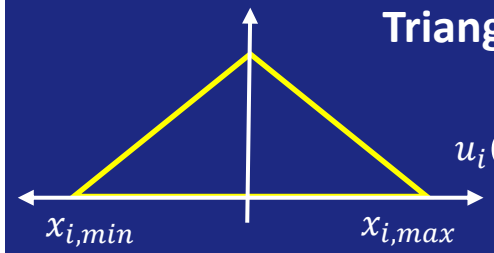
Gaussian (normal) distribution of x_i:

$$u_i(y) = \frac{f(\dots, x_i + u(x_i), \dots) - f(\dots, x_i - u(x_i), \dots)}{2}$$



Rectangular (uniform) distribution of x_i:

$$u_i(y) = \frac{f(\dots, x_{i,max}, \dots) - f(\dots, x_{i,min}, \dots)}{\sqrt{12}}$$



Triangular distribution of x_i:

$$u_i(y) = \frac{f(\dots, x_{i,max}, \dots) - f(\dots, x_{i,min}, \dots)}{\sqrt{24}}$$

Contents

Summary and conclusions

- The traditional GUM approach to uncertainty calculations is “good enough” in many standard situations, but has some limitations:
  - Dominant non-Gaussian input quantities
  - Lack of proper measurement equation, or complex measurement equation
- In the difficult cases, it could be worthwhile to look into Monte Carlo uncertainty propagation
- Sensitivity / “what-if” analysis could also be a useful tool to get an idea of how much the variation of an input parameter affects your final results

- Monte Carlo uncertainty propagation seems to be getting more interest lately. So don’t be surprised if you hear about it in the future
- Don’t be afraid to try it out ☺

Thank you for your attention!
Any questions?

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