

СОФИЙСКИ УНИВЕРСИТЕТ
„СВ. КЛИМЕНТ ОХРИДСКИ“

ФИЗИЧЕСКИ ФАКУЛТЕТ



SOFIA UNIVERSITY
ST. KLIMENT OHRIDSKI

FACULTY OF PHYSICS

Evaluation of uncertainties in measurement

Philippe Cassette

visiting professor at Sofia University "St. Kliment Ohridski"

The easy way to avoid problems...

If your experiment needs statistics, you should have done a better experiment Ernest Rutherford (1871 – 1937)



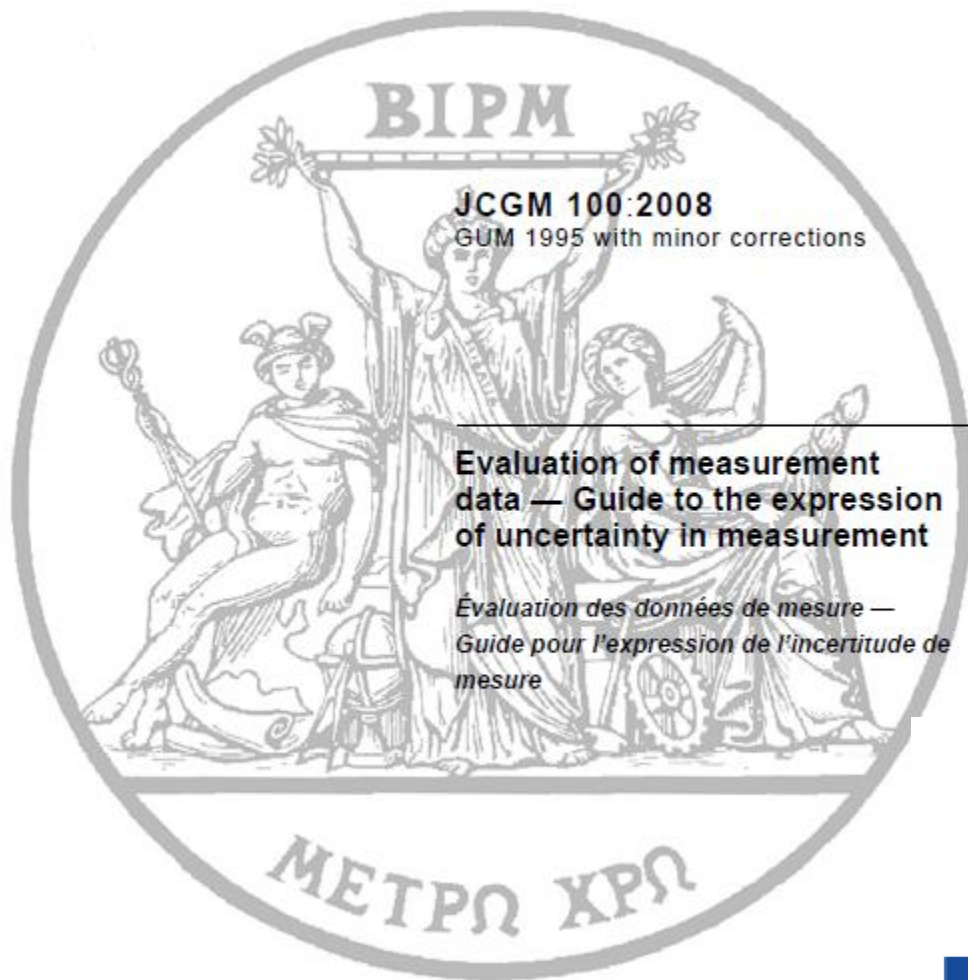
Never repeat a measurement: there is a serious risk that you will not find the same result...

But we are not here to recommend this kind of approach!

Evaluation of uncertainties in measurement

In 1977, recognizing the lack of international consensus on the expression of uncertainty in measurement, the world's highest authority in metrology, the Comité International des Poids et Mesures (CIPM), requested the Bureau International des Poids et Mesures (BIPM) to address the problem in conjunction with the national standards laboratories and to make a recommendation.

- Creation of a working group (CIPM 1977)
- Questionnaire to national metrology laboratories (February 1978)
- Report BIPM 80-3
- Recommendation INC-1 1980 « expression of experimental uncertainties »
- Approbation of INC-1 in 1981 by CIPM
- First publication of the GUM in 1993
- 1995 edition after minor corrections



BIPM: Bureau International des Poids et Mesures

IEC: International Electrotechnical Commission

IFCC: International Federation of Clinical Chemistry

ISO: International Organization for Standardization

IUPAC: International Union of Pure and Applied Chemistry

IUPAP: International Union of Pure and Applied Physics

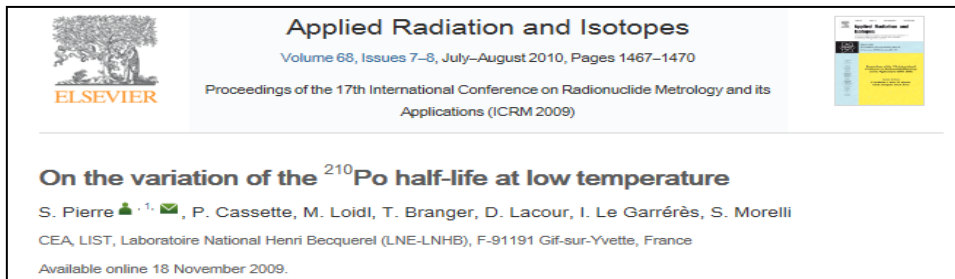
OIML: International Organization of Legal Metrology



Uncertainties in physics

Example of the interest to correctly evaluate the uncertainties

Raiola *et al.* 2007* : decrease of the half-life or alpha radionuclides at low temperature. Experimental observation: decrease of the half-life of ^{210}Po of $(6,3 \pm 1,4) \%$ from 300 K to 12 K.



New experiment at LNE-LNHB in 2009, with exhaustive evaluation of uncertainties. Conclusion: no significant effect!

The measurement uncertainties of the Raiola experiment were under evaluated, and some bias were not taken into account, leading to a wrong scientific conclusion... and a wrong theory to explain this phenomenon.

* F. Raiola et al., Physical Journal A—Hadrons and Nuclei, 32 (2007), pp. 51–53

The ideal method for evaluating and expressing the uncertainty of the result of a measurement should be:

- **Universal:** the method should be applicable to all kinds of measurements and to all types of input data used in measurements.

The actual quantity used to express uncertainty should be:

- **Unique** (*nothing like systematic and random uncertainty*)
- **Internally consistent:** it should be directly derivable from the components that contribute to it, as well as independent of how these components are grouped and of the decomposition of the components into subcomponents
- **Transferable:** it should be possible to use directly the uncertainty evaluated for one result as a component in evaluating the uncertainty of another measurement in which the first result is used.

Concepts and definitions

*The result of a measurement is a random variable...
... and must be processed accordingly*

Error and uncertainty are very different concepts

Error: measured quantity value minus a reference quantity value. As the reference quantity value (true value) is unknown, the error is generally unknown...

If a measurement error (bias) is suspected, it must be corrected... but this does not completely suppress the doubt about the result

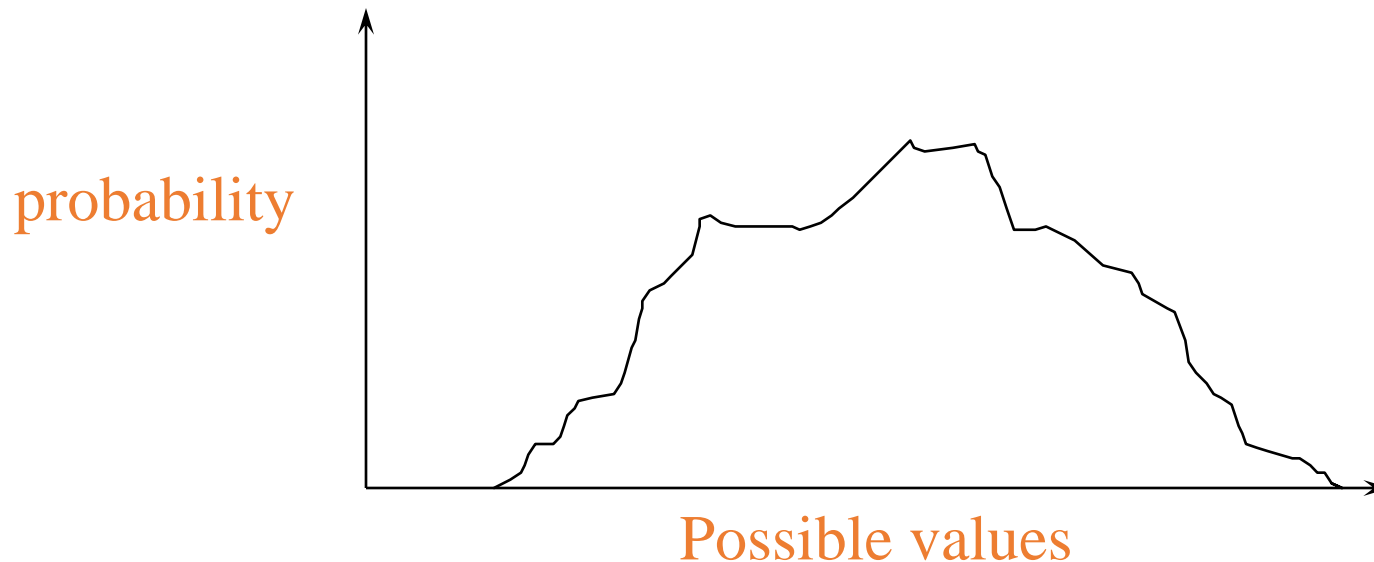
Uncertainty: non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used

The word “uncertainty” means doubt, and thus in its broadest sense “uncertainty of measurement” means doubt about the validity of the result of a measurement.

Random variable

A **random variable**, or **stochastic variable** can be described informally as a **variable whose values depend** on **outcomes** of a **random** phenomenon.

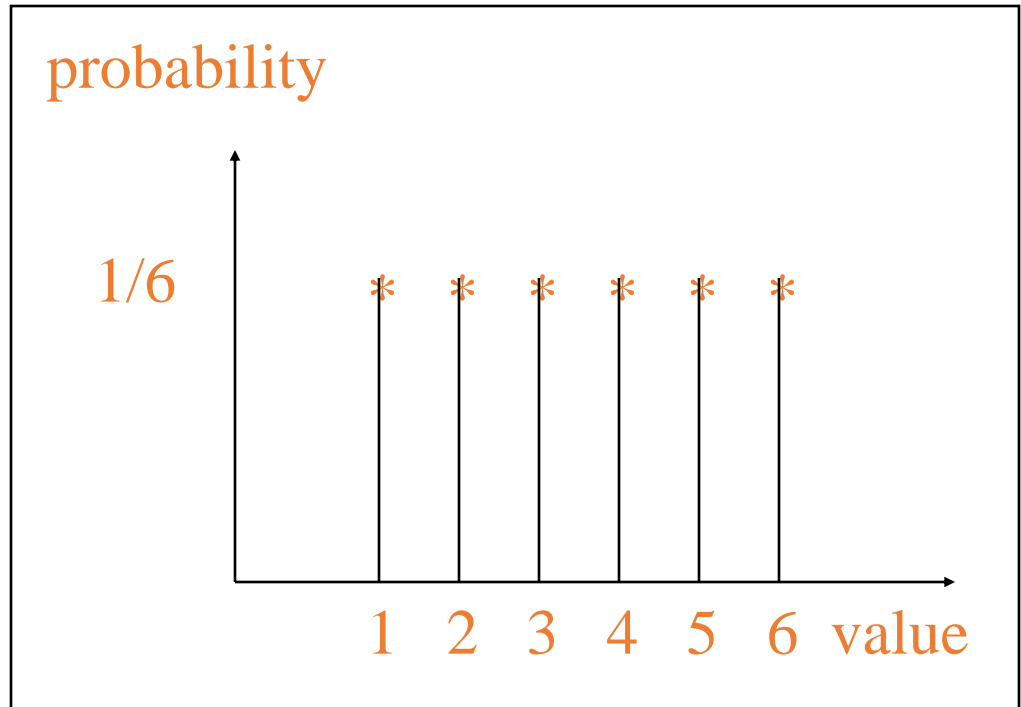
A random variable has a **probability distribution**, which specifies the probability of its range. A probability density function can be defined for continuous random variables



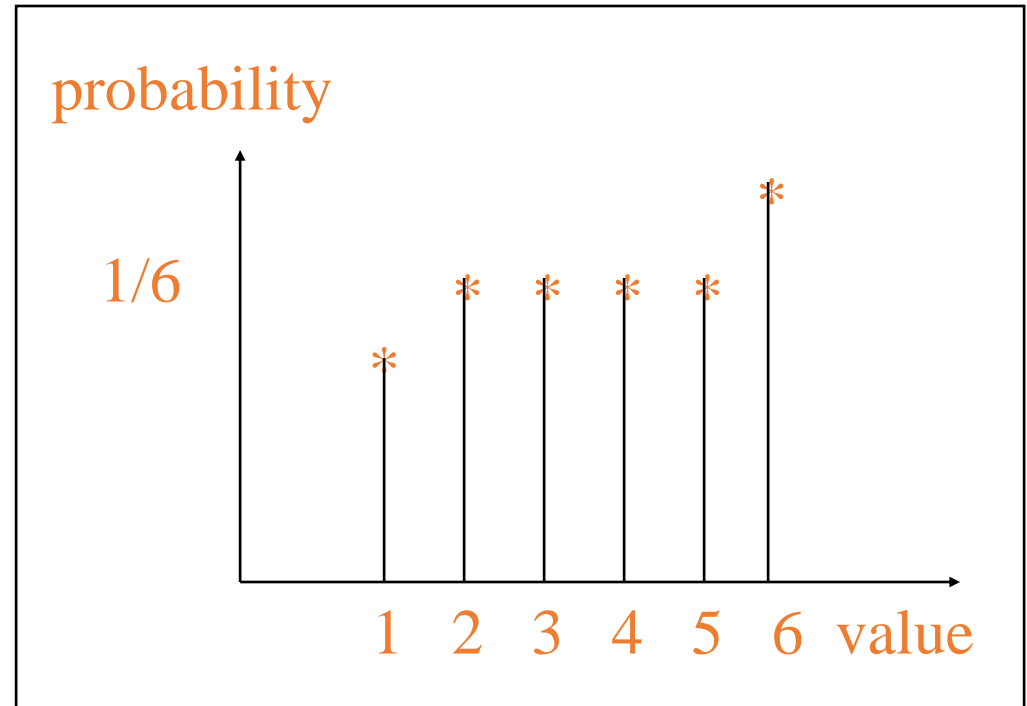
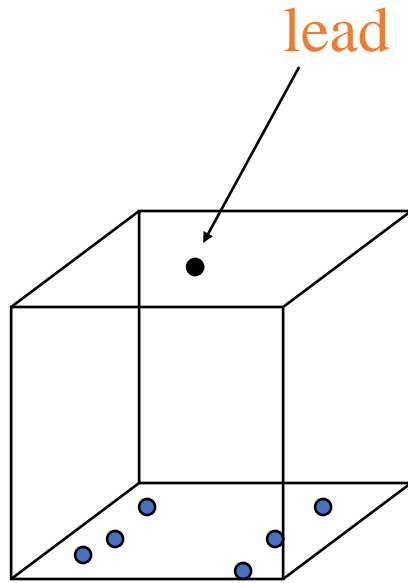
Example of probability distribution: uniform discrete random variable



Playing dice



Other example: the loaded dice



If you change the physics, the probability distribution can change

Other discrete random variable, the Poisson distribution

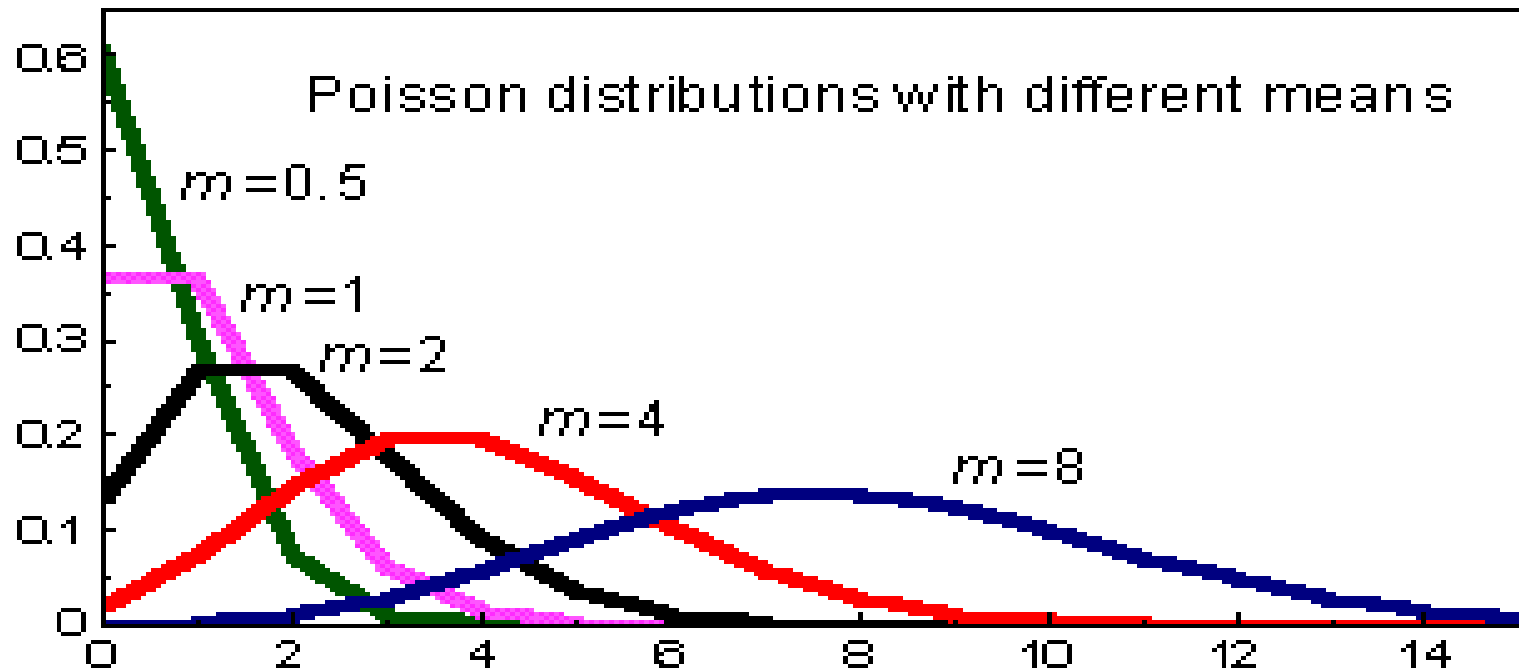
$$P(x, M) = \frac{M^x \times e^{-M}}{x!}$$

$P(x, M)$ is the probability to get the value x for an expected value M

Standard deviation $S = \sqrt{M}$

Poisson distribution

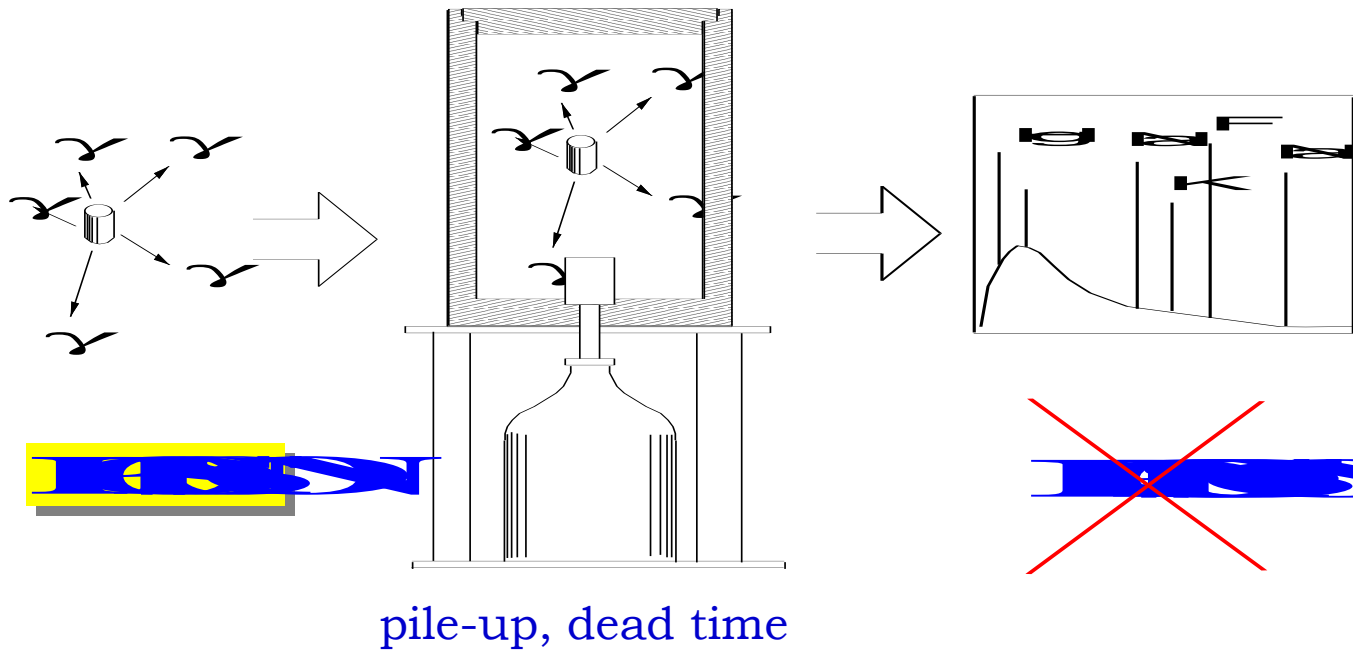
probability distribution that characterizes discrete events occurring independently of one another in time



NOT Poisson distribution:

- **Simultaneous emission of radiation by mother and daughter decay products**
 - dependent increments
- **Cascade of gamma emission, delayed or not**
 - simultaneous : clustering of events
 - delayed states : dependent increments
- **Source decay over a long period ($\sim T_{1/2}$)**
 - not stationary, 'activity' (event rate) diminishes

Non-random count loss

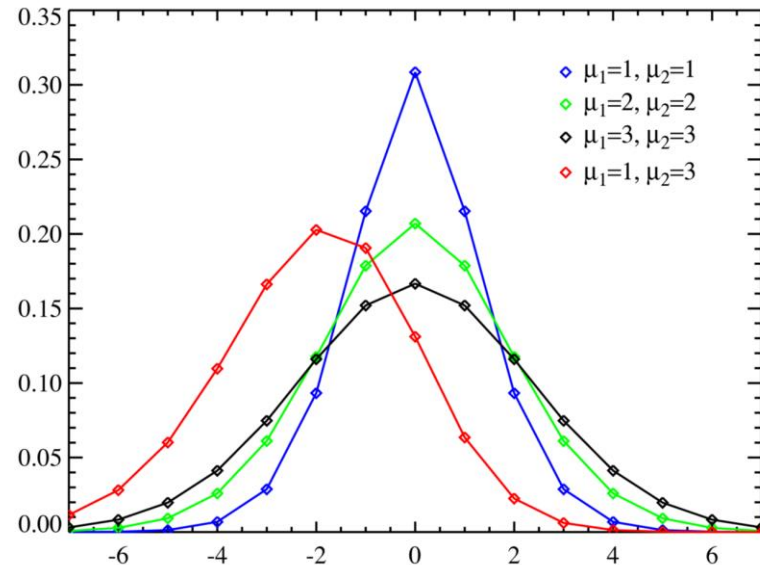


Emission statistics

Counting statistics

Difference of Poisson distributed random variables

The **Skellam distribution** is the discrete probability distribution of the difference $N_1 - N_2$ of two random variables N_1 and N_2 having **Poisson** distributions with expected values μ_1 and μ_2

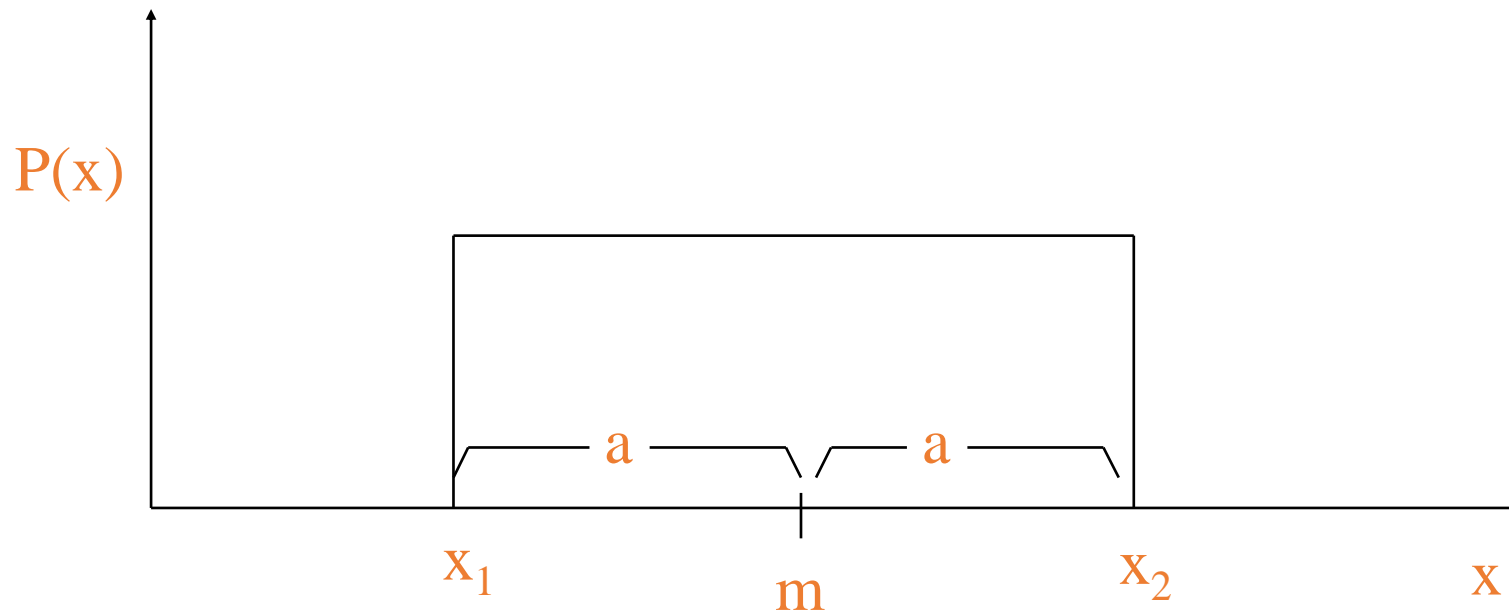


$$P_k(\mu_1, \mu_2) = \sum_{n=-\infty}^{\infty} P_{k+n}(\mu_1)P_n(\mu_2) = e^{-(\mu_1+\mu_2)} \left(\frac{\mu_1}{\mu_2}\right)^{k/2} I_k(2\sqrt{\mu_1\mu_2})$$

where $I_k(z)$ is the modified Bessel function of the first kind.

Any linear combination of two Skellam-distributed variables are again Skellam-distributed.

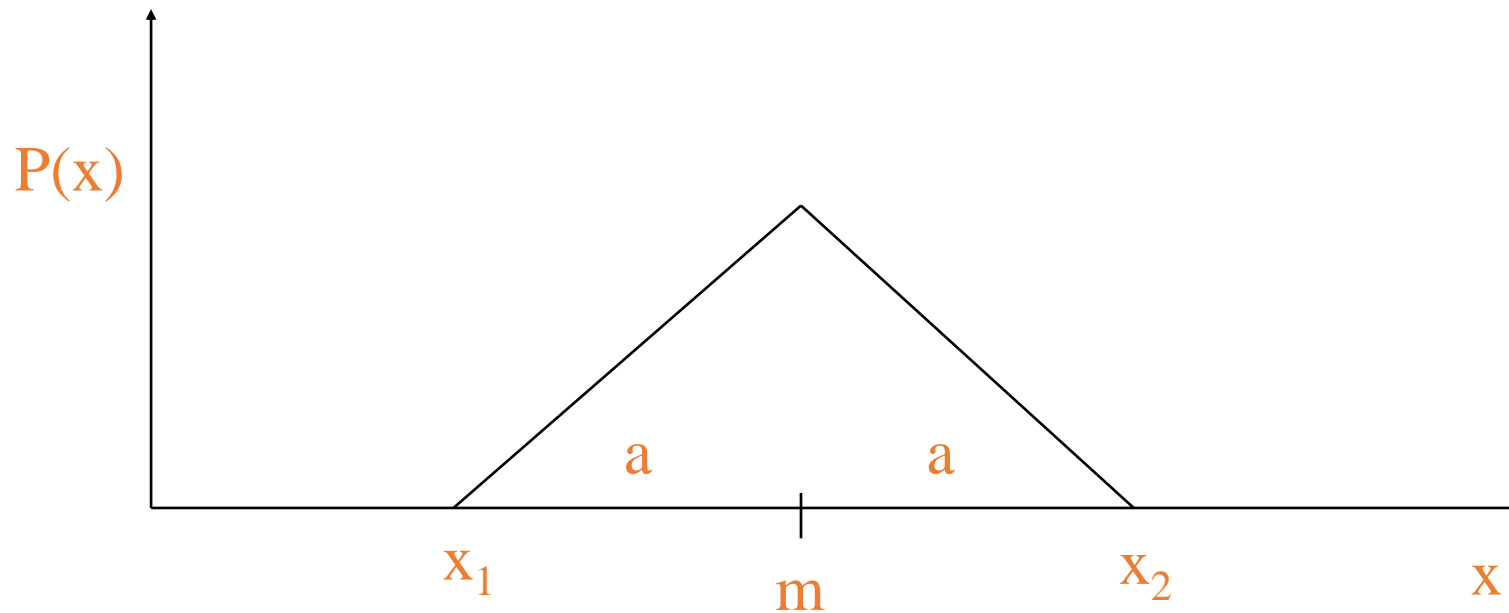
Other example: uniform distribution



$$m = \frac{x_1 + x_2}{2}$$

$$s = \frac{a}{\sqrt{3}}$$

Other example: triangular distribution



$$m = \frac{x_1 + x_2}{2}$$

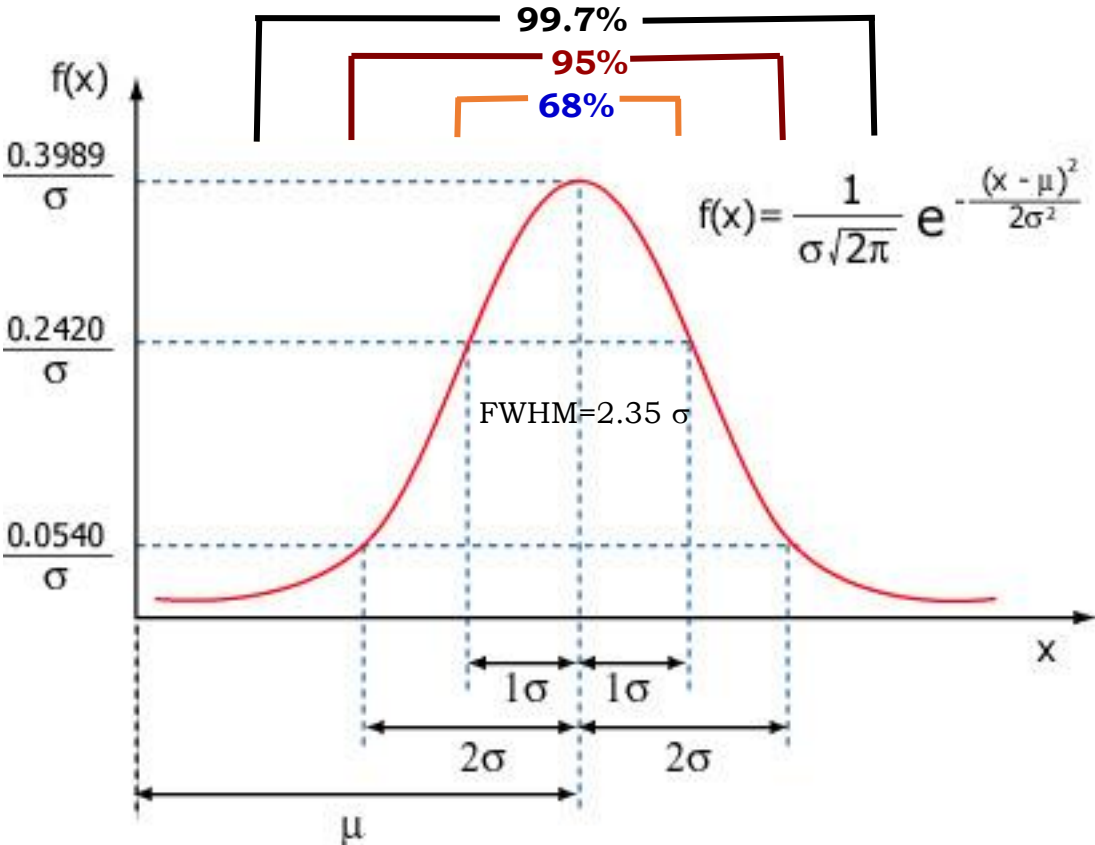
$$s = \frac{a}{\sqrt{6}}$$

Example of continuous random variable, Gaussian (Normal) distribution

$$P(x) = \frac{1}{s\sqrt{2\pi}} e^{-\frac{(x-M)^2}{2s^2}}$$

$P(x)$ is the probability to get the value x of a Gaussian random variable of expected value M and standard deviation s

Normal Distribution



Central Limit Theorem (CLT)

The distribution of an average
will (almost always) tend to be **“NORMAL”**
as the sample size increases, *regardless* of the
distribution from which the average is taken

Let's go back to uncertainties

Reminder:

The uncertainty of a measurement result expresses the reliability of that result or the confidence that we have in it



A measurement result is incomplete without a statement of the corresponding measurement uncertainty

Steps in uncertainty evaluation

- Define the measurand (this is not a trivial task)
- Identify the input quantities and parameters used in the measurement process (experimental data, coefficients, parameter of influence)
- Explicit the relationship between the input quantities and the measurement result
- Evaluate the uncertainties of each input quantity, in terms of standard deviations, and evaluate the covariances between the input quantities
- Propagate the variances and covariances to obtain the standard combined uncertainty
- If necessary, expand the uncertainty with a given coverage factor
- Report the measurement result with the associated uncertainty

Definition of the measurand

- The measurand is the quantity intended to be measured. Before measuring, give a precise and exhaustive definition of the measurand
- Include in the definition the quantities and parameters which could influence the measurement result
- Think about the use of the measurement result in order to avoid any ambiguity on the definition of the measurand

Input quantities

Experimental data:

- Counting rate, mass, volume, peak surface...

Parameters of influence:

- Temperature, pressure, humidity...

Coefficients:

- Correction factors, calibration factors, detection efficiency...

Standards :

- Activity, mass, time...

Theoretical data:

- Emission intensities, decay probabilities, half-life...

Relation between the input quantities and the measurement result

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

y is the measurement result and the x_i are the input quantities

Evaluation of the uncertainties of the input quantities

Each input quantity must be considered as a random variable with a mean value and a standard deviation

The GUM gives two ways to evaluate the input quantities uncertainties:

Type A evaluation method: evaluation of the experimental standard deviation by statistical methods (e.g. by repetition of the measurement)

Type B evaluation method: evaluation of the standard deviation of the input quantity from hypothesis on the statistical distribution of this quantity or by any other information

Warning: *type A and B concerns the evaluation methods and not the uncertainties*

Type A evaluation method

- Repetition of the measurement (sampling of the distribution)
- Calculation of the mean value
- Calculation of the experimental standard deviation
- Calculation of the standard deviation of the mean

If the measurement is repeated in the same conditions, the standard deviation of the mean is a good estimator of the uncertainty

Average, mean value of the distribution

Expected value $E(x)$ (first moment of the distribution)

$$E(x) = \sum_{i=1}^n x_i P(x = x_i)$$

If all values have the same weight

$$P(x_i) = \frac{1}{n}$$

$$E(x) = \sum_{i=1}^n x_i \frac{1}{n} = \frac{1}{n} \sum_{i=1}^n x_i = \text{arithmetic mean} \quad \text{Best estimator of the average value}$$

If the values have different weights

$$\text{Weighted mean } \bar{x} = \frac{\sum_{i=1}^n w_i x_i}{\sum_{i=1}^n w_i} \quad \text{where } w_i = \frac{1}{u(x_i)^2}$$

Dispersion of the distribution

n samples with the same probability: $x_1, x_2, x_3, x_4, \dots, x_n$

Variance (2nd moment of the distribution) $s_x^2(x) = E[(x - E(x))^2]$

$$s_x = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - M)^2}$$

Variance = s^2

s = standard deviation = $\sqrt{\text{variance}}$

Standard deviation of the mean

$$s_{\bar{x}} = \frac{s}{\sqrt{n}}$$

$$s_{\bar{x}} = \sqrt{\frac{1}{n(n-1)} \sum_{i=1}^n (x_i - M)^2}$$

Estimator of the dispersion of the mean

Covariance between quantities(estimated)

$$u(x, z) = \frac{1}{(n-1)} \sum_{i=1}^n (x_i - \bar{x})(z_i - \bar{z})$$

Should we consider the standard deviation or the standard deviation of the mean?

The experimental standard deviation quantifies the dispersion of the random variable

When increasing the number of samples, the standard deviation does not change too much, but is known with better precision...

The standard deviation of the mean quantifies the dispersion of the evaluated mean (which is also a random variable)

When increasing the number of samples, the standard deviation of the mean decreases as the square root of the number of samples (because the mean values is known with better precision)

Example: measurement of the surface contamination of a field Bq/cm²

0,004	0,010	0,004	0,010	0,010	0,003	0,001	0,004	0,009	0,007
0,009	0,004	0,004	0,005	86,485	0,007	0,008	0,001	0,002	0,003
0,005	0,004	0,007	0,009	0,005	0,007	0,002	0,002	0,000	0,001
0,002	0,007	53,528	0,004	0,004	0,006	0,001	0,009	0,005	0,010
0,008	0,005	0,009	0,003	0,003	0,006	23,475	0,009	0,000	0,002
0,003	0,008	0,010	0,008	0,006	0,001	0,004	0,003	0,004	0,001
0,007	88,543	0,008	114,640	0,009	0,003	0,001	0,009	0,002	0,004
0,004	0,010	0,001	0,006	0,008	0,002	0,004	0,007	0,010	0,001
0,005	0,000	0,004	0,005	0,006	0,009	0,010	0,006	0,010	0,002
0,009	0,010	0,009	0,006	0,002	0,006	0,005	0,008	0,009	0,009

Low contamination with hot spots

Evaluation of the results

Mean activity (100 measurement points) :

$$\bar{A} = \frac{1}{100} \sum_{i=1}^{100} A_i = 5,52 \text{ Bq/cm}^2$$

Experimental standard deviation

$$s_A = \sqrt{\frac{1}{100-1} \sum_{i=1}^{100} (A_i - \bar{A})^2} = 25,76 \text{ Bq/cm}^2$$

Standard deviation of the mean

$$s_{\bar{A}} = \sqrt{\frac{1}{100 \cdot (100-1)} \sum_{i=1}^{100} (A_i - \bar{A})^2} = 2,58 \text{ Bq/cm}^2$$

Lets go back to the definition of the measurand

Definition 1 : mean surface activity (mean activity when sampling 1 cm² of soil)
 $A=5,57 \text{ Bq/cm}^2$

Definition 2 : mean surface activity (average activity of the soil) $A= 5,57 \text{ Bq/cm}^2$

Uncertainty: non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used

Uncertainty 1 : experimental standard deviation: $25,76 \text{ Bq/cm}^2$, gives information about the dispersion of surface activity when sampling 1 cm² of soil

Uncertainty 2 : standard deviation of the mean: $2,58 \text{ Bq/cm}^2$, gives information about the dispersion of the average surface activity of the field

What is the best approach?

It depends on what you are looking for

- Both approaches are correct but:
- If you are looking for the mean surface contamination, use uncertainty definition 2
- But, if someone measures the activity contamination and find a hot spot (e.g. 114,64 Bq/cm²). This is 42 standard deviations away from the mean!

Withdrawing a outlier is risky: it could led to underestimate a cause of fluctuation, so to underestimate the uncertainty.
Besides, it could prevent you to discover a new phenomenon...

Type B evaluation methods

Hypothesis on the probability density function (pdf) of the input quantity in order to derive the mean value and the standard deviation

Example: if the input quantity is in the $[M-a, M+a]$ interval

• Uniform pdf:
$$u = \frac{a}{\sqrt{6}}$$

• Triangular pdf:
$$u = \frac{a}{\sqrt{3}}$$

• Gaussian pdf (with 95,5 % confidence interval):
$$u = \frac{a}{\sqrt{9}}$$

Evaluation “as a rule of thumb” is a type B method!

Covariances

- Experimental covariance type A evaluation method

$$s_{x,y} = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{X})(y_i - \bar{Y})}$$

- But covariance can also be estimated (type B evaluation)

Examples :

- related nuclear and atomic data: P_K et ω_K
- coincidence between detectors
- Calibration of gamma detectors using radionuclides with several gamma emissions

Law of propagation of variances

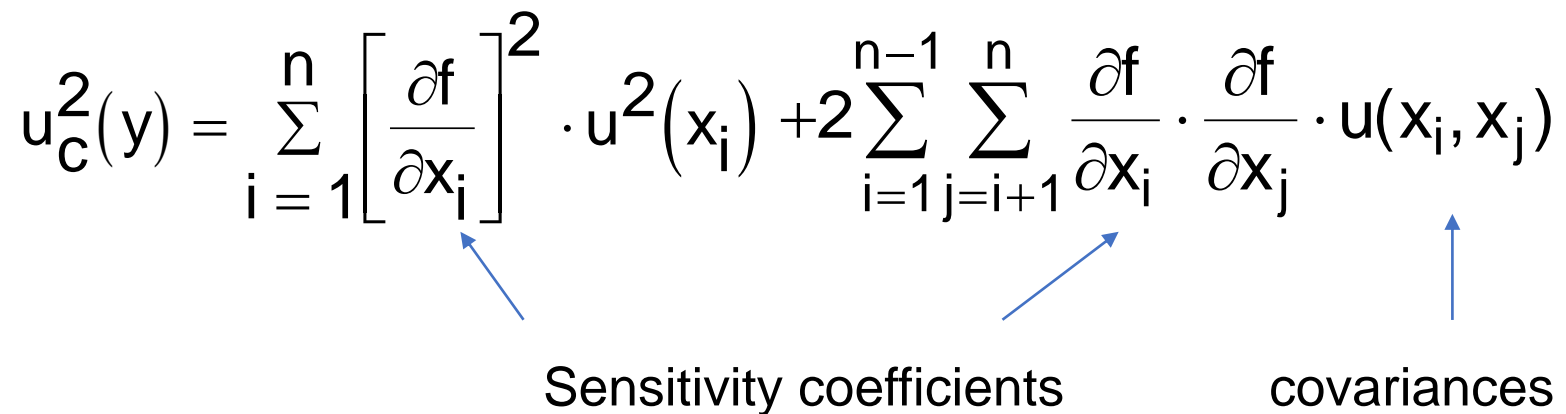
$$y = f(x_1, x_2, \dots, x_n)$$

Hypothesis:

- f is continuous and can be expanded in Taylor series
- Development limited to the 1st order
- Small fluctuations of each input quantity

$$u_c^2(y) = \sum_{i=1}^n \left[\frac{\partial f}{\partial x_i} \right]^2 \cdot u^2(x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^n \frac{\partial f}{\partial x_i} \cdot \frac{\partial f}{\partial x_j} \cdot u(x_i, x_j)$$

Sensitivity coefficients covariances

The diagram shows the equation for the variance of the output y , $u_c^2(y)$. The equation is split into two parts. The first part is $\sum_{i=1}^n \left[\frac{\partial f}{\partial x_i} \right]^2 \cdot u^2(x_i)$. A blue arrow points from the label "Sensitivity coefficients" below to the term $\left[\frac{\partial f}{\partial x_i} \right]^2$. The second part is $+ 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^n \frac{\partial f}{\partial x_i} \cdot \frac{\partial f}{\partial x_j} \cdot u(x_i, x_j)$. A blue arrow points from the label "covariances" below to the term $u(x_i, x_j)$.

Combined standard uncertainty

When the input quantities x_i are not correlated, covariances = 0

$$u_c(y) = \sqrt{\sum_{i=1}^n \left[\frac{\partial f}{\partial x_i} \right]^2 \cdot u^2(x_i)}$$

The combined standard uncertainty $u_c(y)$ is an estimator of the dispersion of the measurand y

Instead of being calculated from the function f , sensitivity coefficients $\partial f / \partial x_i$ are sometimes determined experimentally: one measures the change in y produced by a change in a particular x_i while holding the remaining input quantities constant.

In this case, the knowledge of the function f is accordingly reduced to an empirical first-order Taylor series expansion based on the measured sensitivity coefficients.

Sometimes, the law of propagation of variances cannot be used: hypothesis not fulfilled (large fluctuations, non continuous function, non derivable function, discontinuities...)

Instead a Monte Carlo approach can be used

Examples of propagation of variances (simple cases without covariances)

Sum or difference of terms

$$y = x_1 + x_2 + x_3$$

variance:

$$u_c^2(y) = u^2(x_1) + u^2(x_2) + u^2(x_3)$$

Product or ratio

$$y = x_1 x_2 / x_3$$

Relative variance:

$$\frac{u_c^2(y)}{y^2} = \frac{u^2(x_1)}{x_1^2} + \frac{u^2(x_2)}{x_2^2} + \frac{u^2(x_3)}{x_3^2}$$

Factor

$$y = a x$$

variance:

$$u^2(y) = a^2 \cdot u^2(x)$$

Examples (continued)

Power

$$y=x^p$$

Relative variance

$$\frac{u^2(y)}{y^2} = p^2 \cdot \frac{u^2(x)}{x^2}$$

Exponential

$$y=e^x$$

Relative variance:

$$\frac{u^2(y)}{y^2} = u^2(x)$$

$$y=e^{a/x}$$

relative variance

$$\frac{u^2(y)}{y^2} = \frac{a^2}{x^2} \times \frac{u^2(x)}{x^2}$$

Expanded uncertainty

Although the standard combined uncertainty can be universally used to express the uncertainty of a measurement result, in some commercial, industrial, and regulatory applications, and when health and safety are concerned, it is often necessary to give a measure of uncertainty that defines an interval about the measurement result that may be expected to encompass a large fraction of the distribution of values that could reasonably be attributed to the measurand.

The expanded uncertainty, U , is obtained by multiplying the combined standard uncertainty $u_c(y)$ by a *coverage factor* k :

$$U = k u_c(y)$$

In general, k will be in the range 2 to 3.

However, for special applications k may be outside this range.

Expanded uncertainty

U can be interpreted as defining an interval about the measurement result that encompasses a large fraction p of the probability distribution characterized by that result and its combined standard uncertainty, and p is the *coverage probability* or *level of confidence* of the interval.

More detailed calculations necessitate the knowledge of the *pdf* of the measurand, and the number of degrees of freedom

Warning: the *pdf* of the mean of a random variable can be different than the *pdf* of the random variable.

Example :

- Poisson distribution: the *pdf* of the evaluated mean is a Gaussian distribution
- Gaussian distribution: the *pdf* of the mean is a Student distribution (with n degrees of freedom)

Number of degrees of freedom

Type A evaluation method from n samples:

$$v=n-1$$

Type B evaluation method: no general answer

If the pdf of the measurand is supposed to be Gaussian:

$$v_i \approx \frac{1}{2} \frac{u^2(x_i)}{\sigma^2(u(x_i))} \approx \frac{1}{2} \left[\frac{\Delta u(x_i)}{u(x_i)} \right]^{-2}$$

Uncertainty of the uncertainty

Effective number of degrees of freedom

Welch-Satterthwaite formula :

$$v_{eff} \approx \frac{u_c^4(y)}{\sum_{i=1}^N \frac{u_i^4(y)}{v_i}} \quad \text{with} \quad v_{eff} \leq \sum_{i=1}^N v_i$$

Uncertainty of the uncertainty

The estimated standard uncertainty is a random variable... and thus has an uncertainty!

For a type A evaluation method, if the measurand is supposed to be Gaussian, the relative uncertainty of the uncertainty is a function of the number of repetitions:

Number of repetitions	Relative uncertainty of the uncertainty (%)
2	76
3	52
4	42
5	36
10	24
20	16
30	13
50	10

Consequences

We can assume that for a very good measurement, the relative uncertainty of the uncertainty is seldom less than 25%, so:

- Round up the uncertainty to a maximum of 2 significant digits
- Keep in mind that the uncertainty of the uncertainty also concerns all the uses of the uncertainty, e.g. for the boundary of intervals and for the decision threshold and detection limits. E.g. what is the point to use a Student factor with 3 significant digits?

Rounding up

⇒ *Seldom* justified to quote uncertainties to more than two significant figures

⇒ Practice:

⇒ If 1st significant digit is a 1 or 2, quote two figures, otherwise, quote one figure:

10, 11, 12.....28, 29, 3, 4, 5, 6, 7, 8, 9

⇒ Always round UP (if rounding down decreases uncertainty by more than 5%)

e.g. $0.308 \rightarrow 0.3$ but $0.318 \rightarrow 0.4$

Reporting results

- **$A = 104,7 \text{ Bq/g}$** with a combined standard uncertainty of **$1,5 \text{ Bq/g}$**
- **$A=104,7(15) \text{ Bq/g}$**
- **$A=(104,7 \pm 3,0) \text{ Bq/g}, k=2$**

For an expanded uncertainty, it is mandatory to give the coverage factor k






Good usage of the GUM

Although the GUM provides a framework for assessing uncertainty, it cannot substitute for critical thinking, intellectual honesty and professional skill. The evaluation of uncertainty is neither a routine task nor a purely mathematical one; it depends on detailed knowledge of the nature of the measurand and of the measurement.

The quality and utility of the uncertainty quoted for the result of a measurement therefore ultimately depend on the understanding, critical analysis, and integrity of those who contribute to the assignment of its value.

GUM, 3.4.8

Evolution of the GUM

↙	<i>Evaluation of measurement data – An introduction to the "Guide to the expression of uncertainty in measurement" and related documents</i> JCGM 104:2009	
↙	<i>Evaluation of measurement data – Supplement 1 to the "Guide to the expression of uncertainty in measurement" – Propagation of distributions using a Monte Carlo method</i> JCGM 101:2008	
↙	<i>Evaluation of measurement data – Supplement 2 to the "Guide to the expression of uncertainty in measurement" – Extension to any number of output quantities</i> JCGM 102:2011	
↙	<i>Evaluation of measurement data – The role of measurement uncertainty in conformity assessment</i> JCGM 106:2012	
↙	<i>Guide to the expression of uncertainty in measurement — Part 6: Developing and using measurement models</i> JCGM GUM-6:2020	

Cf. <https://www.bipm.org/en/publications/guides/gum.html>

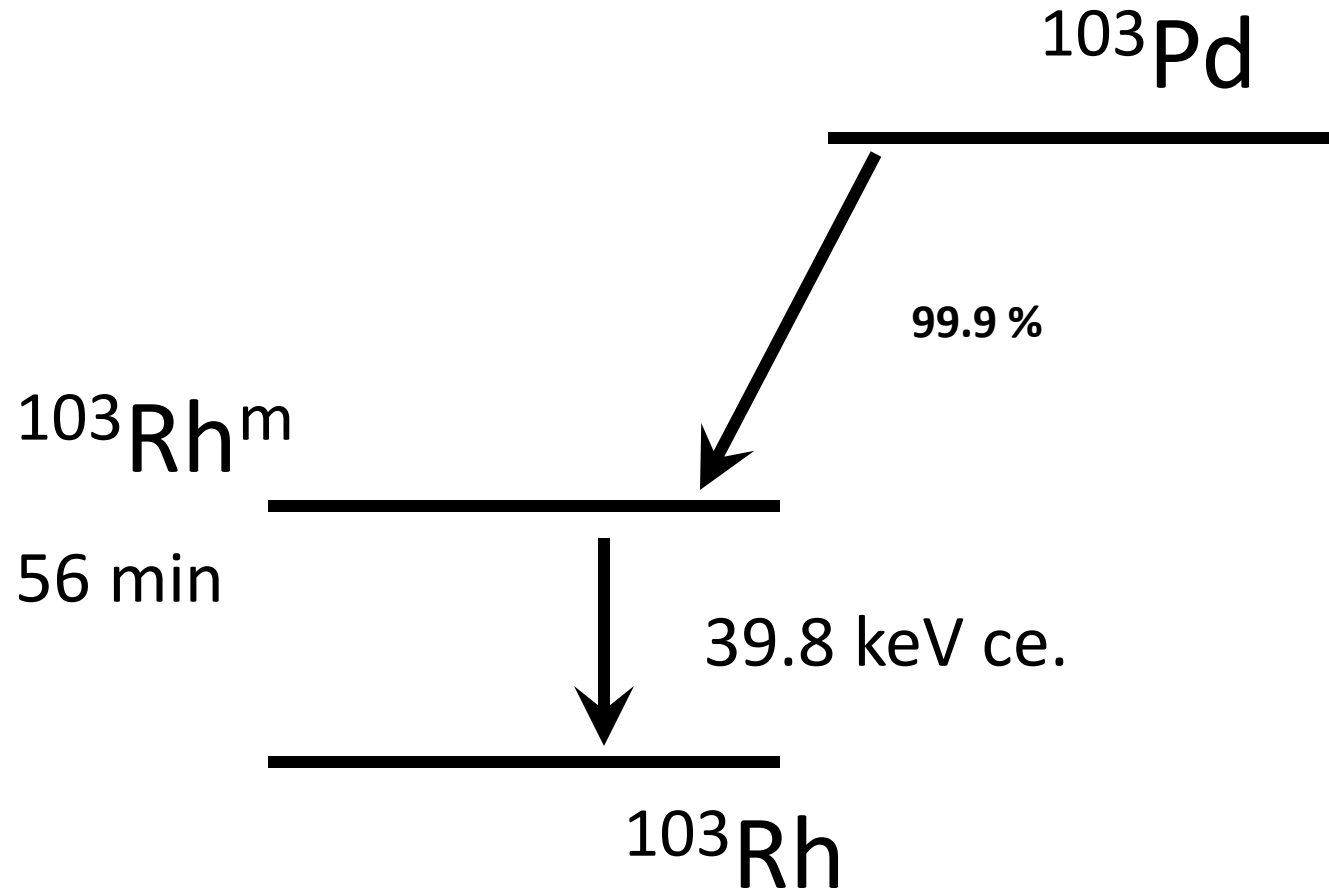
Practical example in
radionuclide metrology
Standardization of a ^{103}Pd
solution

^{103}Pd used in brachytherapy (used to treat prostate cancer)



- Indirect measurement needed (in hospitals) :
 - Ionisation chambers (dose calibrators)
Need of primary standardization and calibration factors
- Standardization :
 - Calorimetry (*not destructive*)
 - Liquid Scintillation Counting (*destructive*)

^{103}Pd simplified decay scheme



The TDCR method in short

For an energy spectrum $S(E)$ absorbed by the scintillator,
Find out the free parameter α for which :

$$\frac{T_{\text{exp}}}{D_{\text{exp}}} = \frac{\int_{\text{spectrum}} S(E)(1 - e^{-\eta})^3 dE}{\int_{\text{spectrum}} S(E)(3(1 - e^{-\eta})^2 - 2(1 - e^{-\eta})^3) dE}$$

with

$$\eta = \alpha \int_0^E \frac{dE}{1 + kB \frac{dE}{dx}}$$

The TDCR method (cont.)

Using this free parameter α , calculate the detection efficiency in double coincidences:

$$\varepsilon_D = \int_{\text{spectrum}} S(E) (3(1 - e^{-\eta})^2 - 2(1 - e^{-\eta})^3) dE$$

with

$$\eta = \alpha \int_0^E \frac{dE}{1 + kB \frac{dE}{dx}}$$

So the energy spectrum absorbed by the LS-cocktail must be calculated...

TDCR method algorithm in practice

$$\frac{R_T}{R_{AB}} = \frac{\int_{\text{spectrum}} S(E)(1 - e^{-\eta_A})(1 - e^{-\eta_B})(1 - e^{-\eta_C}) dE}{\int_{\text{spectrum}} S(E)(1 - e^{-\eta_A})(1 - e^{-\eta_B}) dE}$$

avec

$$\eta_A = \frac{v_A}{3} \int_0^E \frac{AdE}{1 + kB \frac{dE}{dx}}$$

$$\frac{R_T}{R_{BC}} = \frac{\int_{\text{spectrum}} S(E)(1 - e^{-\eta_A})(1 - e^{-\eta_B})(1 - e^{-\eta_C}) dE}{\int_{\text{spectrum}} S(E)(1 - e^{-\eta_B})(1 - e^{-\eta_C}) dE}$$

$$\frac{R_T}{R_{AC}} = \frac{\int_{\text{spectrum}} S(E)(1 - e^{-\eta_A})(1 - e^{-\eta_B})(1 - e^{-\eta_C}) dE}{\int_{\text{spectrum}} S(E)(1 - e^{-\eta_A})(1 - e^{-\eta_{C_B}}) dE}$$

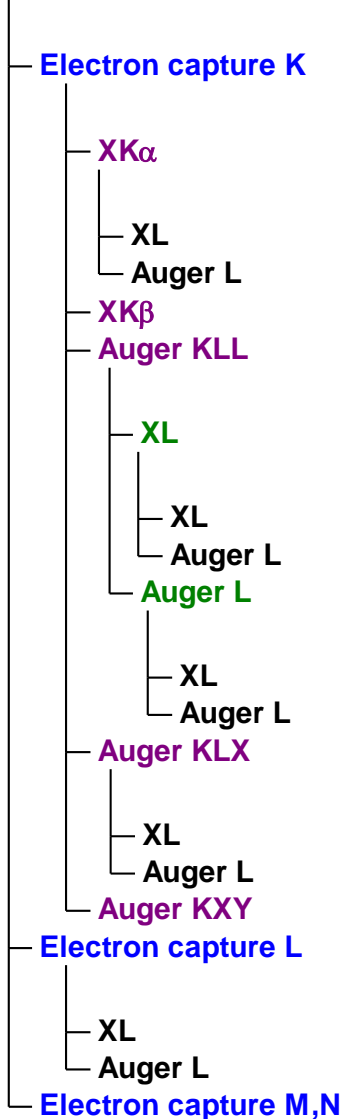
Minimization of:

$$\left(\frac{T_{\text{exp}}}{AB_{\text{exp}}} - \frac{T_{\text{calc}}}{AB_{\text{calc}}} \right)^2 + \left(\frac{T_{\text{exp}}}{BC_{\text{exp}}} - \frac{T_{\text{calc}}}{BC_{\text{calc}}} \right)^2 + \left(\frac{T_{\text{exp}}}{AC_{\text{exp}}} - \frac{T_{\text{calc}}}{AC_{\text{calc}}} \right)^2$$

By downhill simplex algorithm

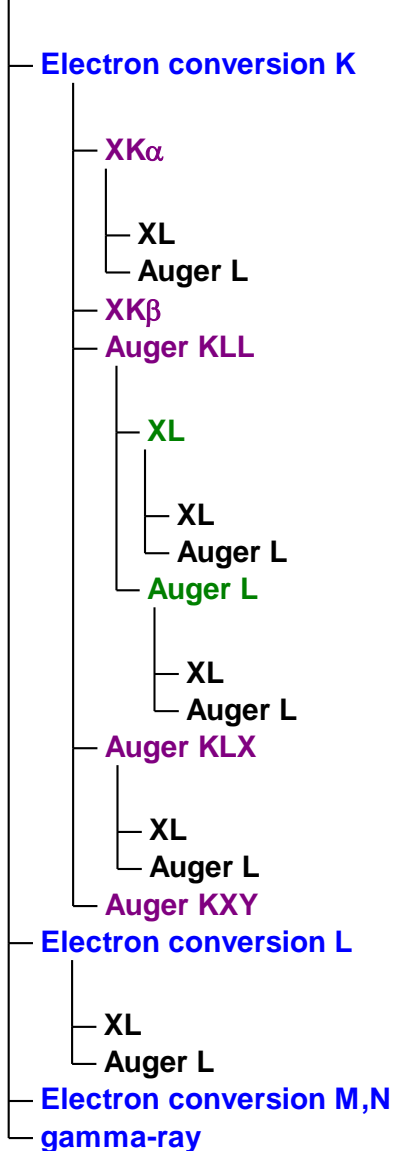
Calculation of the energy spectrum

Pd-103 disintegration



+

Rh-103 desexcitation



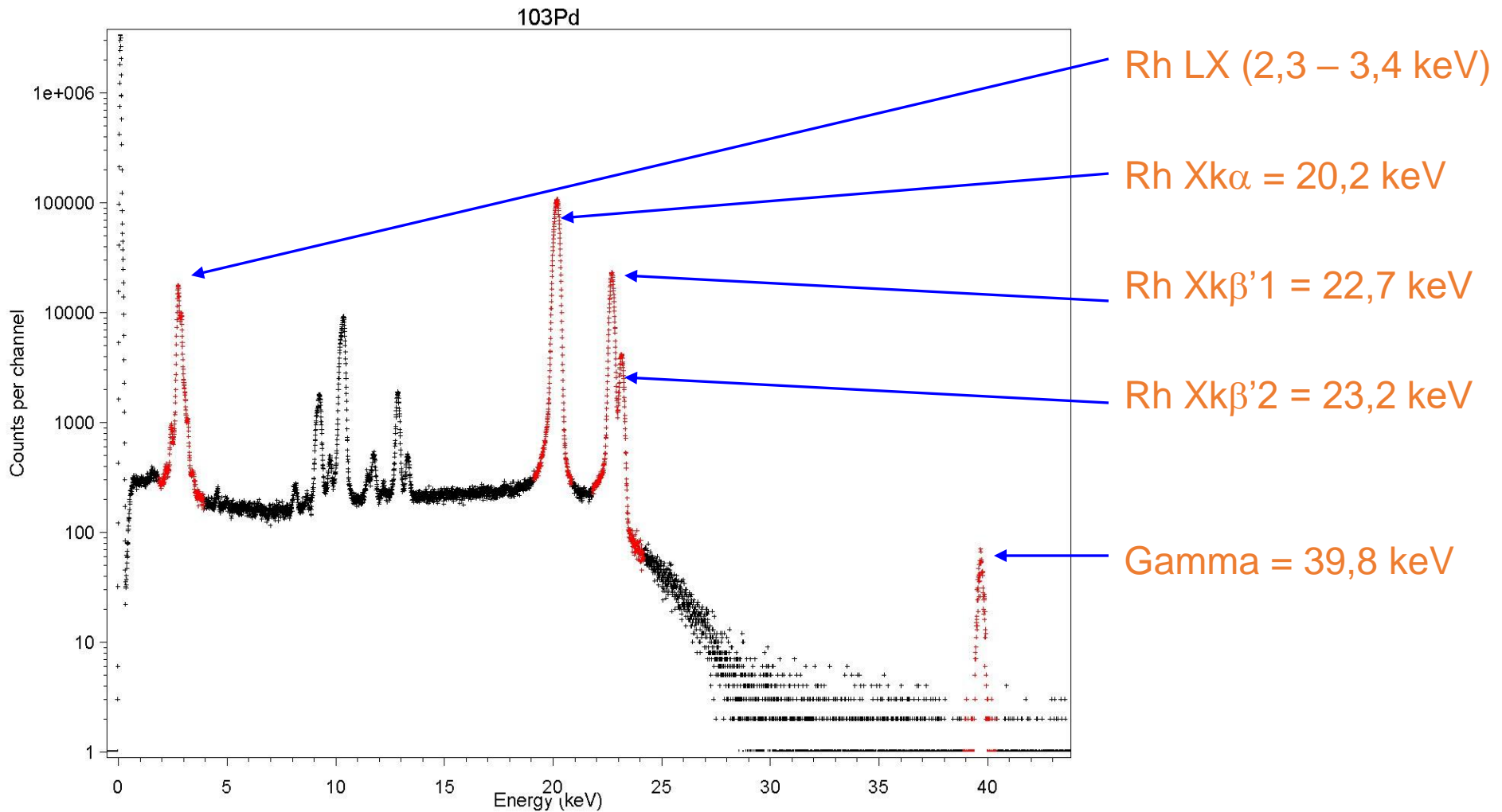
Calculation of the energy spectrum (ec.)

			Energy released	probability
K	XK _α	Absorbed — X _L /Auger L	K _α (Compton+photoelectrique)+X _L /A _L	$P_K * \omega_K * RK_{\alpha} * PK_{\alpha} / PK_{tot}$
		Escape — X _L /Auger L	X _L /A _L	$P_K * \omega_K * (1 - RK_{\alpha}) * PK_{\alpha} / PK_{tot}$
	XK _β	Absorbed —	K _β (Compton+photoelectrique)	$P_K * \omega_K * RK_{\beta} * PK_{\beta} / PK_{tot}$
		Escape —	none	$P_K * \omega_K * (1 - RK_{\alpha}) * PK_{\alpha} / PK_{tot}$
	Auger KLL	X _L /Auger L — XL/Auger L	A _{KLL} +X _L /A _L +X _L /A _L	$P_K * (1 - \omega_K) * P_{KLL} / P_{Ktot}$
	Auger KLY	X _L /Auger L —	A _{KLY} + X _L /A _L	$P_K * (1 - \omega_K) * P_{KLY} / P_{Ktot}$
L	XL/Auger L	—	X _L /A _L	P_L
		—	none	$1 - (P_K + P_L)$
M, N			none	

^{103}Pd decay data (*LNHB evaluation, 2002*)

<u>Parameter</u>	Average value	Standard uncertainty		<u>Parameter</u>	Average value	Standard uncertainty
PK	0.8584	0.0014		$\omega_{M,N}$	0	0
PL	0.1140	0.0011		Xk α relative intensity	0.8283	0.0056
PM,N	0.0232	0.0005		Auger KLL relative intensity	0.686	0.023
K conversion probability	0.0919	0.0028		Auger KLX relative intensity	0.2841	0.0084
L conversion probability	0.732	0.022		Auger KXY relative intensity	0.0295	0.0028
M conversion probability	0.1750	0.0053		Xk α energy	20.17 keV	0.1
ecK energy	16.53 keV	0.33		XK β energy	22.87 keV	0.95
ecL energy	36.54 keV	0.73		Auger KLL energy	16.69 keV	0.33
ecMN energy	39.34 keV	0.79		Auger KLX energy	19.67 keV	0.39

X-ray spectrometry



Calculation of the energy absorbed by the LS-cocktail

Assumptions:

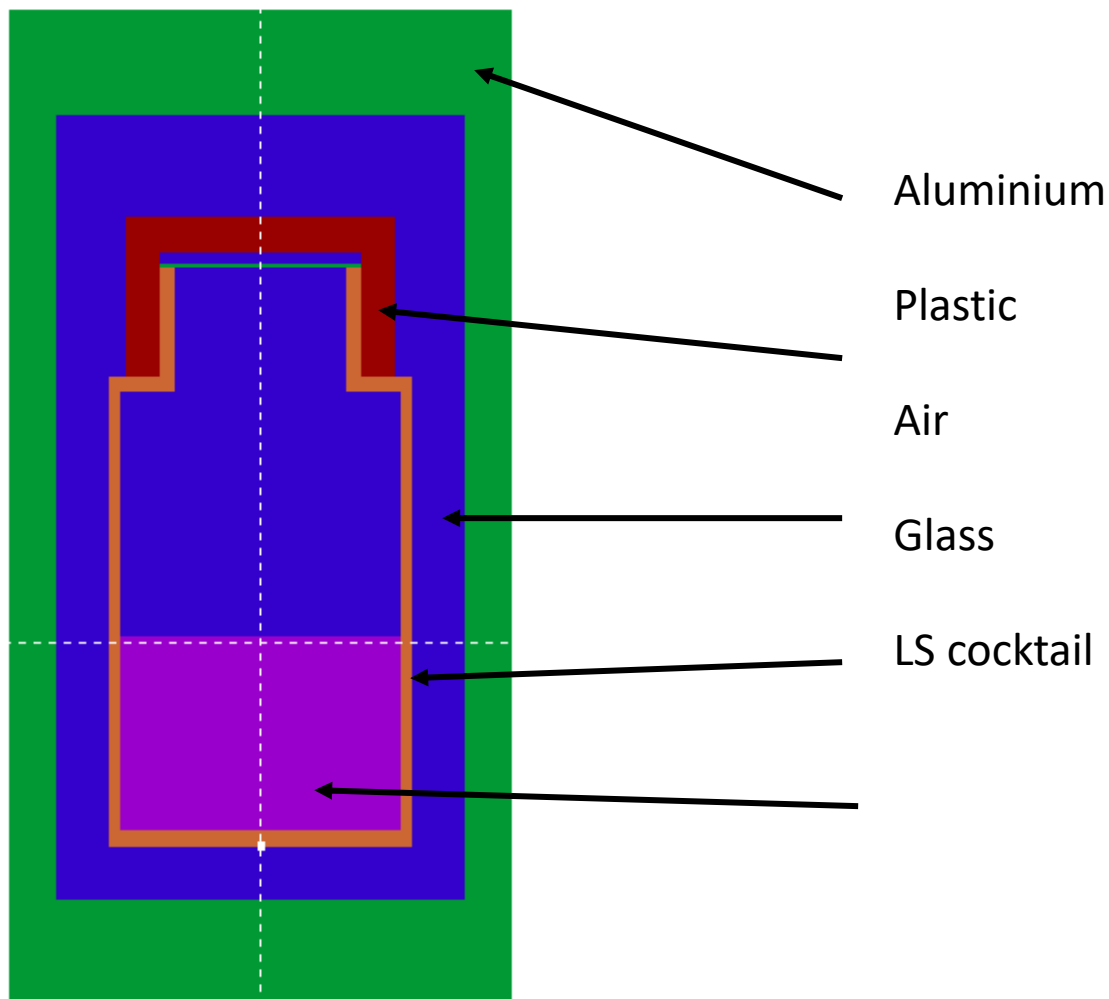
- Auger and conversion electrons totally absorbed
- X_L totally absorbed
- X_K energy transfer calculated using a Monte Carlo model

Dominant decay data parameters:

- $P_K, P_L, P_{M,N}$ (energy available after ec.)
- ω_K (probability of absorption)
- $\alpha_K, \alpha_L, \alpha_{M,N}$ (energy available after ec.)

Monte Carlo simulation of X absorption

Penelope *(Salvat et al.)*



LS-cocktails atomic composition

Elementary composition of the samples

It is useful to have the elementary composition of the scintillator in order to calculate the electron linear energy transfer and photon-interaction cross-sections.

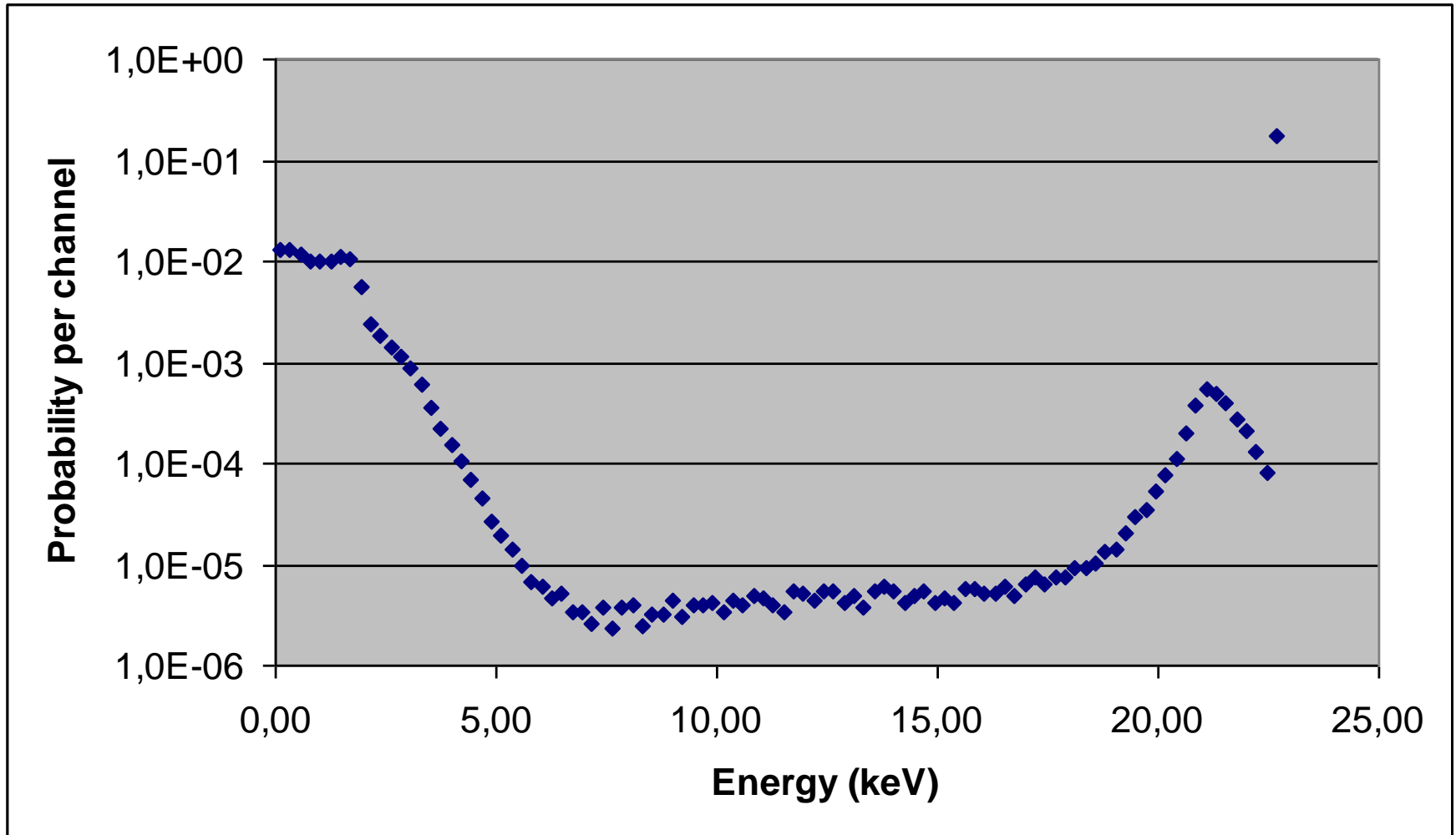
It is necessary to calculate the scintillator-water sample composition individually, using for example, the following compositions kindly provided by J. Thomson, Perkin-Elmer (formerly Packard Bioscience).

Stoichiometric composition and density of various Perkin-Elmer LS-cocktails (stoichiometric formula)

(source : J. Thomson, Perkin-Elmer, formerly Packard Bioscience)

Element	C	H	N	O	P	S	Na	d at 20 °C g/cm ³	Z/A	Molecular weight
Ultima Gold	16,81	24,54	0,040	1,52	0,11	0,02	0,02	0,98	0,5459	255,76
Ultima Gold XR	18,11	29,80	0,035	2,83	0,11	0,03	0,03	0,99	0,5476	297,98
Ultima Gold AB	18,67	28,49	0,010	2,53	0,01	0,00	0,00	0,98	0,5485	293,47
Ultima Gold LLT	18,57	28,43	0,010	2,56	0,01	0,00	0,00	0,98	0,5486	292,68
Insta-Gel Plus	18,53	30,93	0,006	3,90	0,00	0,00	0,00	0,95	0,5490	315,71
Hionic-Fluor	10,83	18,77	0,060	1,97	0,18	0,04	0,04	0,95	0,5449	188,87

Example of energy spectrum transferred to the scintillator by $X_{K\beta}$



Uncertainty evaluation method (GUM)

1. Model the measurement

(get the transfer function between input quantities and measurement result)

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

2. Evaluate standard uncertainties of input quantities

(experimental data, parameters, *etc.*) and covariances between input quantities

3. Combine the standard uncertainties and covariances

$$u_c^2(y) = \sum_{i=1}^n \left[\frac{\partial f}{\partial x_i} \right]^2 \cdot u^2(x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^n \frac{\partial f}{\partial x_i} \cdot \frac{\partial f}{\partial x_j} \cdot u(x_i, x_j)$$

Standard uncertainties on ^{103}Pd input parameters

Experimental :

- Double coincidences : D
- Triple coincidences : T
- TDCR : T/D

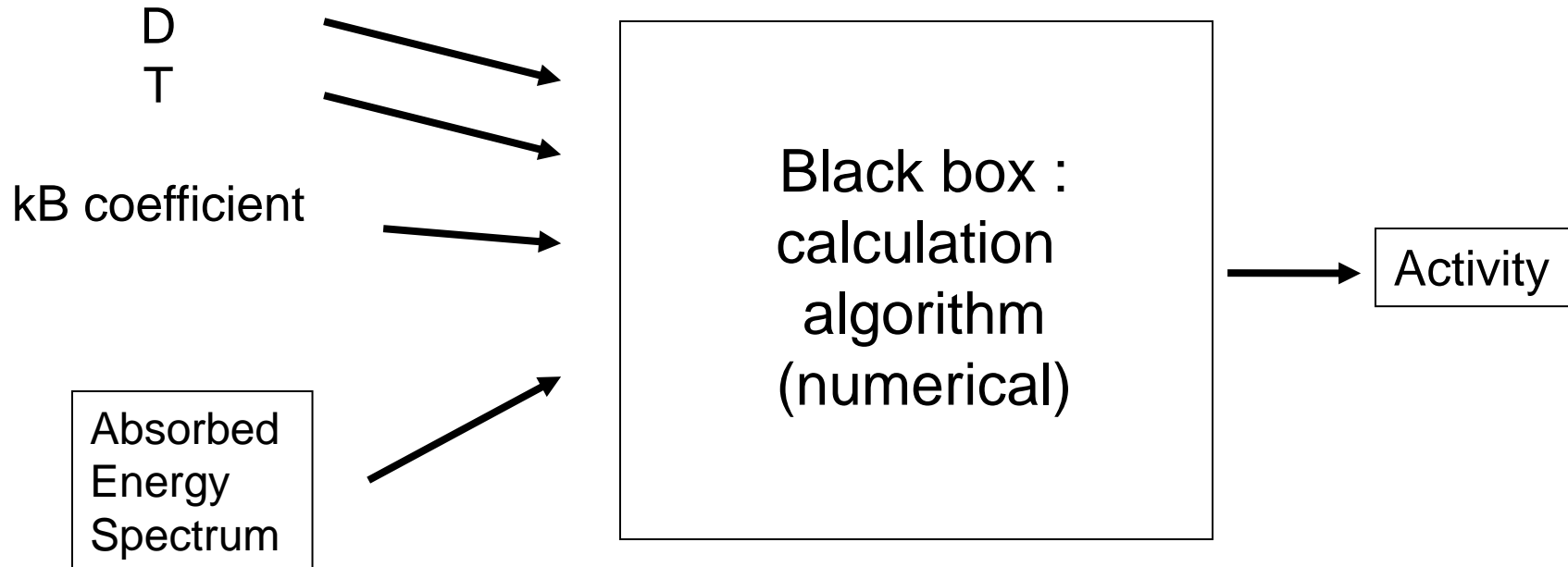
$$s_D^2 = \frac{1}{n-1} \sum_{i=1}^n (D_i - \bar{D})^2$$

$$s_T^2 = \frac{1}{n-1} \sum_{i=1}^n (T_i - \bar{T})^2$$

$$s_{DT} = \frac{1}{n-1} \sum_{i=1}^n (D_i - \bar{D})(T_i - \bar{T})$$

$$s_{TDCR} = TDCR \sqrt{\frac{s_T^2}{T^2} + \frac{s_D^2}{D^2} - \frac{2s_{DT}}{DT}}$$

Measurement function



How to combine the standard uncertainties ?

- Numerical evaluation of the partial derivatives
- Monte Carlo simulation

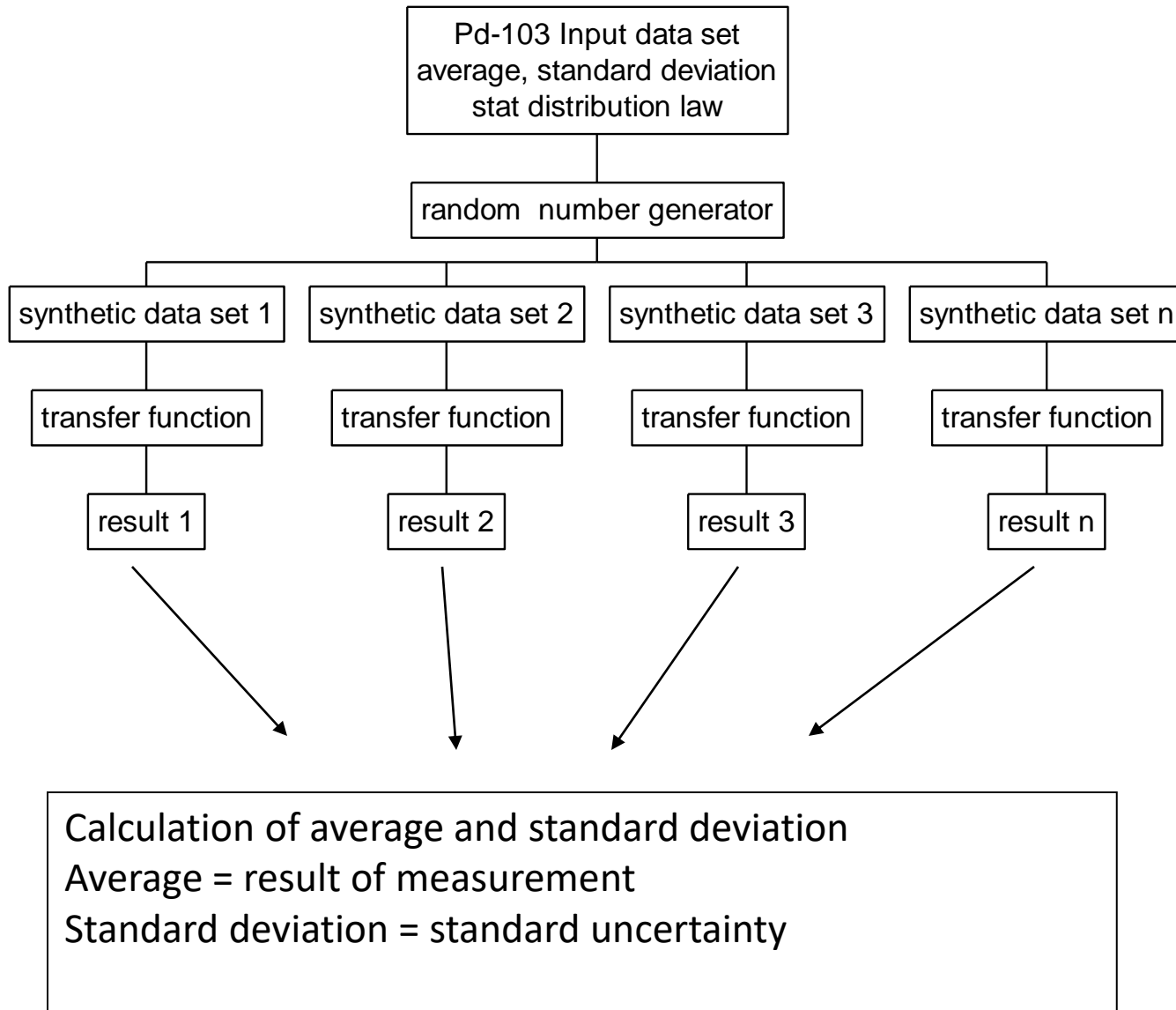
Example of numerical calculation of derivatives

$$\frac{\partial F(x_1, x_2, \dots, x_n)}{\partial x_i} = \frac{F(x_1, \dots, x_i + h, \dots, x_n) - F(x_1, \dots, x_i - h, \dots, x_n)}{2h}$$

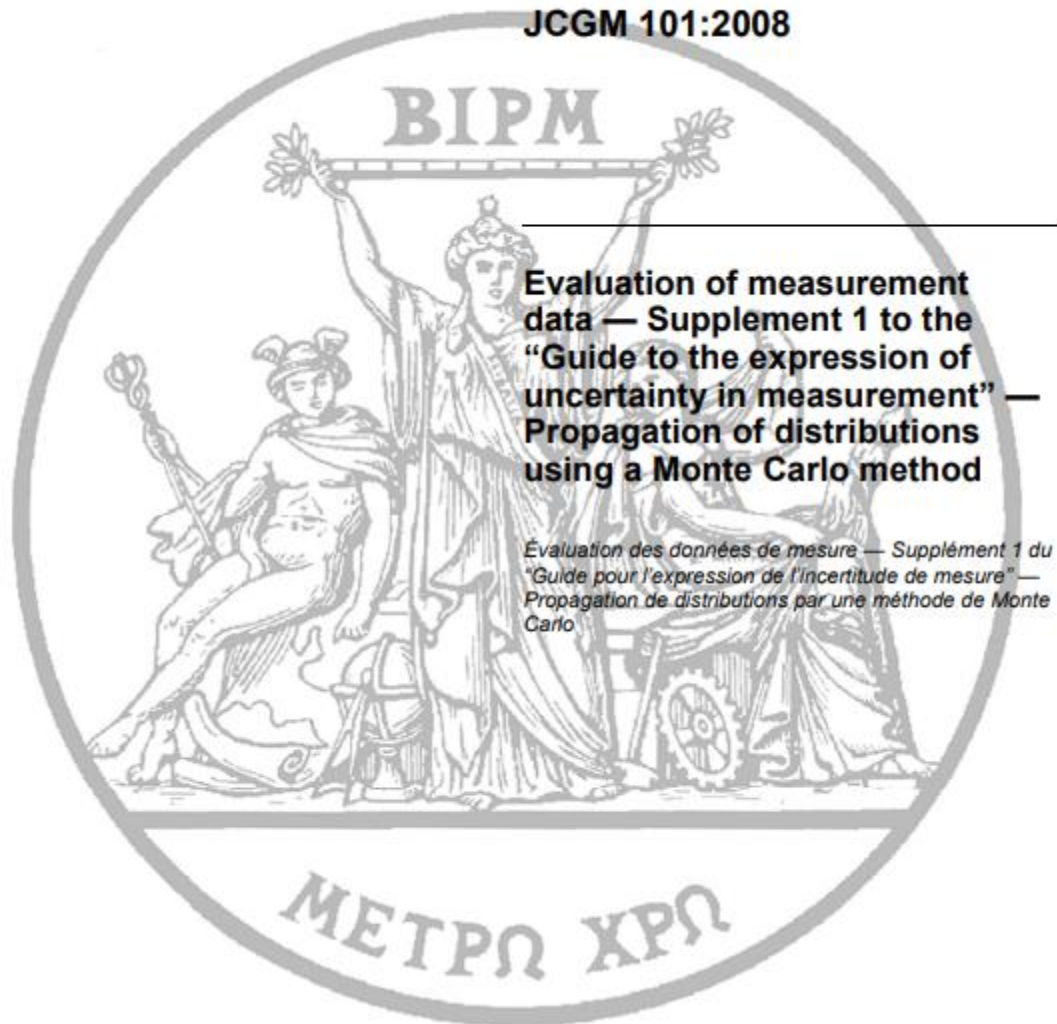
- If ε_F : relative error on the evaluation of F around x_i
- If the choice of h is optimum
 - Then : the relative error on the derivative is about $(\varepsilon_F)^{2/3}$

The number of evaluations of F for each derivative calculation is 6 to 12 with the algorithm used (Numerical recipes, Press et *al.*)

Monte Carlo simulation



JCGM 101:2008



The Monte Carlo method is described in the supplement 1 of the GUM

How to prepare input dataset?

Experimental data: AB, BC, AC, T

Measurement repetition m times, we get m values of (AB, BC, AC, T)

1st method

- calculation of means M_{AB} , M_{BC} , M_{AC} , M_T and experimental standard deviations s_{AB} , s_{BC} , s_{AC} et s_T and covariances
- If we suppose that the values are Gaussian distributed we use a Gaussian random generator to get fluctuation sets of these data

2nd method (bootstrap) :

- random choice of a data set $(AB_{x'}, BC_{x'}, AC_{x'}, T_{x'})$
-
- repetition n times of this random choice (AB_1, BC_1, AC_1, T_1) , $(AB_2, BC_2, AC_2, T_2), \dots$

How to prepare input dataset?

Theoretical or calculated data: kB , dE/dx , atomic and nuclear parameters

- For each data, if we know the mean value M , and the standard deviation s , calculation of a Gaussian distributed random number $G(M,s)$
- If we know the possible range of the data $[a, b]$, calculation of a uniform random number between a and b : $U[a,b]$
- If we have good reasons to consider other *pdf* of the data, use a proper random generator with this *pdf*...

Practical use

(Monte Carlo does not prevent you to think about what you are doing)...)

If the calculation of the measurement function is lengthy, you can quickly do a sensitivity evaluation of what parameters are dominants in the uncertainty

Example, parameter α :

Do 2 calculations with α_{min} and α_{max} , all other parameters kept constant. If the variation of the measurement function is negligible (versus the target uncertainty), you can exclude this parameter from the Monte Carlo procedure.

Possible tools

- Random numbers generators
- Fitting algorithms
- Etc.

•Advantages: the programs are explicit, so you know exactly what you are doing

•Drawback: this needs more efforts than using a ready-to-use library...

NUMERICAL RECIPES

The Art of Scientific Computing

Third Edition

William H. Press

*Raymer Chair in Computer Sciences and Integrative Biology
The University of Texas at Austin*

Saul A. Teukolsky

*Hans A. Bethe Professor of Physics and Astrophysics
Cornell University*

William T. Vetterling

*Research Fellow and Director of Image Science
ZINK Imaging, LLC*

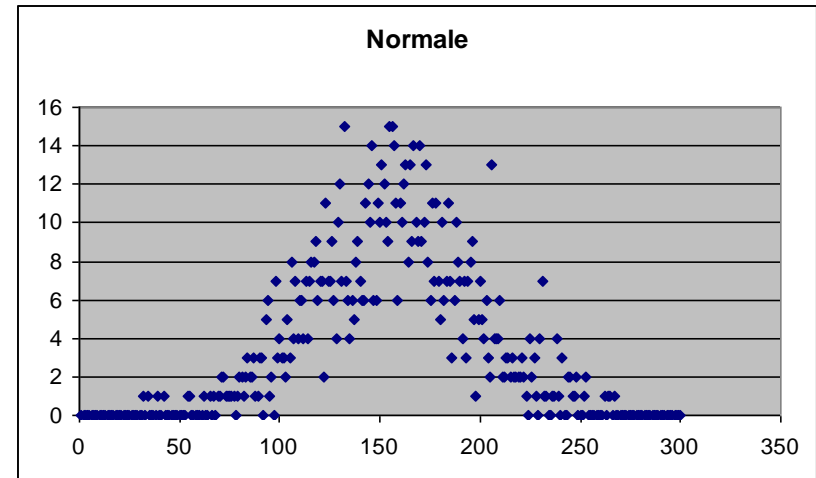
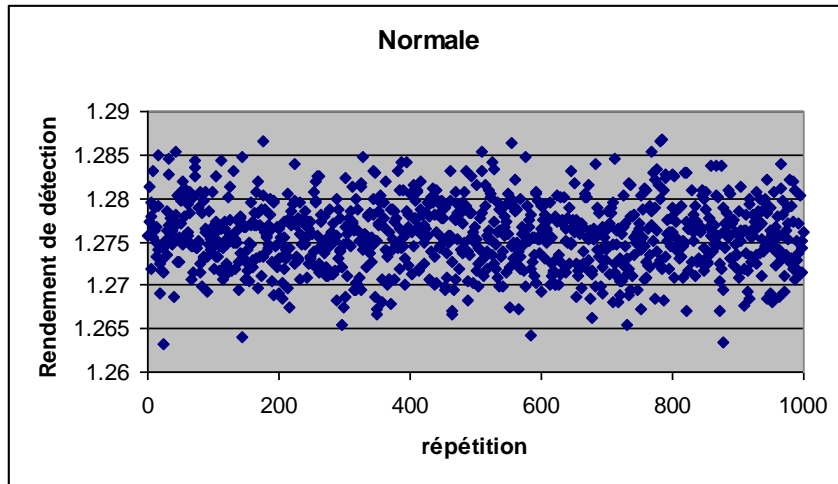
Brian P. Flannery

*Science, Strategy and Programs Manager
Exxon Mobil Corporation*

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Detection efficiency, ^{103}Pd

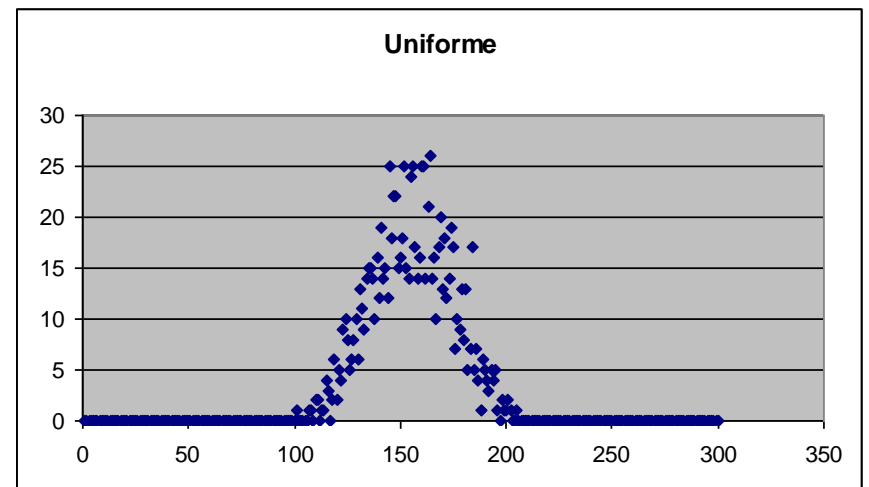
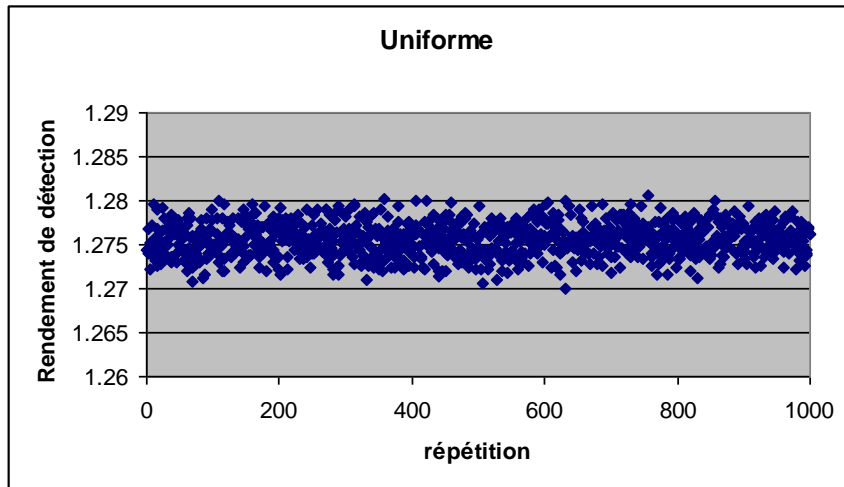
Gaussian distribution of the input quantities



$$\varepsilon_D = 1.2757 (39)$$

Detection efficiency, ^{103}Pd

Uniform distribution of the input quantities



$$\varepsilon_D = 1.2756 \pm 0.0019$$

Other useful tool: the NIST uncertainty machine

The screenshot shows the NIST Uncertainty Machine web application. At the top left is the NIST logo and the text "Uncertainty Machine". At the top right is a language selector set to "English". Below the header are two tabs: "About" and "App", with "App" being the active tab. The main content area is divided into three sections:

- Introduction:** Contains a paragraph describing the tool, a dashed box for uploading a configuration file with the text "Drop configuration file here or click to upload", a "Reset" button, and a link to the user's manual.
- 1. Select Inputs & Choose Distributions:** Includes a dropdown for the number of input quantities (set to 1), a text input for names (containing "x0"), a dropdown for the distribution type (set to "Gaussian (Mean, StdDev)"), and two input fields for parameters (set to 0 and 1). There is also a "Correlations" toggle switch.
- 2. Choose Options:** Includes a text input for the number of realizations (set to 1000000), a text input for the random number generator seed (set to 96), and a "Symmetrical coverage intervals" toggle switch.

The third section, "3. Write the Definition of Output Quantity", contains a text area with the expression "x0" and a "Run the computation" button at the bottom.

<https://uncertainty.nist.gov/>

Comment on the *pdf* of the input quantities

Criteria:

- on physical basis
- at best (maximum of entropy, rule of thumb)

For ^{103}Pd there are two dominant input quantities, so:

- uniform distributions will give a triangular distribution (convolution of two uniform distributions)
- Gaussian distributions will give a Gaussian distribution

Thus the *pdf* of the result also depends on the *pdf* of the input quantities...
or illustrate the central limit theorem

Conclusions

In case of complicated measurement (e.g. ^{103}Pd) the Monte Carlo method is the best (or even only) way to evaluate uncertainties. This approach is well documented in the supplement 1 of the GUM.

Advantages:

- The numerical methods to use are generally simple and straightforward
- The input quantities could have big fluctuations
- The measurement function can be non-linear, non derivable, etc.
- This method is universal and can also be applied for any measurement

But:

- The delicate problem is still the evaluation of the variances and covariances of the input quantities. Sometimes simplifying hypothesis are necessary...
- The *pdf* of the result depends on the *pdf* considered for the input quantities.

Last but important final comment

Generally, uncertainties are evaluated and not strictly calculated.

Empirical approaches and guess estimates cannot always be avoided and uncertainty evaluation is not only a question of statistics but rely on the knowledge of the measurement procedure and models.

It is generally accepted that a measurement with a relative uncertainty of the uncertainty of about 25% to 30% is a very good measurement.

This should suggest humility in uncertainty evaluation and even allow to use some simplifications and shortcuts.

The uncertainty is just an expression of the doubt we have on a measurement. It is important to evaluate it in a proper way, to explicit the evaluation procedure in order to be understood by others. This is why the GUM is useful.