DE LA RECHERCHE À L'INDUSTRIE

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Evaluation of uncertainties, the Monte Carlo method (GUM supplement 1)

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LNE
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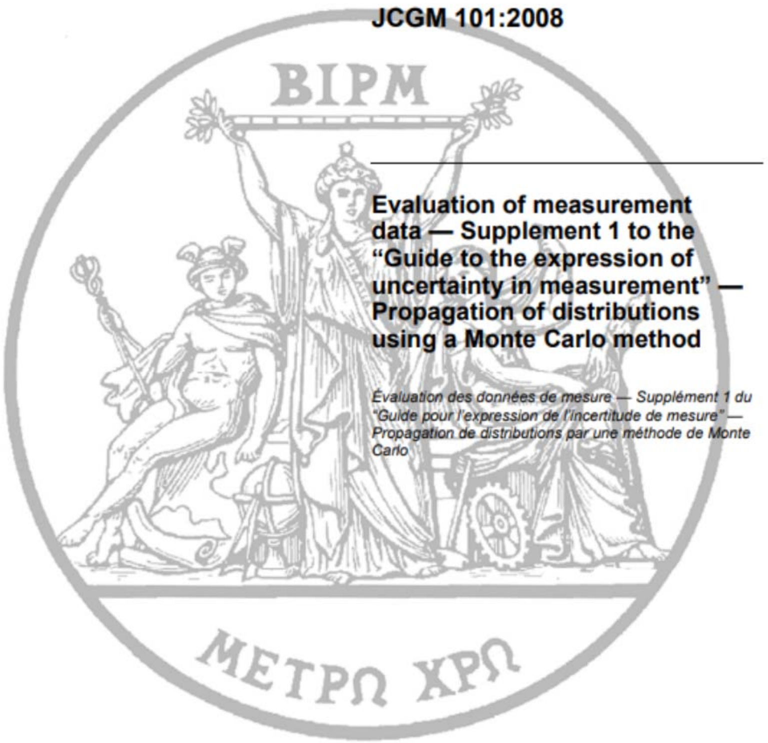
Supplement 1 to the GUM

https://www.bipm.org/utils/common/documents/jcgm/JCGM_101_2008_E.pdf

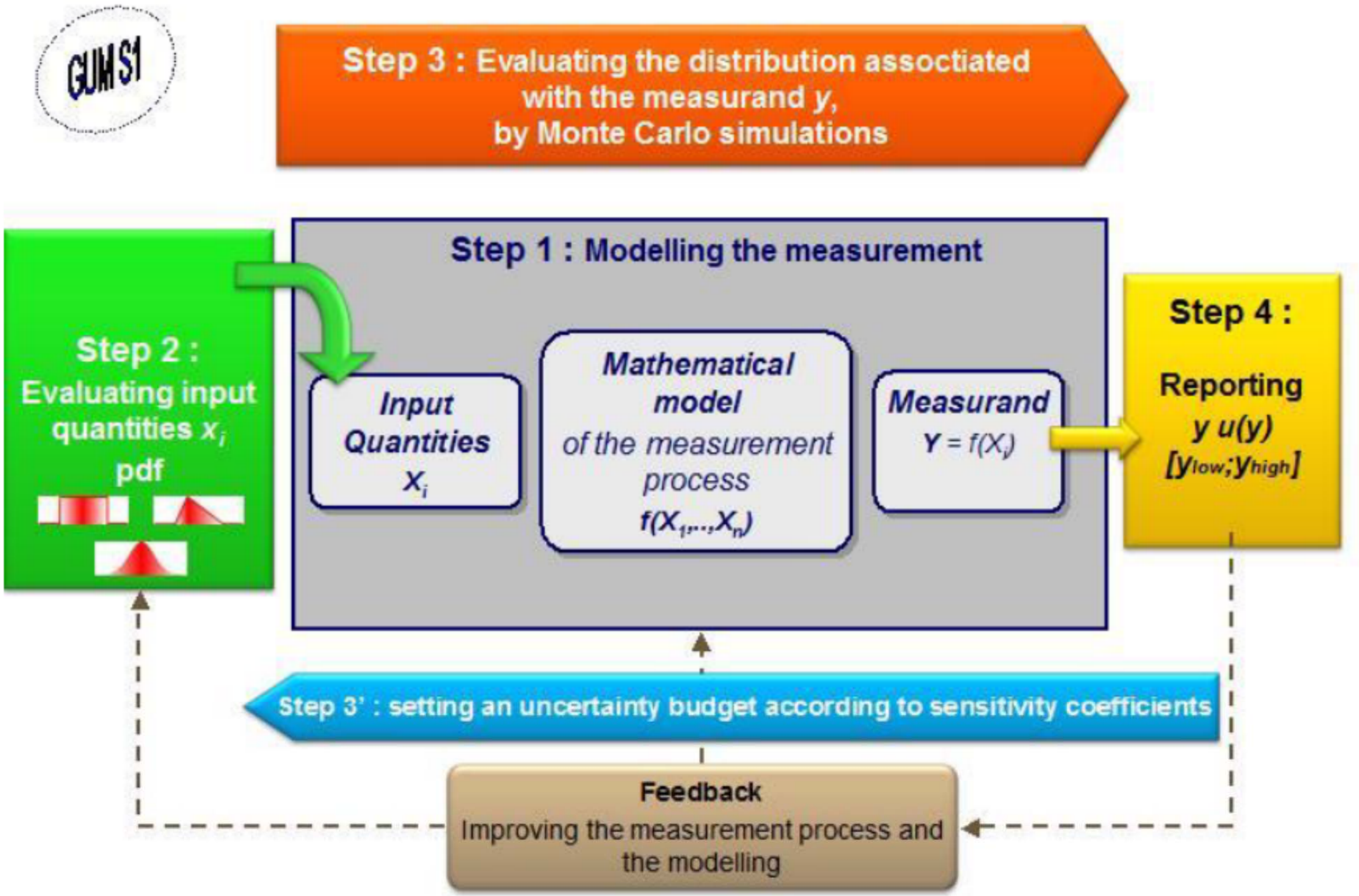


JCGM 101:2008

Evaluation of measurement data — Supplement 1 to the "Guide to the expression of uncertainty in measurement" — Propagation of distributions using a Monte Carlo method

Évaluation des données de mesure — Supplément 1 du "Guide pour l'expression de l'incertitude de mesure" — Propagation de distributions par une méthode de Monte Carlo

First edition 2008


GUM S1
Step 3 : Evaluating the distribution assoctiated with the measurand y, by Monte Carlo simulations
Step 2 : Evaluating input quantities x_i pdf
Step 1 : Modelling the measurement
Input Quantities X_i
Mathematical model of the measurement process $f(X_1,..,X_n)$
Measurand $Y = f(X_i)$
Step 4 : Reporting y $u(y)$ $[y_{low};y_{high}]$
Step 3' : setting an uncertainty budget according to sensitivity coefficients
Feedback
Improving the measurement process and the modelling

MONTE CARLO METHOD (PRINCIPLE)

- mean of each input quantity
- covariance matrix
- *pdf* of each quantity (assumed)
- random number generator

n data sets

AB_1	AB_2	AB_3	…	AB_n
BC_1	BC_2	BC_3		BC_n
AC_1	AC_2	AC_3		AC_n
T_1	T_2	T_3		T_n
kB_1	kB_2	kB_3		kB_n
$S(E)_1$	$S(E)_2$	$S(E)_3$		$S(E)_n$
etc.	etc.	etc.		etc.

n calculations

Measurement model (analytical or numerical)

n results

mean

Standard deviation

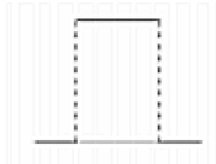
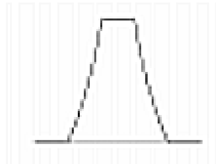
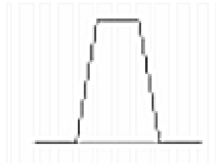
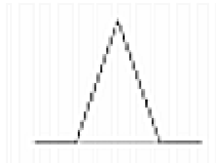
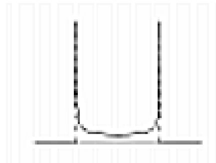
Pdf of the results ?

INPUT QUANTITIES DATA SET

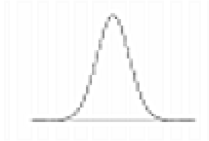
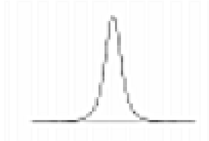
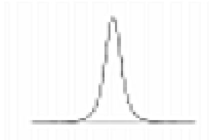
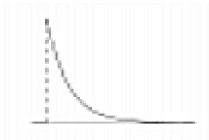
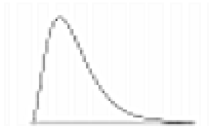
- Experimental data: random sampling of available data
- Parameters : GUM supplement 1 recommendation (maximum of entropy):
  - If the mean and the variance are known, use Gaussian *pdf* *G(M,s)*
  - If realistic boundaries are known, *[a, b],* use uniform *pdf* *U[a,b]*
  - If other *pdf* are suitable, use them!

Subjective evaluation cannot be excluded

GUM supplement 1 recommendations

Available information	Assigned PDF and illustration (not to scale)	
Lower and upper limits a, b	Rectangular: $\mathrm{R}(a, b)$	
Inexact lower and upper limits $a \pm d$, $b \pm d$	Curvilinear trapezoid: $\mathrm{CTrap}(a, b, d)$	
Sum of two quantities assigned rectangular distributions with lower and upper limits a_1, b_1 and a_2, b_2	Trapezoidal: $\mathrm{Trap}(a, b, \beta)$ with $a = a_1 + a_2$, $b = b_1 + b_2$, $\beta = \lvert(b_1 - a_1) - (b_2 - a_2)\rvert/(b - a)$	
Sum of two quantities assigned rectangular distributions with lower and upper limits a_1, b_1 and a_2, b_2 and the same semi-width ($b_1 - a_1 = b_2 - a_2$)	Triangular: $\mathrm{T}(a, b)$ with $a = a_1 + a_2$, $b = b_1 + b_2$	
Sinusoidal cycling between lower and upper limits a, b	Arc sine (U-shaped): $\mathrm{U}(a, b)$	

GUM supplement 1 recommendations

Available information	Assigned PDF and illustration (not to scale)	
Best estimate x and associated standard uncertainty $u(x)$	Gaussian: $\mathrm{N}(x, u^2(x))$	
Best estimate $\boldsymbol{x}$ of vector quantity and associated uncertainty matrix $\boldsymbol{U_x}$	Multivariate Gaussian: $\mathrm{N}(\boldsymbol{x}, \boldsymbol{U_x})$	
Series of indications $x_1, \ldots, x_n$ sampled independently from a quantity having a Gaussian distribution, with unknown expectation and unknown variance	Scaled and shifted t: $t_{n-1}(\bar{x}, s^2/n)$ with $\bar{x} = \sum_{i=1}^{n} x_i/n$, $s^2 = \sum_{i=1}^{n} (x_i - \bar{x})^2/(n-1)$	
Best estimate x, expanded uncertainty U_p, coverage factor k_p and effective degrees of freedom ν_{eff}	Scaled and shifted t: $t_{\nu_{\mathrm{eff}}}(x, (U_p/k_p)^2)$	
Best estimate x of non-negative quantity	Exponential: $\mathrm{Ex}(1/x)$	
Number q of objects counted	Gamma: $\mathrm{G}(q+1, 1)$	

CORRELATED INPUT QUANTITIES

- Experimental data: calculate experimental covariance
- Parameters: example P_K, P_L *et* P_M *for electron capture*

$$\sum_i P_i = 1$$

In a first approximation consider uncorrelated values of P_K and P_L and calculate $P_M=1-(P_K+P_L)$

Unfortunately, the decay data evaluations do not provide the covariance matrix, but only the diagonal terms (variances)

PRACTICAL TOOLS 1

The LNE-MCM software https://www.lne.fr/en/node/1263
(presently in French, but the LNE-Uncertainty software in English will be released soon)

17th International Congress of Metrology, 02012 (2015)
DOI: 10.1051/metrology/201502012

A user-friendly software for a simple and validated implementation of GUM Supplement 1

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[1]*Laboratoire national de métrologie et d'essais, Trappes, France*

Le progrès, une passion à partager

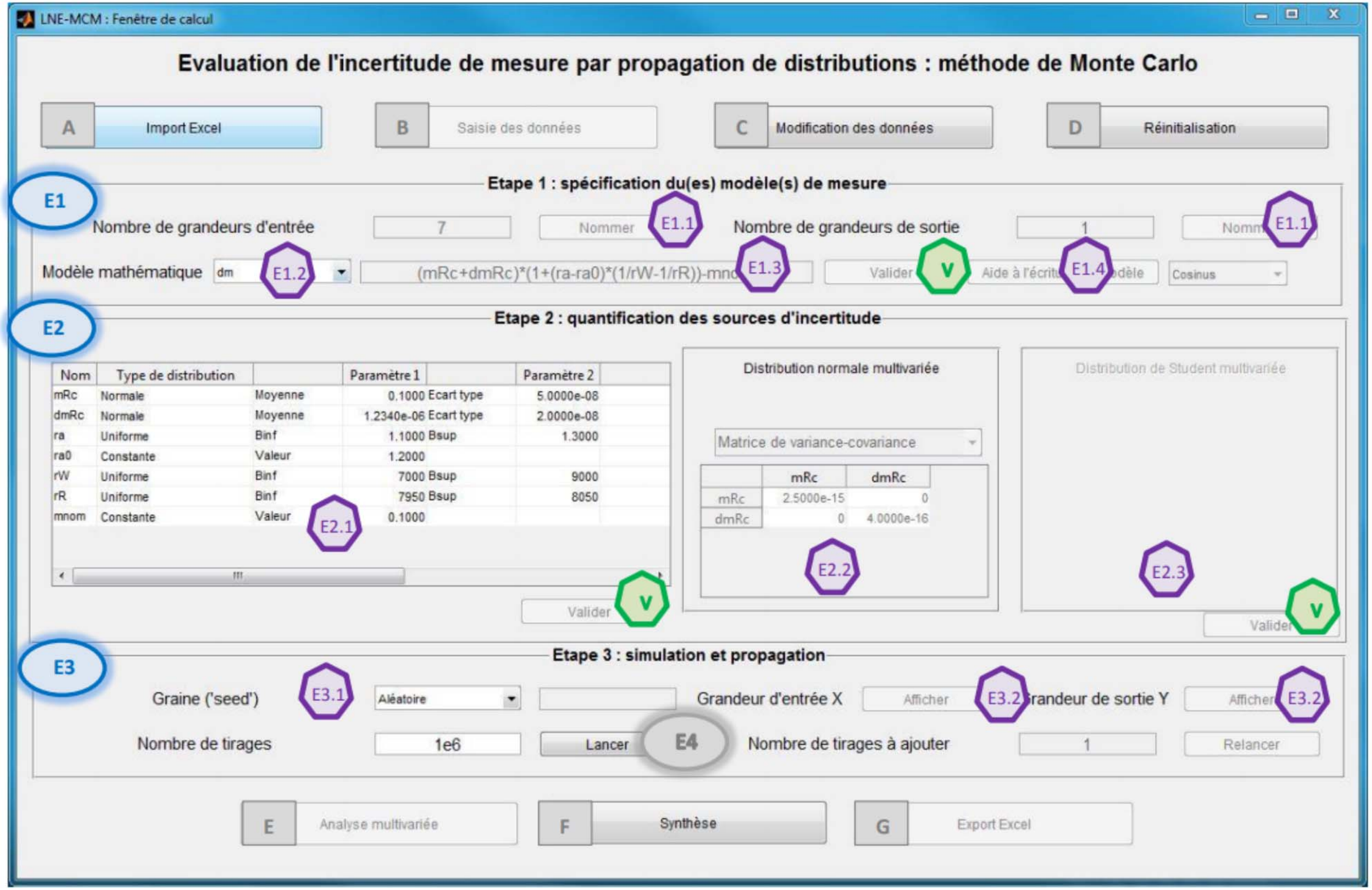
MANUEL DE L'UTILISATEUR

LOGICIEL LNE-MCM 1.0

décembre 2015

LNE - MCM

VERSION 1.0

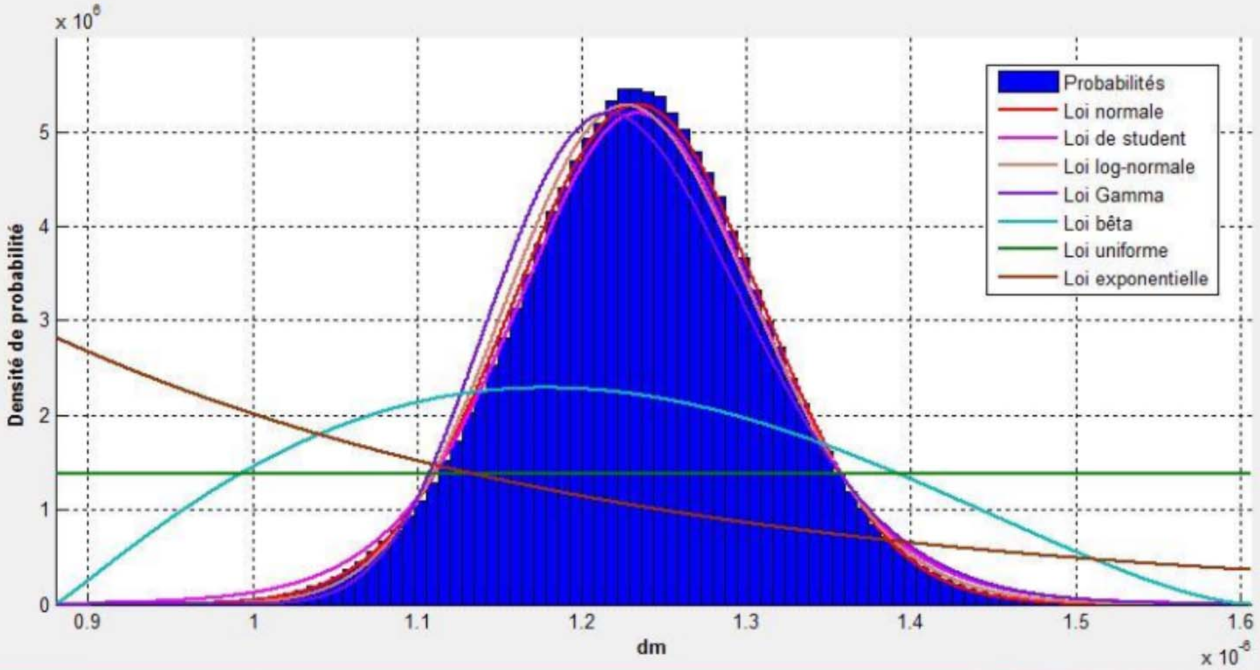

LNE-MCM : Fenêtre de calcul
Evaluation de l'incertitude de mesure par propagation de distributions : méthode de Monte Carlo
A Import Excel
B Saisie des données
C Modification des données
D Réinitialisation
E1
Etape 1 : spécification du(es) modèle(s) de mesure
Nombre de grandeurs d'entrée
7
Nommer
E1.1
Nombre de grandeurs de sortie
1
E1.1
Modèle mathématique
dm
E1.2
(mRc+dmRc)*(1+(ra-ra0)*(1/rW-1/rR))-mno
E1.3
Valider
V
E1.4
Cosinus
E2
Etape 2 : quantification des sources d'incertitude
Nom | Type de distribution | | Paramètre 1 | | Paramètre 2
mRc | Normale | Moyenne | 0.1000 | Ecart type | 5.0000e-08
dmRc | Normale | Moyenne | 1.2340e-06 | Ecart type | 2.0000e-08
ra | Uniforme | Binf | 1.1000 | Bsup | 1.3000
ra0 | Constante | Valeur | 1.2000
rW | Uniforme | Binf | 7000 | Bsup | 9000
rR | Uniforme | Binf | 7950 | Bsup | 8050
mnom | Constante | Valeur | 0.1000
E2.1
Valider
V
Distribution normale multivariée
Matrice de variance-covariance
mRc | dmRc
mRc | 2.5000e-15 | 0
dmRc | 0 | 4.0000e-16
E2.2
Distribution de Student multivariée
E2.3
Valider
V
E3
Etape 3 : simulation et propagation
Graine ('seed')
E3.1
Aléatoire
Grandeur d'entrée X
Afficher
E3.2
Grandeur de sortie Y
Afficher
E3.2
Nombre de tirages
1e6
Lancer
E4
Nombre de tirages à ajouter
1
Relancer
E Analyse multivariée
F Synthèse
G Export Excel

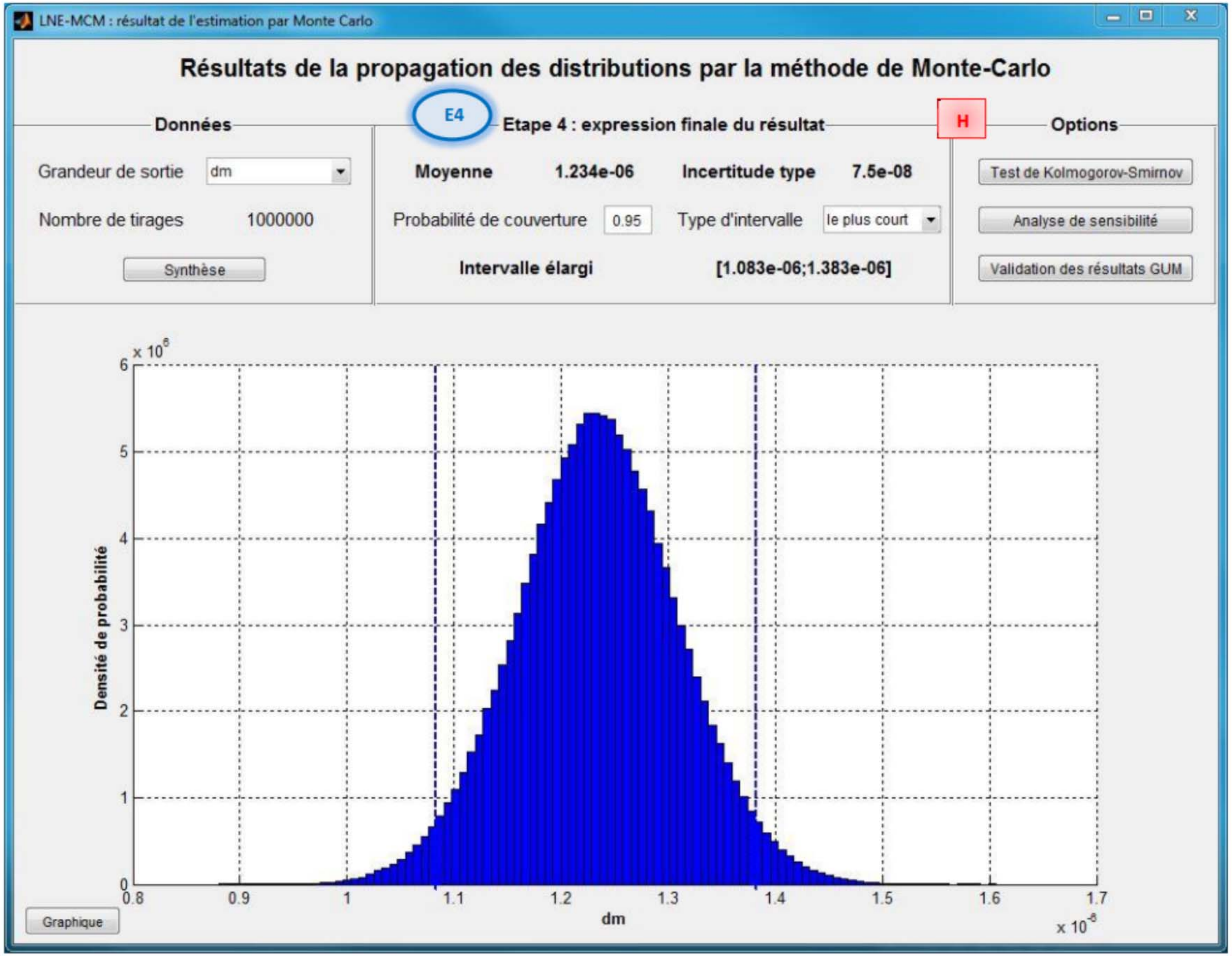
LNE-MCM : Test de Kolmogorov-Smirnov

Test d'adéquation de Kolmogorov-Smirnov

Grandeur de sortie dm

	Loi	p-value	statistique de test		Paramètre 1		Paramètre 2		Paramètre 3
1	Normale	< 1e-6	0.0050	Moyenne	1.2340e-06	Ecart type	7.5481e-08		
2	Student	< 1e-6	0.0142	Shift	1.2340e-06	Scale	7.4905e-08	ddl	10
3	Log-normale	< 1e-6	0.0150	Moyenne	-13.6071	Ecart type	0.0615		
4	Gamma	< 1e-6	0.0343	K	20.3692	Thêta	1.7372e-08		
5	Bêta	< 1e-6	0.2580	Alpha	2.1082	Bêta	2.5924		
6	Uniforme	< 1e-6	0.2911	Borne inf	8.8015e-07	Borne sup	1.6061e-06		
7	Exponentielle	< 1e-6	0.4272	Lambda	2.8260e+06				




LNE-MCM : résultat de l'estimation par Monte Carlo
Résultats de la propagation des distributions par la méthode de Monte-Carlo
Données
E4
Etape 4 : expression finale du résultat
H
Options
Grandeur de sortie
dm
Nombre de tirages
1000000
Synthèse
Moyenne
1.234e-06
Incertitude type
7.5e-08
Probabilité de couverture
0.95
Type d'intervalle
le plus court
Intervalle élargi
[1.083e-06;1.383e-06]
Test de Kolmogorov-Smirnov
Analyse de sensibilité
Validation des résultats GUM
Densité de probabilité
x 10^6
dm
x 10^-6
Graphique

PRACTICAL TOOLS 2

The NIST uncertainty machine https://uncertainty.nist.gov/

NIST Uncertainty Machine — User's Manual

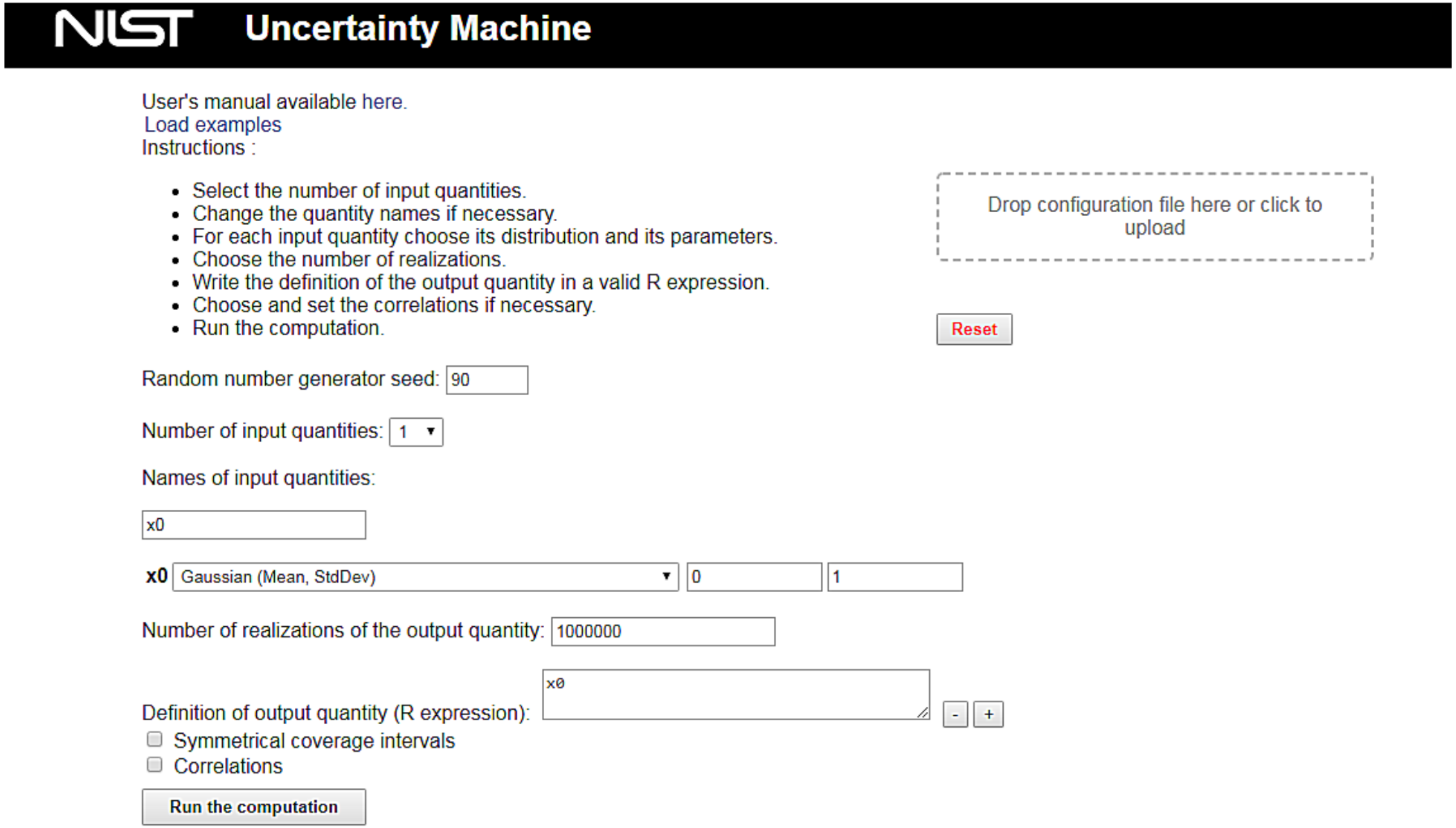
Thomas Lafarge Antonio Possolo

Statistical Engineering Division
Information Technology Laboratory
National Institute of Standards and Technology
Gaithersburg, Maryland, USA

March 10, 2018

1 NIST Uncertainty Machine for the Impatient

- Using a Web browser, visit `https://uncertainty.nist.gov/`.
- Choose the number of input quantities from the drop-down menu, and give them names if desired.
- Select a probability distribution for each of the input quantities, and enter values for its parameters (in the absence of cogent reason to do otherwise, assign Gaussian distributions to the input quantities, with means equal to estimates of their values, and standard deviations equal to their standard uncertainties);
- Specify the size of the Monte Carlo sample to be drawn from the probability distribution of the output quantity (no larger than 5 000 000).
- Enter one or more valid R expressions (one per line) into the box labeled **`Value of output quantity (R expression)`** such that the last line evaluates to $f(x_1, \ldots, x_n)$, the right-hand side of the measurement equation. (Refer to (U-8) on Page 11 for the case when the output quantity is a vector.)
- If there are correlations between the input quantities, then check the box marked **`Correlations`**, enter the values of the non-zero correlations, and select a copula to apply them with (*cf.* Figure 6 on Page 26).
- Click the button labeled **`Run the computation`**.



Uncertainty Machine

User's manual available here.
Load examples
Instructions :

- Select the number of input quantities.
- Change the quantity names if necessary.
- For each input quantity choose its distribution and its parameters.
- Choose the number of realizations.
- Write the definition of the output quantity in a valid R expression.
- Choose and set the correlations if necessary.
- Run the computation.

Drop configuration file here or click to upload

Reset

Random number generator seed: 90

Number of input quantities: 1

Names of input quantities:

x0

x0 Gaussian (Mean, StdDev) 0 1

Number of realizations of the output quantity: 1000000

Definition of output quantity (R expression): x0

- +

☐ Symmetrical coverage intervals
☐ Correlations

Run the computation

NIST Uncertainty Machine

User's manual available here.
Load examples
Instructions :

- Select the number of input quantities.
- Change the quantity names and update them if necessary.
- For each input quantity choose its distribution and its parameters.
- Choose the number of realizations.
- Write the definition of the output quantity in a valid R expression.
- Choose and set the correlations if necessary.
- Run the computation.

Drop configuration file here or click to upload

Reset

Random number generator seed: 5

Number of input quantities: 3

Names of input quantities:

a | b | c

a	Gaussian (Mean, StdDev)	32	0.5
b	Uniform (Mean, StdDev)	0.9	0.025
c	Triangular -- Symmetric (Mean, StdDev)	1	0.3

Number of realizations of the output quantity: 1000000

Definition of output quantity (R expression): `a*b/c`

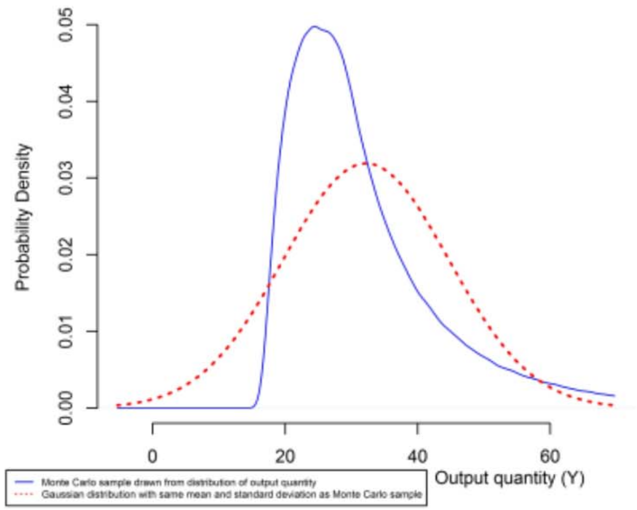
- [ ] Symmetrical coverage intervals
- [ ] Correlations

Run the computation

OUTPUT

NIST Uncertainty Machine

```
===== RESULTS ==============================

Monte Carlo Method

Summary statistics for sample of size 1000000

ave     = 32.2
sd      = 13
median  = 28.8
mad     = 8.9

Coverage intervals

99% (    17.1,       85)       k =      2.7
95% (    18.2,       67)       k =        2
90% (    19.1,     57.9)       k =      1.6
68% (    21.8,     42.4)       k =     0.82

ANOVA (% Contributions)

            w/out Residual w/ Residual
a                     0.22        0.18
b                     0.62        0.52
c                    99.16       81.89
Residual                NA       17.42

-------------------------------------------

Gauss's Formula (GUM's Linear Approximation)

        y  = 28.8
     u(y) = 8.7

             SensitivityCoeffs Percent.u2
a                          0.9       0.27
b                         32.0       0.85
c                        -29.0      99.00
Correlations                NA       0.00
===========================================
```



Download binary R data file with Monte Carlo values of output quantity
Download a text file with Monte Carlo values of output quantity
Download text file with numerical results shown on this page
Download JPEG file with plot shown on this page
Download configuration file

DE LA RECHERCHE À L'INDUSTRIE

NIST Uncertainty Machine

User's manual available here.
Load examples
Instructions :

- Select the number of input quantities.
- Change the quantity names if necessary.
- For each input quantity choose its distribution and its parameters.
- Choose the number of realizations.
- Write the definition of the output quantity in a valid R expression.
- Choose and set the correlations if necessary.
- Run the computation.

Drop configuration file here or click to upload

Reset

Random number generator seed: 90

Number of input quantities: 2

Names of input quantities:

x0 | x1

x0	Student t (Mean, StdDev, No. of degrees of freedom)	1	2	3
x1	Rectangular (Left Endpoint, Right Endpoint)	-1	1	

Number of realizations of the output quantity: 1000000

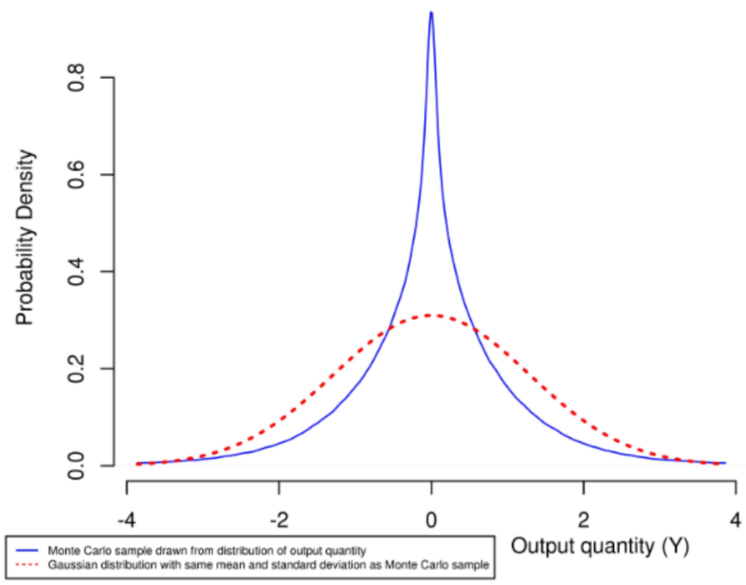
Definition of output quantity (R expression): `x0*x1` - +

- [ ] Symmetrical coverage intervals
- [ ] Correlations

Run the computation

NIST Uncertainty Machine

```
===== RESULTS ==============================

Monte Carlo Method

Summary statistics for sample of size 1000000

ave     = 0.001
sd      = 1.3
median  = -3e-05
mad     = 0.72

Coverage intervals

99% (    -4.4,      4.4)        k =      3.4
95% (    -2.5,      2.5)        k =      1.9
90% (    -1.8,      1.8)        k =      1.4
68% (   -0.86,     0.86)        k =     0.67

ANOVA (% Contributions)

            w/out Residual w/ Residual
x0                    0.08        0.02
x1                   99.92       19.99
Residual                NA       80.00

--------------------------------------------

Gauss's Formula (GUM's Linear Approximation)

        y  = 0
      u(y) = 0.58

             SensitivityCoeffs Percent.u2
x0                           0          0
x1                           1        100
Correlations                NA          0
============================================
```



Download binary R data file with Monte Carlo values of output quantity
Download a text file with Monte Carlo values of output quantity
Download text file with numerical results shown on this page
Download JPEG file with plot shown on this page
Download configuration file

PRACTICAL CONSIDERATIONS

Do not start with a brute force approach: sometimes it is not necessary to vary all the input quantities, but only those which could have a significant influence on the result

A preliminary calculation with extreme values, or a physical evaluation, can indicate the main input quantities to consider

Example, parameter α :

Make two calculations with α_{min} and α_{max} (keeping constant the other input data). If the difference is small (versus the target uncertainty) it is not useful to vary α in the Monte Carlo process

Application to measurements with no explicit transfer function

Example : activity measurement of ^{55}Fe with the TDCR method in LSC

AB, BC, AC

T

kB

$$\frac{dE}{dx}$$

Energy spectrum *S(E)*

Numerical model
(minimization)

Activity

Numerical model
(Monte Carlo simulation)

Decay scheme parameters
P_K, P_L, P_M, ω_K,…
Scintillator composition, geometry…

EXAMPLE OF A NUMERICAL MODEL

$$\begin{cases} \dfrac{R_T}{R_{AB}} = \dfrac{\int_{spectrum} S(E)(1-e^{-\eta_A})(1-e^{-\eta_B})(1-e^{-\eta_C})\ dE}{\int_{spectrum} S(E)(1-e^{-\eta_A})(1-e^{-\eta_B})dE} \\ \dfrac{R_T}{R_{BC}} = \dfrac{\int_{spectrum} S(E)(1-e^{-\eta_A})(1-e^{-\eta_B})(1-e^{-\eta_C})\ dE}{\int_{spectrum} S(E)(1-e^{-\eta_B})(1-e^{-\eta_C})dE} \\ \dfrac{R_T}{R_{AC}} = \dfrac{\int_{spectrum} S(E)(1-e^{-\eta_A})(1-e^{-\eta_B})(1-e^{-\eta_C})\ dE}{\int_{spectrum} S(E)(1-e^{-\eta_A})(1-e^{-\eta C_B})dE} \end{cases}$$

with

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

Solution: minimization of $\boxed{\left(\dfrac{T_{\exp}}{AB_{\exp}} - \dfrac{T_{calc}}{AB_{calc}}\right)^2 + \left(\dfrac{T_{\exp}}{BC_{\exp}} - \dfrac{T_{calc}}{BC_{calc}}\right)^2 + \left(\dfrac{T_{\exp}}{AC_{\exp}} - \dfrac{T_{calc}}{AC_{calc}}\right)^2}$

e.g. with the “downhill simplex” algorithm

UNCERTAINTY DETERMINATION

Evaluation of the input quantities: same as the conventional GUM approach

Variance propagation?

- 1st option: numerical evaluation of partial derivatives
- 2nd option: Monte Carlo method

The 2nd option is by far quicker and more exact

EXAMPLE OF ^{55}FE

Activity $A=N/R$

The counting uncertainty is negligible *vs.* the detection efficiency uncertainty

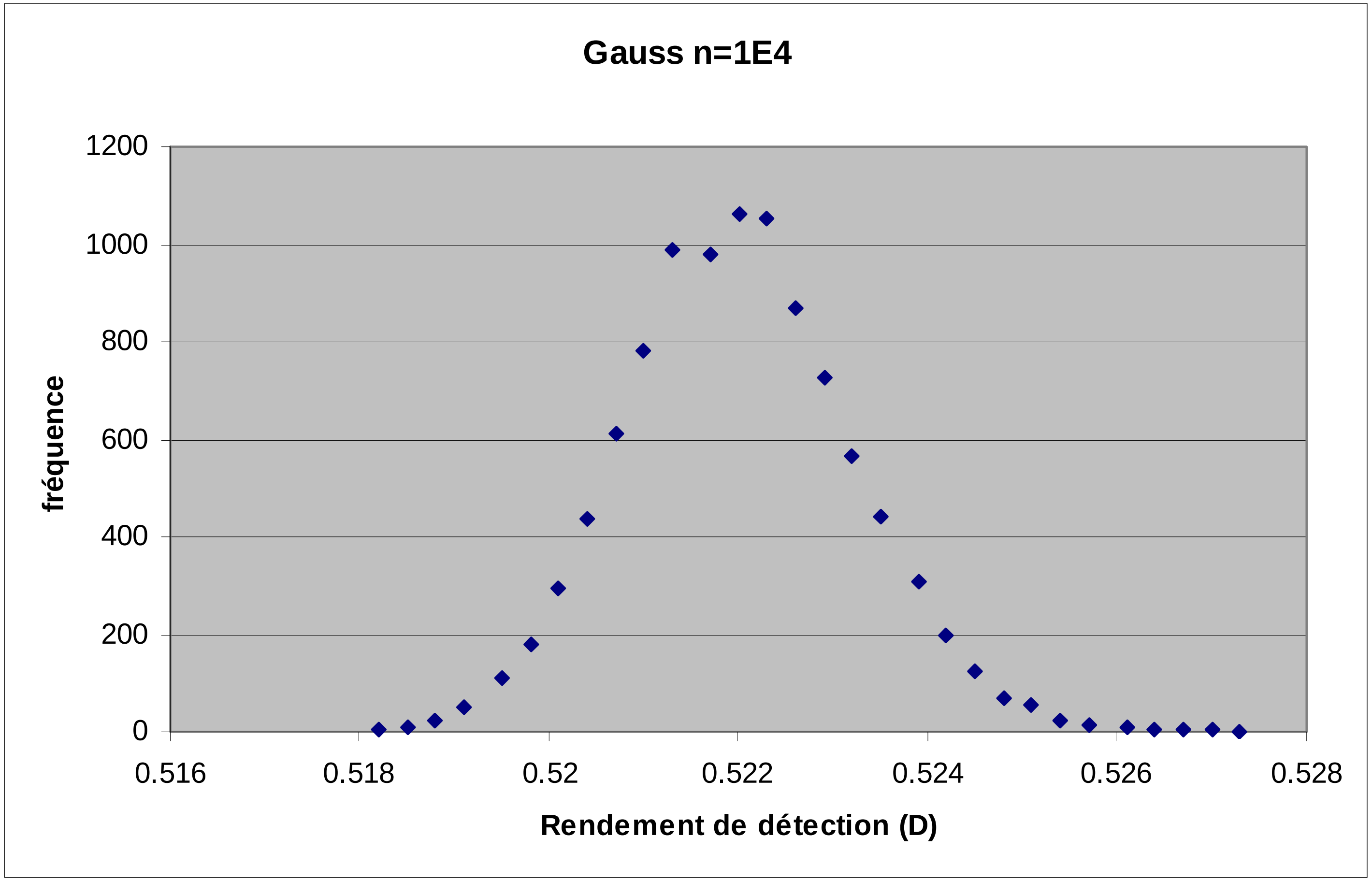
This simplifies the problem, as with this method *N* and *R* are correlated

Sometimes, there is no real reason to choose one articular *pdf* for the input quantities, and several choices are possible (e.g. if the minimum and maximum values of a parameter are known, several interpretations are possible:

- With no other information: uniform *pdf*
- If the mean value is more probable: triangular or Gaussian *pdfs*

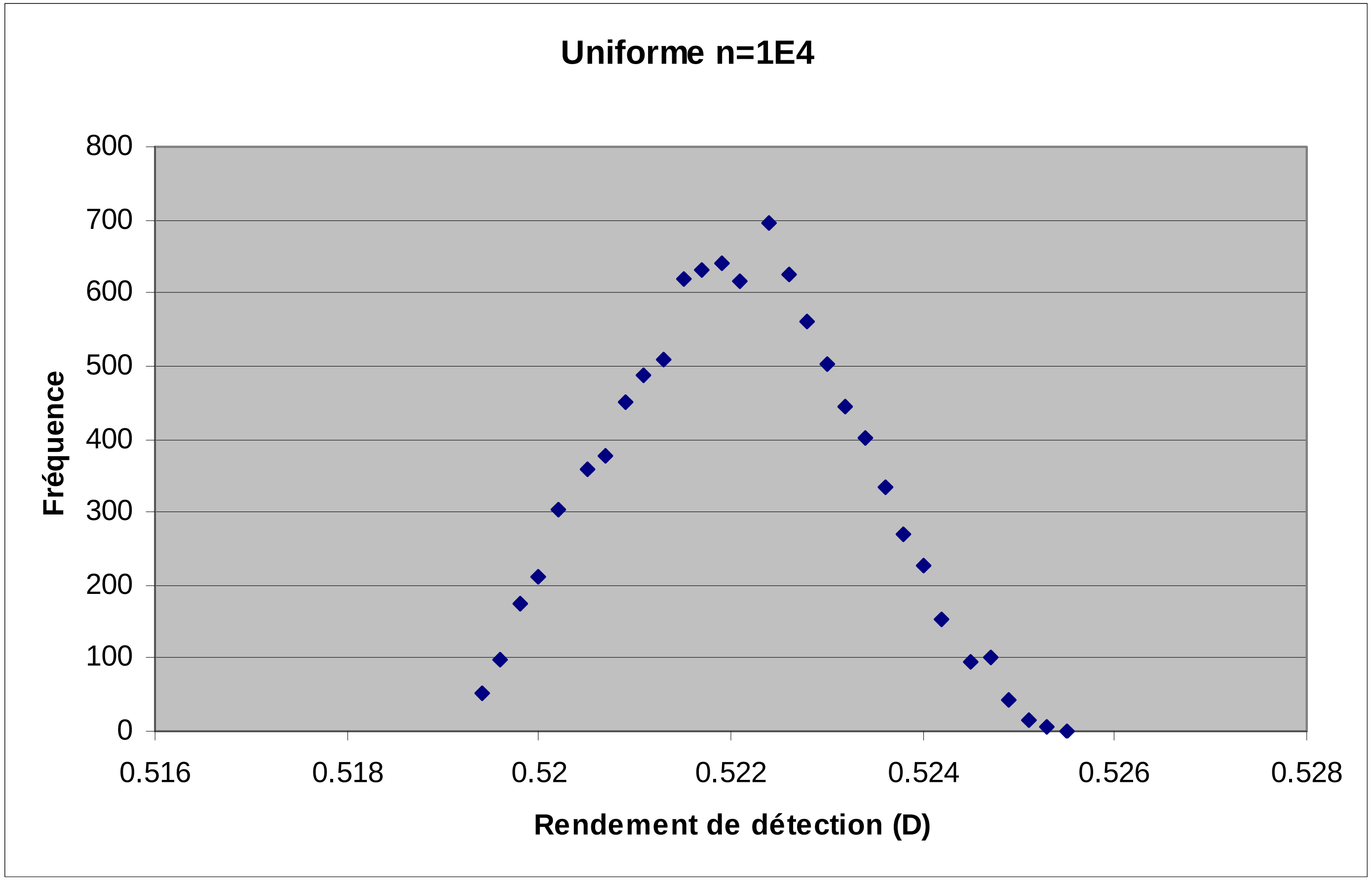
Here, test with 2 different *pdf*s: Gaussian or uniform

GAUSSIAN FLUCTUATIONS OF THE INPUT QUANTITIES



$\boxed{\varepsilon_D = 0.5219\ (8)}$

UNIFORM FLUCTUATIONS OF THE INPUT QUANTITIES



ε_D=0.5222 (12)

COMMENTS

For ^{55}Fe *a posteriori* analysis shows that there are 2 dominant factors in the uncertainty budget

Consequences:
- uniform *pdf* → triangular *pdf*
- Gaussian *pdf* → Gaussian *pdf*

- The transfer function induces the convolution of the pdfs of the input quantities

Thus, the pdf of the result is the consequence of the pdfs of the input quantities

Some statisticians would try to convince us that there is an univocal choice of the pdfs, thus that the pdf of the result is objective and that there is no uncertainty of the uncertainty…

My personal opinion (you could disagree) is that there is some subjectivity in this choice, and what you get from the Monte Carlo method is only a result of your hypothesis on the pdfs

CONCLUSIONS

The Monte Carlo method given in the supplement 1 of the GUM is a very powerful and simple tool to propagate uncertainties, especially when the measurement function is complex or non-analytical. In the latter case, this is the only possible method

Advantages of this method:

- Calculation algorithms are simple and explicit and can be easily incorporated in the codes used for the calculation of the measurement result
- This method overcomes the limitation of the usual formula of propagation of variances: some parameters could have a dominant influence on the uncertainty and the measurement model could be non-linear, discontinuous, non-analytical, non-derivable

But:

- The evaluation of the values and pdfs of the input quantities remain the biggest challenge and some simplifications can be necessary
- The *pdf* of the result is just a consequence of the *pdfs* of the input quantities, or an illustration of the central limit theorem!

Perspectives (personal view)

The GUM framework is a sound approach to the determination of uncertainties. The supplement 1 gives a powerful tool in most cases

I am not convinced that the determination of the pdf of the result gives much more information than an expression of the result as a mean value and associated standard deviation, except if confidence intervals have to be evaluated

There is a real risk that some Bayesian extremists will use this approach to redefine the measurement result as a *pdf* and not only from its mean value and uncertainty. In my opinion, this could ruin more than 20 years of effort in the rationalization of uncertainty determination in the field of metrology

Thank you for your attention