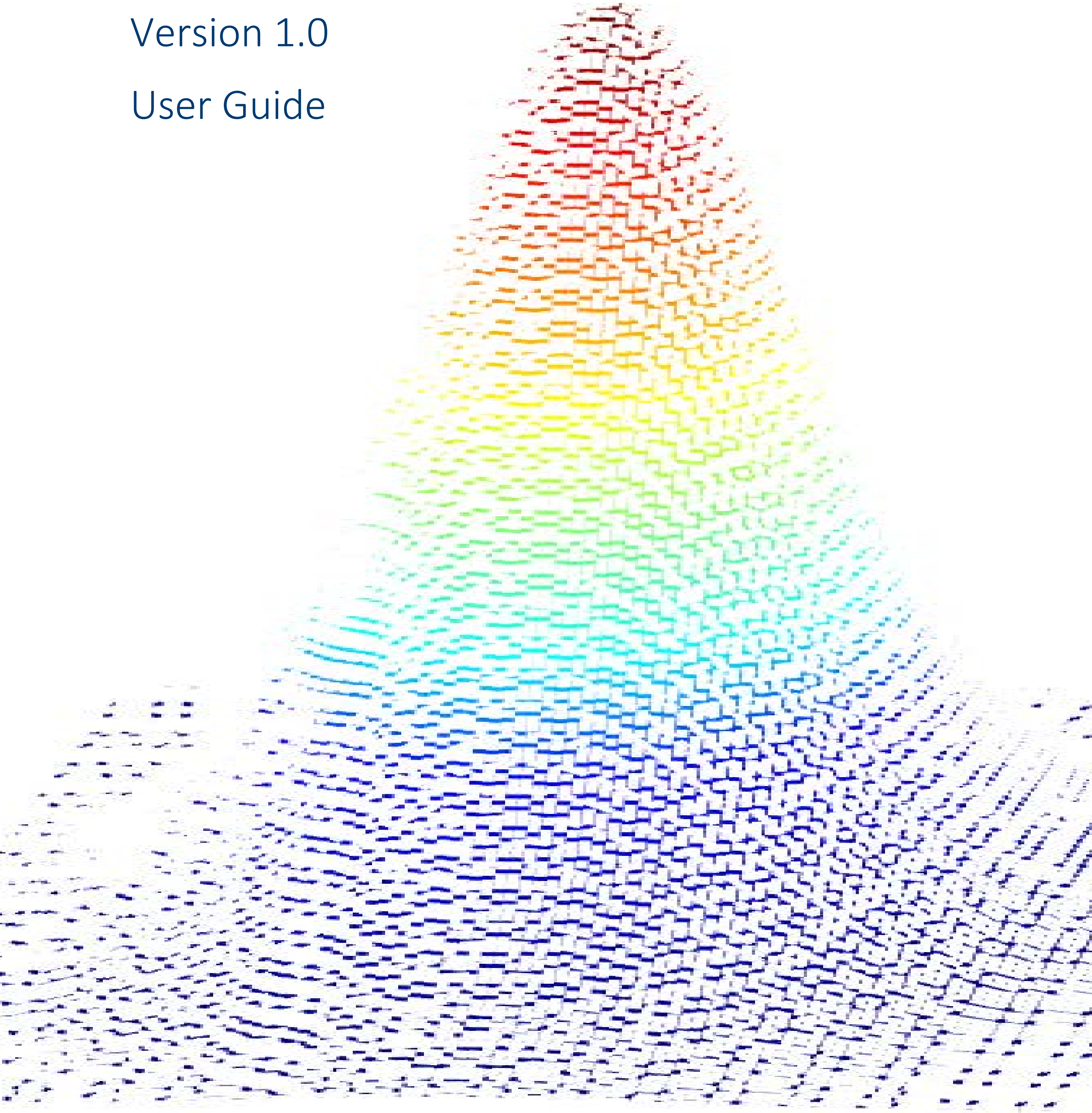
LNE Uncertainty

Version 1.0

User Guide



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LABORATOIRE NATIONAL DE MÉTROLOGIE ET D'ESSAIS

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I. Foreword

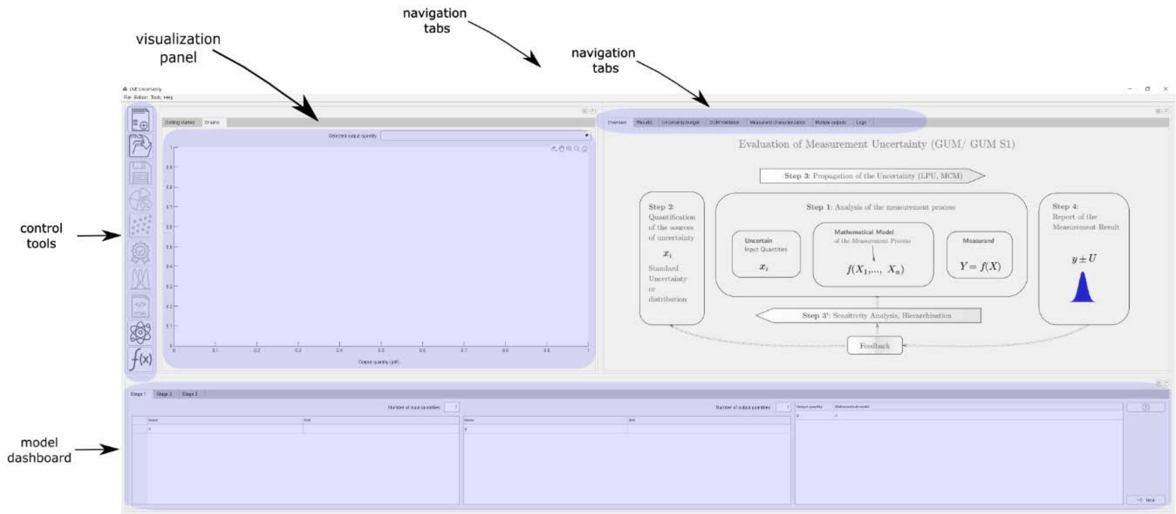
LNE Uncertainty is a free standalone application developed by the Laboratoire National de métrologie et d'essais (LNE) which enables measurement uncertainty to be estimated by propagation of variances or distributions using Monte Carlo simulations in accordance with the methods described in the Guide to the expression of uncertainty in measurement, GUM (JCGM100:2008, 2008), and its supplement 1 (JCGM101:2008, 2008). This software can be downloaded from the LNE website.

In addition to the evaluation of measurement uncertainty, LNE Uncertainty allows to:

- verify the validity of the results obtained with the GUM method according to the criteria described in GUM Supplement 1,
- process several output quantities simultaneously. The user can refer to the GUM Supplement 2 for the concept of multiple measurands (JCGM102:2011, 2011),
- establish an uncertainty budget by carrying out a sensitivity analysis using three methods: GUM, Spearman method based on rank correlation coefficients and Sobol method (Saltelli, Chan and Scott, 2000)
- determine the distribution of the output quantity by checking with the Kolmogorov-Smirnov test the adequacy to different theoretical distributions (Massey, 1951).

The software is a MATLAB executable. It has been tested against a series of examples of the literature (examples are available on Zenodo platform following this link).

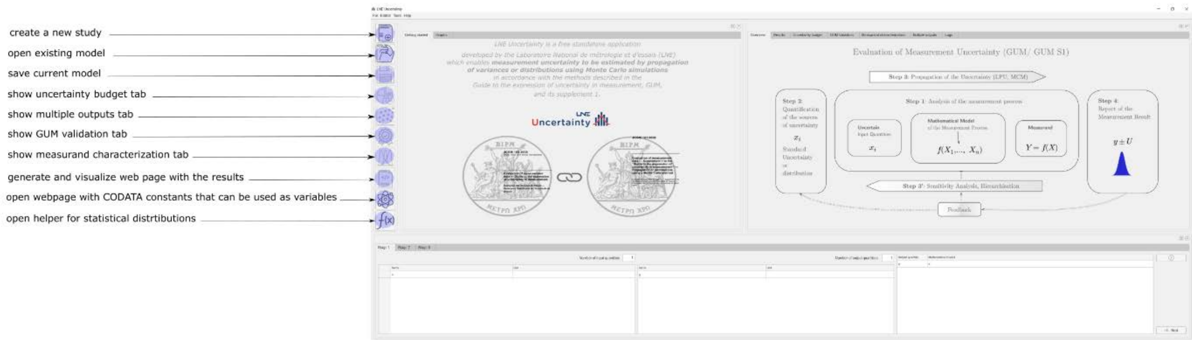
II. Global overview



The software is made of four resizable and dockable windows:

- control tools
- model dashboard
- navigation tabs
- visualization panel

III. Control tools



List of the actions the control tools allow the user to perform:

- ✓ Create new study
- ✓ Open existing model
- ✓ Save current model
- ✓ Show uncertainty budget tab
- ✓ Show GUM validation tab
- ✓ Show Measurand characterization tab

- ✓ Show Multiple outputs tab
- ✓ Generate and visualize html web page with the current results

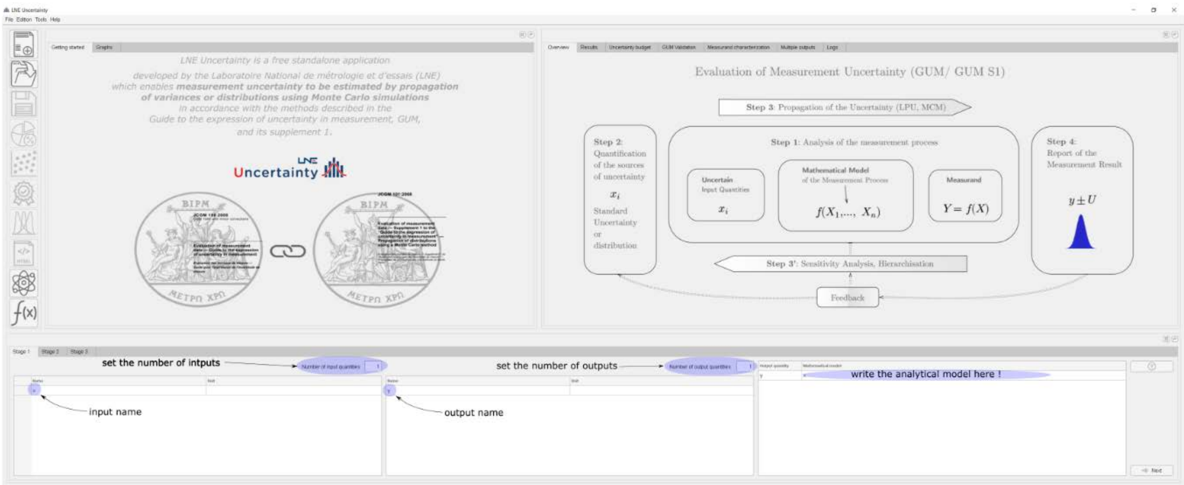
- ✓ Open web page with CODA constants list of variables that are reserved variables in the application

IV. Model dashboard

i. Step 1: specification of the measurement model(s)

The number of input quantities as well as the number of output quantities are displayed in the dedicated frames. You can assign names (and optionally units) to the input and output variables. The default names are X1, X2,... and Y1, Y2,... . The user must define the analytical model to relate the inputs to the outputs (the model can use standard math functions such as cos, sin, tan, tanh ...)

NB: In the case of measurement models with intermediate measurands, the user must ensure that each quantity entered in the frame is defined beforehand, otherwise you'll get an error.



ii. Step 2: quantification of sources of uncertainty

To assign a distribution to the input quantities, 14 probability distributions are available:

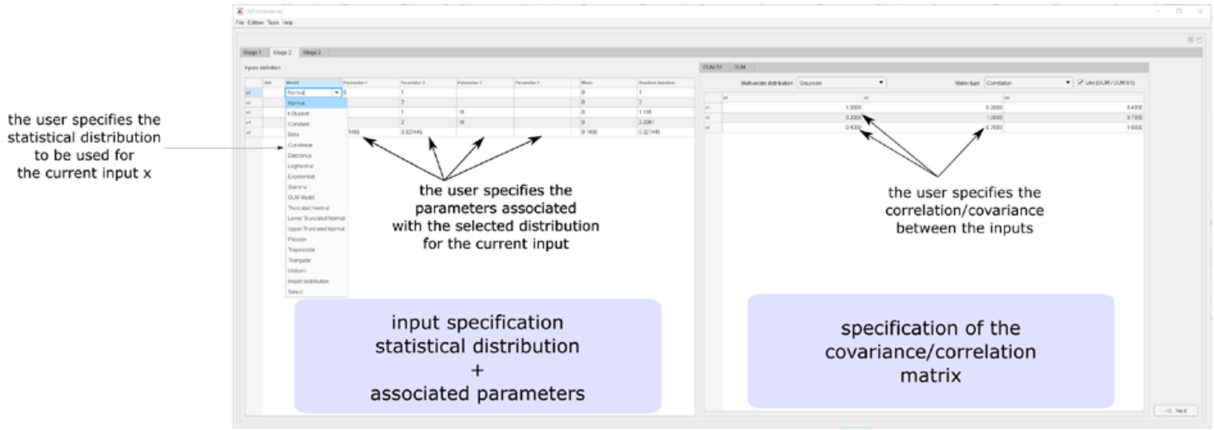
- *Normal,*
- *t-Student,*
- *Beta,*
- *Curvilinear trapezoïd,*
- *U-shaped,*
- *Exponential,*
- *Gamma,*
- *LogNormal,*
- *Truncated Normal,*
- *Lower Truncated Normal,*
- *Upper Truncated Normal,*
- *Poisson,*
- *Triangular,*
- *Trapezoidal,*
- *Uniform,*
- *Constant*

For each distribution, the table recalls the parameter(s) to be filled in. It contains a specific line for constant input quantities.
LNE Uncertainty software allows correlations between input quantities modelled by :

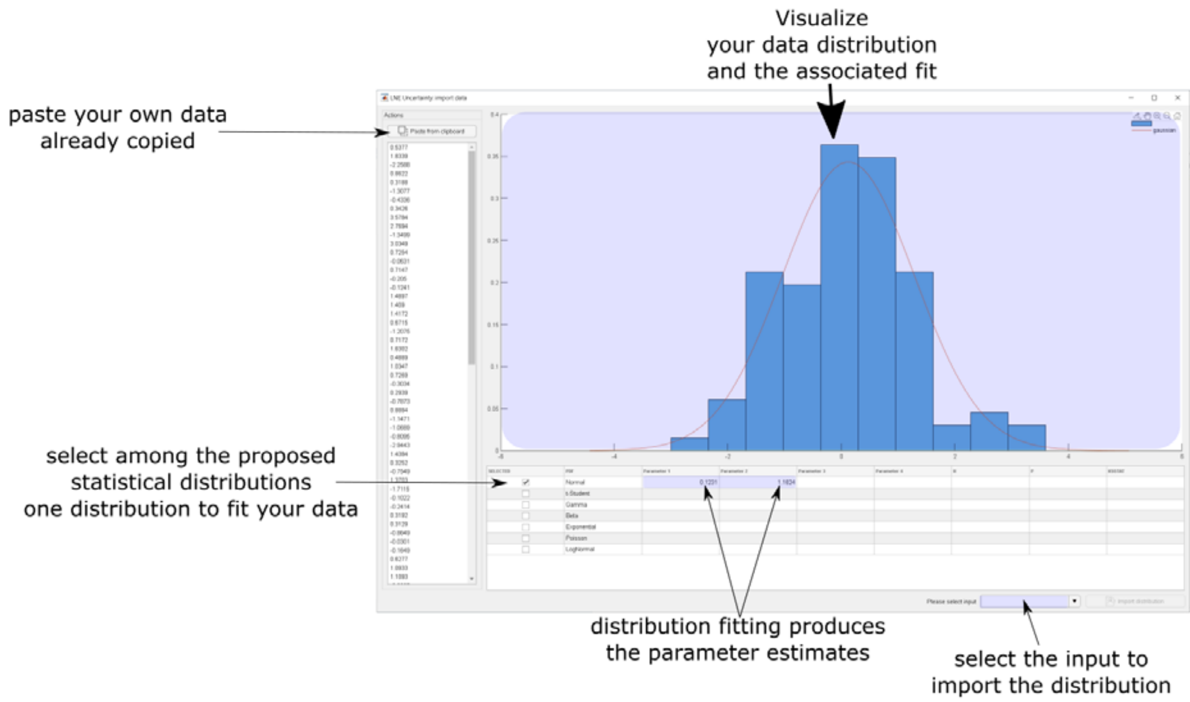
- normal distributions: ***multivariate normal distribution .***
  The user can fill in either the correlation matrix or the variance-covariance matrix.

- Student's distributions: ***multivariate Student distribution .***
  The user only fills in the correlation matrix.

NB: In the case of the multivariate Student distribution, the dependence between input variables is modelled using a Gaussian copula with Student marginals (Possolo, 2010).



The user can also import its own data and fit the provided data using the field <<import data>> in the dropdown list

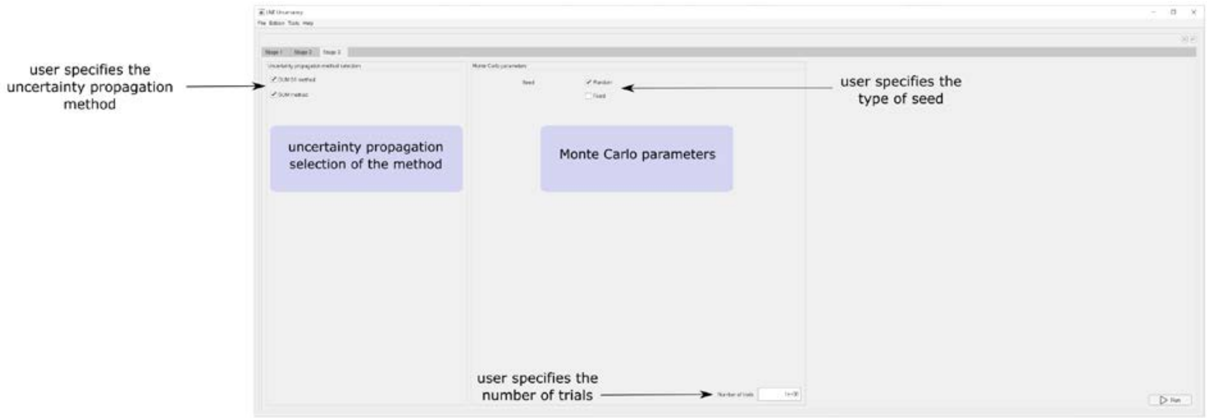


iii. Step 3: simulation and propagation

The user can:

- select between GUM and GUM S1 uncertainty propagation methods (as a default, both are used)
- configure the seed:
  - *Fixed* and chosen by the user. Two simulations with the same seed will have the same results
  - *Random (default)* and calculated from the computer clock to avoid repetition of random series
- specify the number of trials (as a default, 10^6 trials are computed)

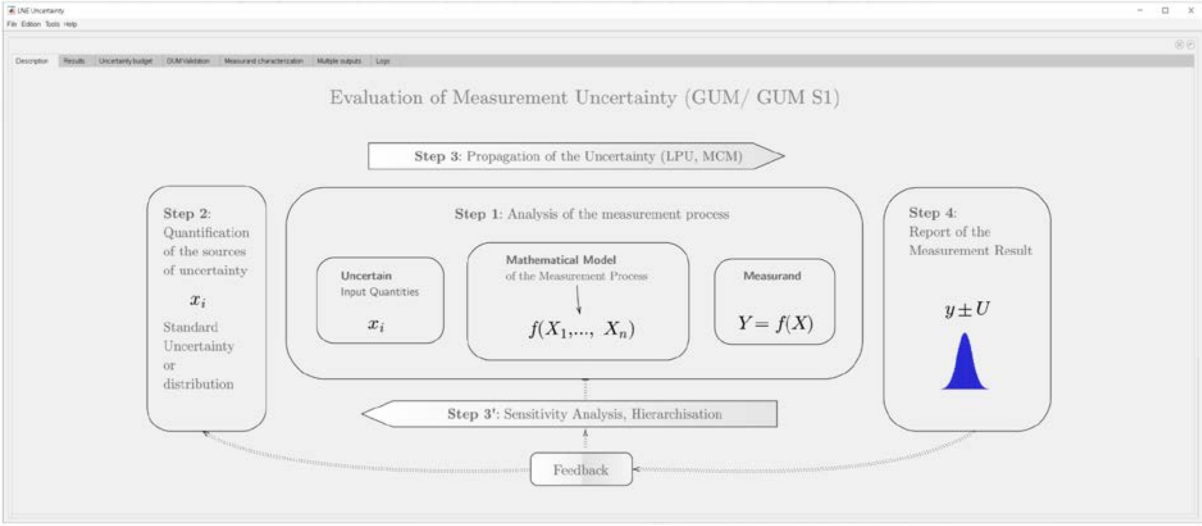
Once steps 1 to 3 have been performed, you can press the button Run to launch the simulation process.



V. Navigation tabs

i. Description

- Displays an image showing the methodology for the Evaluation of Measurement Uncertainty (GUM /GUM S1)



ii. Results

Results tab summarizes the information related to the current output variable. It displays the results for both the GUM and GUM S1 (if both are selected at step 3 in the model dashboard).

For the GUM results, the user can specify the coverage factor k. For the GUM S1, the user can specify the coverage probability and the type of confidence interval to compute. The coverage interval $[y_{\text{inf}}; y_{\text{sup}}]$ of probability p $(0 \leq p \leq 1$) is an interval that contains $100 \times p\%$ *of* the values from the Monte Carlo simulation. It can be:

- symmetric (in probability) in which case it is obtained by taking the quantile of order $1 - p/2$ as y_{inf}, and the quantile of order $p/2$ as y_{sup},

- the shortest in which case it is obtained by determining α $(0 \leq \alpha \leq 1 - p)$ such that the interval constituted by the order quantiles α and $1 - \alpha$ is as short as possible.

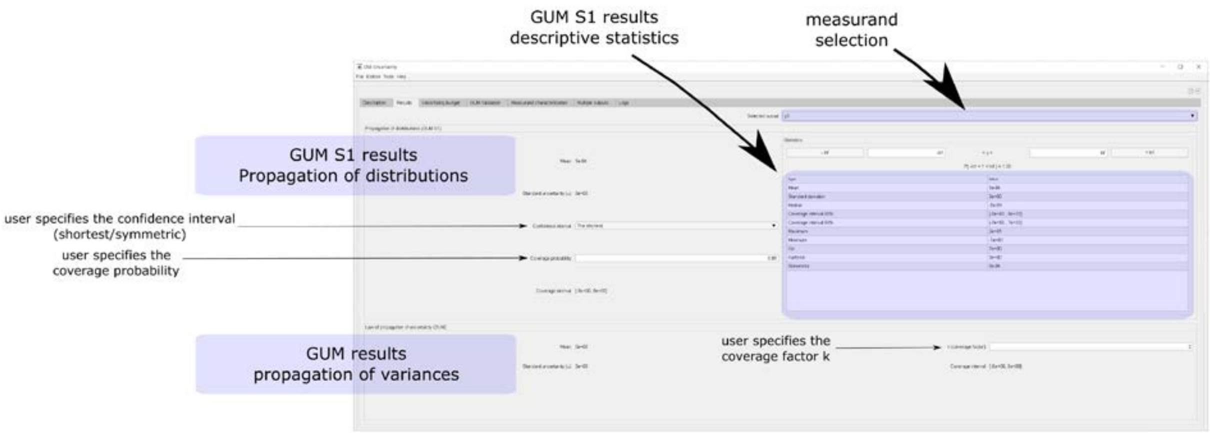
From GUM S1 results, the user can also compute $P(a \leq y \leq b)$ and specify (a, b) where y is the current measurand under study and (a, b) stand as some lower and upper bound, respectively. As a default, $a = -\infty, b = +\infty$.

GUM results

- mean,
- standard uncertainty,
- expanded uncertainty

GUM S1 results

- mean,
- standard uncertainty,
- coverage interval,
- confidence interval,
- summary statistics
    - ✓ mean,
    - ✓ standard deviation,
    - ✓ median,
    - ✓ coverage interval 95%
    - ✓ coverage interval 99%
    - ✓ maximum,
    - ✓ minimum,
    - ✓ variance,
    - ✓ skewness,
    - ✓ kurtosis



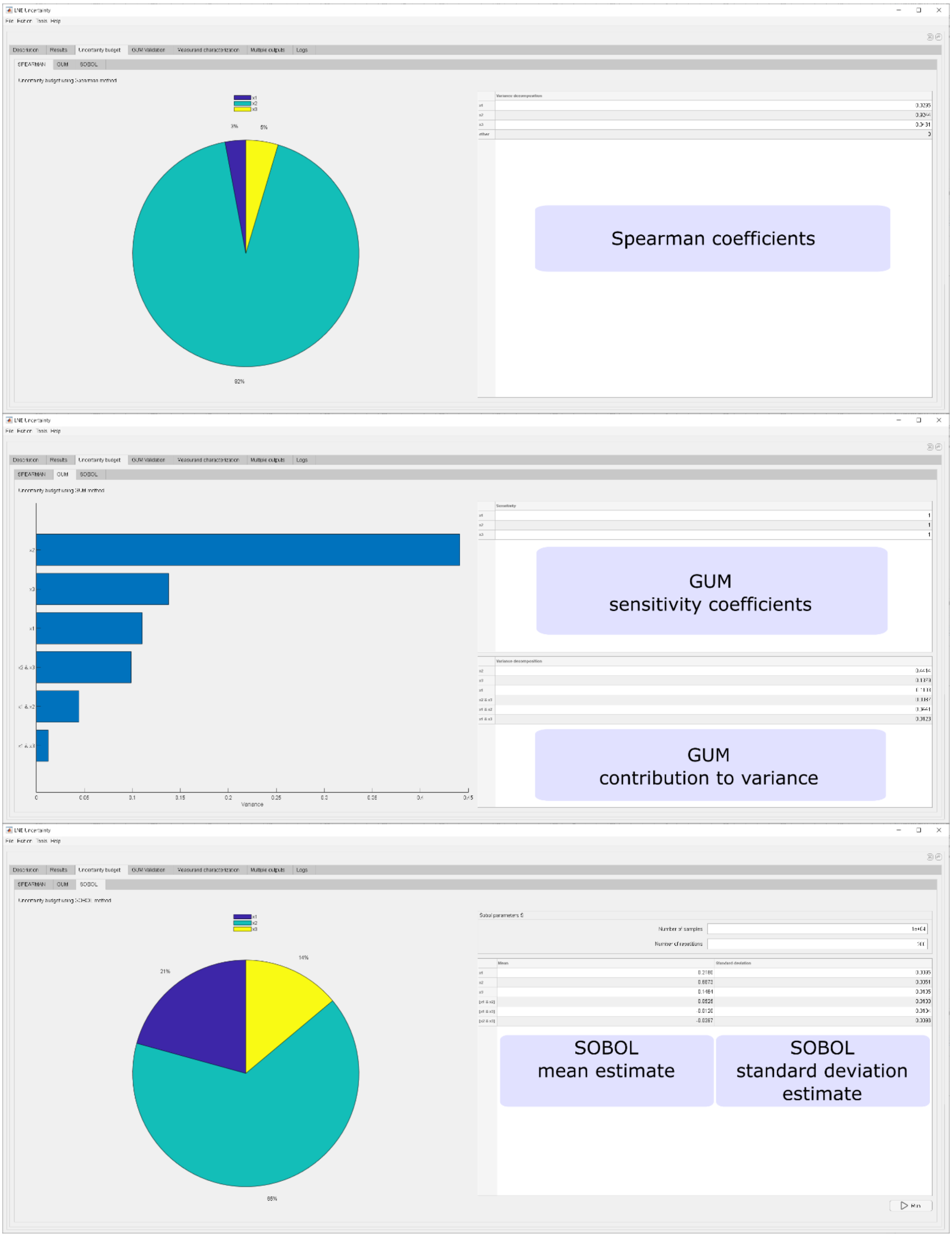
iii. Uncertainty budget

Sensitivity analysis allows the uncertainty budget to be established by ranking the input quantities in relation to their contribution to the variance of the output quantity. Three methods are available in LNE Uncertainty software: GUM method, Spearman correlation coefficients and Sobol' indices. A tab is dedicated to each method so the user can navigate among the three tabs to check the results.

Regarding Spearman's correlation coefficients, the calculation is not very time-consuming. However, the interpretation of these coefficients only makes sense in the case of a monotonic measurement model.

On the other hand, Sobol' indices make it possible to evaluate the contribution of each source of uncertainty, as well as possible interactions, without any particular hypothesis on the properties of the measurement model apart from continuity. Estimating these indices requires additional Monte Carlo runs, which significantly increases the calculation time.

NB: It is important to note that the interpretation of the results is delicate if there are significant correlations between the input quantities. In this case, it is not possible to dissociate the individual effects from the correlated input quantities.


Spearman coefficients
GUM
sensitivity coefficients
GUM
contribution to variance
SOBOL
mean estimate
SOBOL
standard deviation
estimate

iv. GUM validation

The Monte Carlo method has a wider scope of application than the GUM method. In order to study the validity of the results obtained by the GUM method, GUM Supplement 1 defines a validation criterion. This is based on a comparison of the 100% wider intervals obtained by the two methods (p is the coverage probability).

In practice the differences $dinf = |y - Up - yinf|$ and $dsup = |y + Up - ysup|$ are calculated, where $yinf$ and $ysup$ represent the lower and upper limits of the expanded interval obtained by the Monte Carlo method and $[y - Up;\ y + Up]$ represents the symmetrical expanded interval around the value assigned to the measurand obtained by the GUM method.

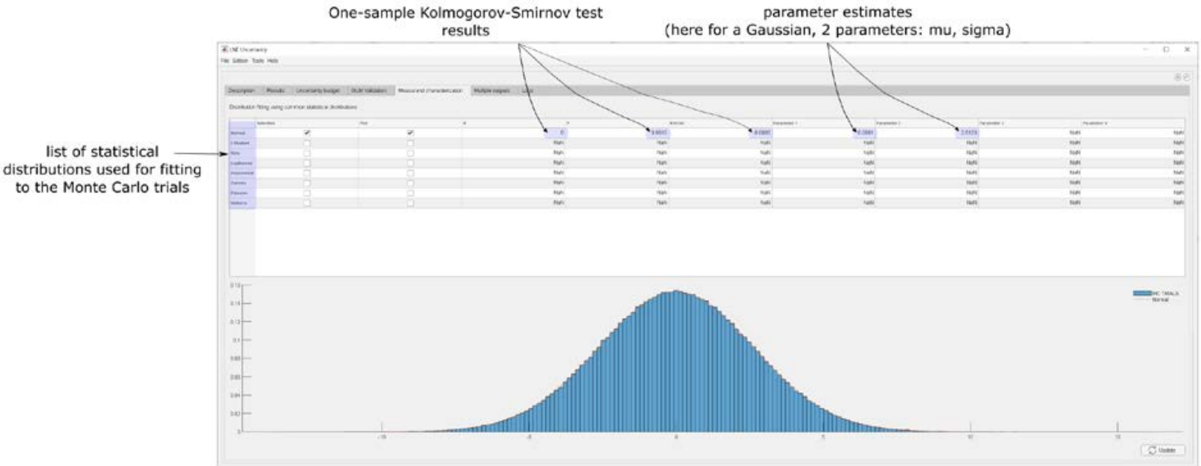
We compare $dinf$ and $dsup$ to a numerical tolerance $\delta = 0{,}5 \times 10^{-1}$ calculated from the standard deviation of the values assigned to the output quantity obtained by the Monte Carlo method. In fact, one poses $\mathrm{u(y)} = \mathrm{c} \times 10^{-1}$ with c an integer consisting of one or two digits depending on whether it is validated with one or two significant digits.

Usually the comparison is made over intervals expanded to 95%, in which case the coverage factor (k) of the combined uncertainty calculated by the GUM method is classically taken to be equal to 2.

NB: The user must configure the simulation to use both propagation methods in order to perform the validation procedure (step 3 in the main dashboard).

v. Measurand characterization

- Displays the histogram of the Monte Carlo trials
- Allows to select among common statistical distributions (Normal, Student, Beta, LogNormal, Gamma, Poisson and Uniform) those to use to fit the Monte Carlo trials and displays the estimated parameters as well as statistical hypothesis test results (*h, p, ksstat*) for selected statistical distributions

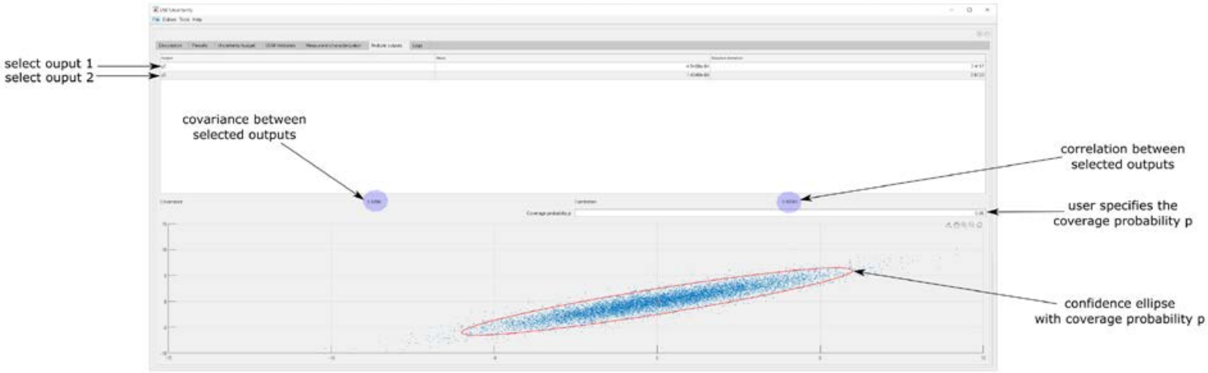


vi. Multiple outputs

LNE Uncertainty software allows a multivariate analysis of the output quantities. The reader is referred to supplement 2 of the GUM dealing with multiple measurands.

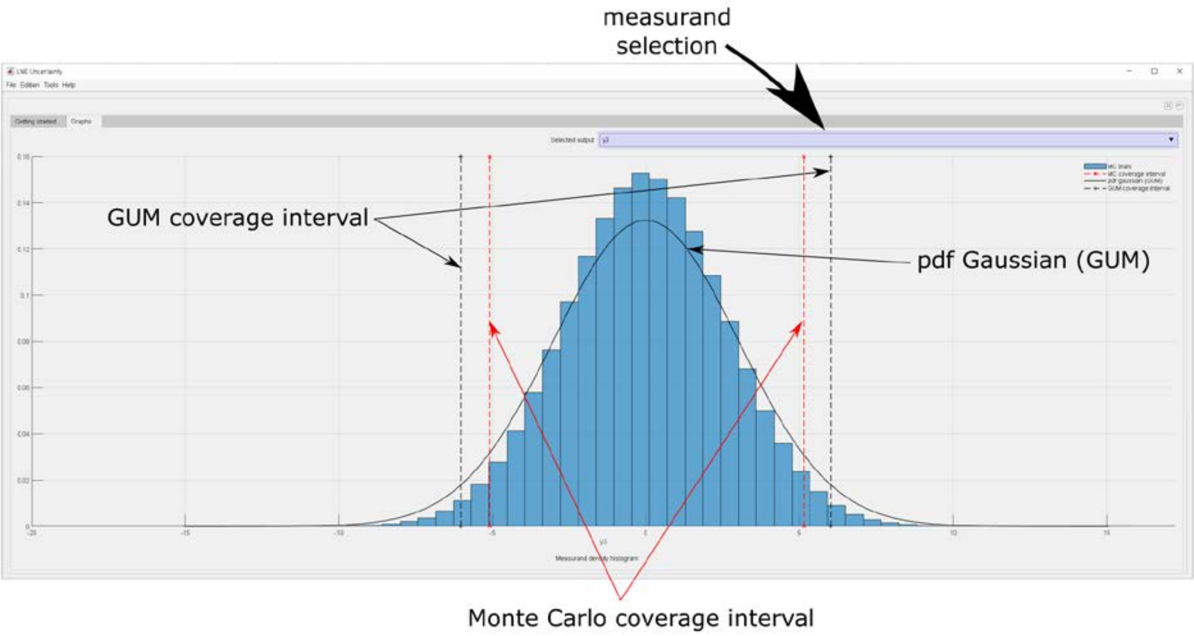
Results are presented in pairs of output quantities. The measurement result box displays the estimated mean and standard deviation for the output quantities of interest and gives their covariance and linear correlation coefficient. The graph displays the confidence ellipse computed according to the user-specified coverage probability p. It allows to quickly identifying the direction and intensity of the correlation of the two selected output quantities.

<u>NB:</u> In accordance with Supplement 2 of the GUM, there is an arbitrary number of regions of confidence or 100% enlarged regions. LNE Uncertainty proposes to use a confidence ellipse. The length of the half-axes is equivalent to the value of the standard deviation of each of the selected output quantities. In the case where the output quantities are approximately Gaussian, the Confidence Ellipse represents accurately the expanded region at $100\times p\%$. In other cases, the confidence ellipse may not be informative.



VI. Visualization panel

- plots the histogram for the selected measurand with mean, standard uncertainty when GUM is selected at step 3 in the model dashboard
- plots the histogram for the selected measurand with mean, standard uncertainty and confidence interval when GUM S1 is selected at step 3 in the model dashboard



VII. Additional information

i. Kolmogorov Smirnoff fit test

LNE Uncertainty allows checking the adequacy of the distribution of the output quantity to a probability distribution according to the Kolmogorov-Smirnov test. Seven distributions are proposed:

- *normal*,
- *uniform*,
- *exponential*,
- *log-normal*,
- *Gamma*,
- Beta,
- *Student*.

The principle of the Kolmogorov-Smirnov test is to compare the simulated distribution function $F_M(y) = \frac{1}{M}\sum_{j=1}^{M} 1_{\{Y_j \leq y\}}$ of the output variable with the cumulative distribution function F_0 of the theoretical distribution. The quantity M represents the number of Monte Carlo trials and Y_j stands as the j^{th} value of the simulated sample.

The parameters of the theoretical distribution are estimated from the sample of simulated values.
The statistic of the Kolmogorov-Smirnov test is given by the following formula:

$$D_M = \max_{1 \leq i \leq M}\{|F_0(Y_i) - F_M(Y_i)|\}$$

If the differences between the two distribution functions are too great, then the test leads to the conclusion that the output quantity does not follow the theoretical distribution considered at the specified risk level. Default is 0.05.

LNE Uncertainty gives the values of the test statistic and the p-value for each theoretical distribution. The p-value is the probability of obtaining a value of the test statistic greater than or equal to D_M under the assumption that the simulated values are distributed according to the theoretical distribution. In other words, the smaller the value, the greater the deviations between the output quantity distribution and the theoretical distribution.

The results are summarized in a table with a graph representing the probability density of the calculated output quantity and the densities of the selected theoretical probability distributions.

The common practice is to reject the theoretical distribution if the p-value is less than 0.05.

NB: In a Monte Carlo simulation with a large number of prints, the test is very sensitive to minute deviations from the theoretical distribution and the p-value values are overwhelmingly small. For this reason, it is also important to look at the value of the test statistic, since the lower the value, the closer the theoretical distribution is to the value of the output quantity.

ii. Spearman rank correlation coefficient

When the mathematical model is monotonous, the Spearman correlation coefficient calculation is used to perform a sensitivity analysis. This method consists of calculating the correlation coefficient between the ranks associated with each of the quantities involved. The correlation coefficient between $\mathrm{X_i}$ and *Y* is given by the following formula:

$$\rho(X_i;Y) = 1 - \frac{6\sum_{j=1}^{M}\left(RX_i^j - RY^j\right)^2}{M(M^2-1)}$$

with $\mathrm{RX_i}$ the row vector of the input quantity $\mathrm{X_i}$, RY the vector of the rows of the output size *Y*, j the j^{th} Monte Carlo trial and M the total number of Monte Carlo trials. The correlation coefficients thus obtained are normalised to obtain an estimate of the relative contribution of each input quantity to the variance of the output quantity *Y.* The sensitivity indices are thus obtained, which are given by the following formula:

$$S_i^{Spearman} = \frac{\rho^2(X_i;Y)}{\sum_{j=1}^{n}\rho^2\left(X_j;Y\right)}$$

with n the number of inputs. The index $\mathrm{S_i^{Spearman}}$ represents the contribution of the input quantity $\mathrm{X_i}$ to the variance of *Y*. All of these sensitivity indices together constitute the uncertainty budget associated with the output quantity *Y*.

iii. Sobol method

Sobol method allows the detection of significant interactions between input quantities. The estimation of the sensitivity index $\mathrm{S_i^{Sobol}}$ between the output variable Y and the input variable X_i is based on the use of two noted samples $\left(\mathrm{x_{ij}}\right)_{\substack{\mathrm{i=1,\dots,n}\\ \mathrm{j=1,\dots,M}}}$ and $\left(\mathrm{x_{ij}}'\right)_{\substack{\mathrm{i=1,\dots,n}\\ \mathrm{j=1,\dots,M}}}$.

This is obtained by the following formula:

$$\mathrm{S_i^{Sobol}} = \frac{\widehat{\mathrm{D}}_\mathrm{i}}{\widehat{\mathrm{D}}} = \frac{\frac{1}{\mathrm{M}}\sum_{\mathrm{j=1}}^{\mathrm{M}} \mathrm{f}\left(\mathrm{x_{1j}},\dots,\mathrm{x_{nj}}\right)\mathrm{f}\left(\mathrm{x'_{1j}},\dots,\mathrm{x_{ij}},\dots,\mathrm{x'_{nj}}\right) - \hat{\mathrm{f}}_0^{\,2}}{\frac{1}{\mathrm{M}}\sum_{\mathrm{j=1}}^{\mathrm{M}} \mathrm{f}^2\left(\mathrm{x_{1j}},\dots,\mathrm{x_{nj}}\right)}$$

where n is the number of inputs, M the total number of Monte Carlo trials and $\hat{\mathrm{f}}_0 = \frac{1}{\mathrm{M}}\sum_{\mathrm{j=1}}^{\mathrm{M}} \mathrm{f}\left(\mathrm{x_{1j}},\dots,\mathrm{x_{nj}}\right)$ an estimate of the average output quantity.

This estimation method is, however, costly in terms of the number of model evaluations. Thus, LNE Uncertainty proposes to repeat this calculation several times on samples of size $M_s \ll M$ and then, to calculate the average index for each input quantity.

The standard deviation of the values of this index is also calculated in order to control the stability of the estimate.

The user can therefore specify two parameters:

- the **number of repetitions** of the estimate
- the s**ample size** M_s representing the number of values present in both samples $(x_{ij})_{\substack{i=1,\dots,n \\ j=1,\dots,M_s}}$ and $(x_{ij}')_{\substack{i=1,\dots,n \\ j=1,\dots,M_s}}$.

LNE Uncertainty software also calculates second order indices, which represent the interactions between two input quantities. For sake of clarity, the reader is referred to Saltelli's book (Saltelli, Chan and Scott, 2000) to obtain the formulas for second-order indices.

The results are displayed in the form of a pie chart representing the uncertainty budget and a data table containing the contribution to variance and standard deviation (on the values of each index) of the ^{1st} and ^{2nd} order Effects where applicable.

NB: The interaction between X_i and X_j is displayed as X_i, X_j.

VIII. References

JCGM100:2008 (2008) 'Evaluation of measurement data — Guide to the expression of uncertainty in measurement', *International Organization for Standardization Geneva ISBN*, 100(September). doi: 10.1373/clinchem.2003.030528.

JCGM101:2008 (2008) 'Supplement 1 to the ''Guide to the Expression of Uncertainty in Measurement" - Propagation of distributions using a Monte Carlo method', *International Organization for Standardization Geneva ISBN*, 101.

JCGM102:2011 (2011) 'Evaluation of measurement data – Supplement 2 to the "Guide to the expression of uncertainty in measurement" – Extension to any number of output quantities', *International Organization for Standardization Geneva ISBN*, 102(October), pp. 1–72.

Massey, F. J. (1951) 'The Kolmogorov-Smirnov Test for Goodness of Fit', *Journal of the American Statistical Association*, 46(253), pp. 68–78. doi: 10.1080/01621459.1951.10500769.

Possolo, A. (2010) 'Copulas for uncertainty analysis', *Metrologia*. IOP Publishing, 47(3), pp. 262–271. doi: 10.1088/0026-1394/47/3/017.

Saltelli, A., Chan, K. and Scott, M. (2000) 'Sensitivity analysis, Probability and Statistics series', in.