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Comprehensive Exordium of Monte Carlo Simulation Technique: An Alternative Approach for Measurement Uncertainty Evaluation

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Precise and accurate measurements are essential for reliable experimental investigations and establishments of immaculate scientific theories. It has been realized that the measurement observations are always accompanied by certain reservations, hence to provide quality measurements, systematic assessment of these uncertainties is of much significance. This article attempts to demonstrate the detailed procedure for measurement uncertainty evaluation using Monte Carlo Simulation (MCS) technique as per the recommendations of JCGM 101: 2008 using Microsoft Excel. Interestingly, it has been perceived that the expanded uncertainty values and histograms acquired using Law of Propagation of Uncertainties (LPU) and Monte Carlo Simulation (MCS) are distinctive.

Keywords: Metrology, Measurement, Uncertainty, Law of Propagation of Uncertainties, Probability Distribution Function, Monte Carlo Simulation, Random Number Generation

1 Introduction

Metrology is defined as the science of measurement and its applications. To understand the measurement observations appropriately, computation of associated measurement uncertainty is crucial. According to the international vocabulary of metrology (VIM), measurement uncertainty is defined as "non-negative parameter characterizing the dispersion of the quantity values being attributed to a measure and, based on the information used"¹. The measurement uncertainty occurrence may be attributed to undefined measure and, indistinct approximations, numerous assumptions formulated during measurements, significant deviation in measurement outcomes, instrument bias, erroneous measurement methodologies and environmental conditions, hence, the measurement observations are recommended to be expressed in a standard manner with distinctive quantitative proclamation characterizing their degree of accuracy. Measurement uncertainty evaluation is comprised of exhaustive statistical analysis of measurement observations followed by compendious elucidation of the final outcome.

The conventional method of measurement uncertainty evaluation in accordance with Guide to the Expression of Uncertainty in Measurement (GUM) is

known as Law of Propagation of Uncertainties (LPU). This approach has been extrapolated from a set of approximations to simplify the computations and justifies a wide range of models¹. In LPU technique, the measure and model is expanded as per the Taylor to propagate uncertainties followed by series simplification of the expression by considering the first order term only, however considering the higher order terms may enhance the accuracy of measurements. This approximation stands conceivable here, as the uncertainty values are very small in comparison of the corresponding quantities and leads to a general expression for propagation of uncertainties. Though, the GUM/LPU technique is a well-established and authentic approach for measurement uncertainty computation, however, there are numerous constraints associated with it. The model function used for measure and calculation must have inconsequential non-linearity, so that the approximation made by considering only the first order term of Taylor series in LPU method may estimate the uncertainty output accurately. The law of propagation of uncertainty endorses the central limit theorem; stating that the convolution of various distributions results into normal distribution, substantiating that the probability distribution of measure and is approximately normal and can be demonstrated by a t-distribution. However, in

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several cases, the resultant probability distribution may exhibit a skewed nature and does not demonstrate a normal distribution necessarily, hence challenging the central limit theorem. The LPU technique, after calculating the standard uncertainties, follows welch-Satterthwaite equation for computation of effective degree of freedom, required to obtain the expanded uncertainty. Additionally, the GUM/LPU methodology may not stand valid, if some of the input quantities are bigger in comparison of others or when the probability distributions of input sources are asymmetric or the order of magnitude of the estimated measurand and associated uncertainty are nominally indistinguishable. In order to surmount expostulations existing with LPU method, Monte Carlo Simulation (MCS) technique was adopted as an alternative approach for measurement uncertainty evaluation^{2,3}. Name of this method was embraced form the Monte Carlo Casino in Monaco. Monte Carlo Simulation approach is based on a computational algorithm, in which repeated random sampling is carried out for result computation and is preferred when an exact result computation through a deterministic algorithm is not achievable. It is an extremely flexible method with unlimited analysis amplitude and remarkable empirical distribution handling capability.

2 Materials and Methods

2.1 Method for measurement Uncertainty Evaluation using Monte Carlo Simulation Technique

The general LPU expression has been demonstrated by Equation 1.

$$u_y^2 = \sum_{i=1}^N \left(\frac{\partial f}{\partial x_i}\right)^2 u_{x_i}^2 \qquad \dots (1)$$

Where, u_y represents the combined uncertainty of output (Y) and u_{xi} represents the standard uncertainty for ith input quantity.



Fig. 1 — LPU approach for measurement uncertainty.

The LPU approach follows the route exhibited in Fig. 1.

For measurement uncertainty evaluation, Monte Carlo Simulation technique was adopted because it can conduct the random sampling from input quantities probability distributions^{4,5}, hence, evading the need of calculating the first order derivatives or sensitivity coefficients and effective degrees of freedom. Furthermore, it provides the probability distribution of the measured quantity along with its graphical representation for determination of coverage interval. In Monte Carlo Simulation procedure, generation of numerous pseudo random numbers for various inputs parameters with explicit probability distribution functions stabilizes the measurement uncertainty assessment⁶. The steps adopted in Monte Carlo Simulation for measurement uncertainty evaluation are exhibited by Fig. 2. In present investigation, we consider a hypothetical case for measurement uncertainty evaluation using the two approaches; LPU and MCS. Various error sources contributing towards the measurement uncertainty in this suppositional case, have been identified and demonstrated in the fishbone diagram shown in Fig. 3.

3 Results and Discussion

The hypothetical model function for current exercise is established in Equation 2, whereas a







Fig. 3 — Error sources contributing towards measurement uncertainty.

Table $1 - A$ typical uncertainty budget as per law of propagation of uncertainties							
Sources of Error	Limits	Probability Distribution	Factor	Sensitivity coefficient	Standard Uncertainty	Uncertainty contribution (µm)	Degree of freedom
Repeatability	0.1	Normal	1	1	0.100	0.100	9
Error due to temperature variation	1.1	Rectangular	1.7321	1	0.635	0.635	œ
Reproducibility	0.1	U-shaped	1.4142	1	0.071	0.071	œ
Misalignment	0.1	Triangular	2.4495	1	0.041	0.041	8
Uncertainty of the standard used	0.01	Normal	2	1	0.005	0.005	∞
Combined uncertainty $u_c = \pm 0.65$ un	nit						
Expanded uncertainty at a coverage	e interval of	f 95% (<i>k</i> =2) U _E	$=\pm 1.3$ unit				

detailed uncertainty budget as per GUM/LPU has been presented in Table 1.

$$Y = (\delta_R \times \delta_t) + (\delta_{MA} \times \delta_{US} / \delta_{RP}) \qquad \dots (2)$$

Where Y, is Output; δ_R , Repeatability; δ_t , Error due to temperature deviation; δ_{MA} , Error due to misalignment; δ_{US} , Error due to uncertainty of standard used; δ_{RP} , Error due to reproducibility

Here, the average value of output from 10 repeatable measurements is = 87.13 unit, with standard deviation 0.3 unit.

The reported measurement result for dimensional measurement in case of LPU is = 87.13 ± 1.3 unit.

Further, the measurement uncertainty evaluation is carried out using MCS, in order to obtain more reliable outcomes through a set of randomly generated numbers with numerically approximated probability distribution functions of the measure and. To initiate with, the number of Monte Carlo Trials "M" is chosen followed by generating random numbers for each input quantity according to respective probability distribution functions, and repeating this process for M times for each input. Using the model function, output value is calculated for each input sample vector, which has been drawn repeatedly through the random number generator^{7,8}. The appropriate random distribution of measure and is approximated using empirical distribution of "M" output sample vectors. The recommended number of trials "M" can be acquired using Equation 3.

$$M > \frac{10^4}{1-p}$$
 ... (3)

Where, p represents the coverage interval.

For a coverage interval of 95%, M=2, 00, 000. Hence, to carry out MCS for measurement uncertainty evaluation at coverage interval of 95%, the number of trials should be at least 2, 00, 000. Each input quantity is considered one by one for MCS.



Fig. 4 — Repeatability histogram.

3.1 Repeatability

As per the repeatability calculation, the mean measured value obtained for this particular investigation is = 87.13 unit and the standard deviation = 0.3 unit. Steps involved for random number generation for repeatability with normal distribution are described below:

- i) Open Microsoft office excel
- ii) Go to "Data" tab
- Select "Random number generation" iii)
- iv) For 2, 00, 000 iterations, put suitable number of variables and number of random numbers to give an array of 2, 00, 000 random numbers
- Select the distribution as "Normal" v)
- Put the mean value and standard deviation vi)
- vii) Select the output range and press "OK"
- viii) Now plot the histogram, by selecting the input range, bin range, output range and chart output from array. The histogram for repeatability data is shown in Fig. 4.

3.2 Error due to temperature variation

Repeat the steps from i to iv, followed by selecting "Uniform" distribution, and range, now select output range and press "OK". We get an array B of 2, 00, 000 random numbers. The histogram shown in Fig. 5 can be plotted by following the steps explained above (step viii).

3.3 Reproducibility

Microsoft excel does not have a direct provision to generate random numbers with U-shaped distribution, hence there is a need to apply a formula. Repeat the steps from i to iv. Select distribution "Uniform", from -3.14 to 3.14. We get an array, now here in this case we keep minimum value 0.0001 and maximum value 0.1. Apply the formula for U-distribution in the first cell and continue to obtain the final array containing 2, 00, 000 random numbers with U-shaped distribution. The histogram demonstrated in Fig. 6 can be plotted using step viii, discussed previously.

3.4 Misalignment

Similar to U-shaped distribution random number generation inadequacy, Microsoft excel cannot generate random numbers with triangular distribution. Here also we repeat the steps from i to iv, followed by selecting distribution "Uniform" from 0.0001 to 1 for this particular case and obtaining an array. Now keep minimum value 0.0001, maximum value 0.1, average value 0.05 and apply the formula for triangular distribution in the first cell and continue to acquire the final array containing 2, 00, 000 random numbers with triangular distribution. The histogram exhibited in Fig. 7 can be plotted following the step viii explained above.

3.5 Uncertainty of the standard used

Repeat steps from i to v, put mean value 0.0001 and standard deviation 0.005 for this particular

Fig. 5 — Histogram for error due to temperature variation.



Fig. 6 — Reproducibility histogram.

hypothetical case. Select the output range and press "OK". We get an array E of 2, 00, 000 random numbers with normal distribution, with histogram plotted using step viii, as displayed in Fig.8.

As per the model function presented by Equation 2, we produced Monte Carlo Simulation array E with 2, 00, 000 random numbers for measurement uncertainty evaluation. 10 iterations out of 2, 00, 000 iterations are shown in Table 2.

Next, the average measured value for MCS array E for this distinct hypothetical case is computed; $Y_{Average}$ = 91.46 unit, whereas the expanded uncertainty calculated for MCS array E is U_{exp} = ±5.08 unit. Further we calculated measurand values at 95% coverage interval using formula; Percentile (MCS array, 0.975) for Y_{High} and Percentile (MCS array, 0.025) for Y_{Low} .

The measurand histogram plotted by selecting input range, bin range, output range and chart output from MCS array, is demonstrated in Fig. 9, where Y_{High} and Y_{Low} values have been highlighted by increased frequencies.

In this investigation for measurement uncertainty evaluation of a typical hypothetical case, through Monte Carlo simulation approach, the MCS outcome has been noticed in form of a trapezoidal histogram





Fig. 8 — Histogram for uncertainty of the standard used.

			Table 2 — Monte	e Carlo Simulatio	on iterations		
Trials	Repeatability	Error due to temperature variation	Reproducibility	Misalignment	Uncertainty of the standard used	Mean Measured value (unit)	Expanded uncertainty (unit)
1	87.12	1.06	0.01	0.015	0.003	93.21	4.78
2	86.93	1.04	0.0005	0.014	-0.0042	98.05	5.29
3	86.58	1.09	0.05	0.008	0.007	78.95	4.71
4	87.34	1.09	0.05	0.010	-0.002	87.60	4.77
5	86.85	1.04	0.05	0.014	-0.009	81.30	5.84
6	87.29	1.00	0.01	0.009	0.002	90.69	5.27
7	87.75	1.01	0.05	0.008	0.003	86.41	4.10
8	87.00	1.00	0.01	0.014	0.0003	84.66	3.86
9	87.10	1.05	0.01	0.014	0.002	85.57	5.14
10	87.99	1.03	0.005	0.015	0.006	77.18	5.26



Fig. 9 — MCS histogram.

(not essentially with normal distribution as in case of LPU). The MCS findings are summarized in Table 3.

4 Conclusion

In present investigation, a simplified procedure for measurement uncertainty evaluation using Monte Carlo Simulation approach has been discussed in detail using Microsoft Office excel. Input quantities with different probability distribution functions have been identified and exhibited through an arrow diagram, followed by random number generation and their consolidation as per the model function. The MCS array obtained has been further analysed to compute average measured value and expanded uncertainty along with output histogram. This is to be realized, that the mean measured values and expanded measurement uncertainty values attained through LPU and MCS approaches are not same in this suppositional case. Additionally, it is evident that the MCS histogram, obtained for this hypothetical case is

Table 3 — Monte Carlo Simulation outcomes

Parameters	MCS results
Mean measured value (unit)	91.46
Expanded uncertainty (unit)	± 5.08
Low end point (unit)	87.29
High end point (unit)	95.70

somewhat trapezoidal, hence does not necessarily advocate the central limit theorem for measurand probability distribution.

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