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SOME REMARKS ON THE USE OF U-SHAPE PROBABILITY DISTRIBUTION FUNCTIONS IN MONTE CARLO SIMULATION

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Abstract – Although Monte Carlo simulation (MCS) has been applied to the calculation of measurement uncertainties in metrology problems, its use has generally been restricted to cases where the distributions assigned to the pdf's of the input quantities are the more common Gaussian, rectangular and triangular distributions. However, cases exist where the distributions of the input quantities are more complex, such as U-shape (e.g. electrical metrology), and combinations of this and the above and other distributions. This study will establish procedures for sampling from and using such distributions and develop appropriate algorithms.

In particular, this paper will concentrate on approaches that are free from the assumptions inherent in the GUM-based procedures that are conventionally used. Those procedures are at the moment "taken as read" by many laboratories when, in fact, the conditions for their application do not necessarily apply (e.g. normality of distributions involved, input quantities uncorrelated). Thus, simulations will be carried out based on a U-shape probability distribution function, to investigate the validity of the GUM approach using the MCS technique as the validation tool.

Keywords: Measurement uncertainty, Monte Carlo simulation, probability distribution function.

1. INTRODUCTION

The use of U-shaped probability distribution functions is common in some domains of metrology, and is considered as an adequate model to represent probability related with random variables in cases where the probability of finding the value of the quantity next to the limits of its specified interval is far greater than finding it closer to its central value.

Although Monte Carlo simulation (MCS) has been applied to the calculation of measurement uncertainties in metrology problems, its use has generally been restricted to cases where the distributions assigned to the pdf's of the input quantities are the more common Gaussian, rectangular and triangular distributions. However, cases exist where the probability distributions of the input quantities exhibit a different behaviour, such as U-shape (e.g. electrical metrology), and combinations of this and the above and other distributions. This study will establish procedures for sampling from and using such distributions and develop appropriate algorithms.

Not only does MCS produce results that tend to the exact solution, depending on the number of MC trials taken, but it provides much richer information about the model being analysed. Essentially, MCS is a sampling technique that provides an alternative approach to the propagation of uncertainties through a Taylor-series approximation to the measurement model as in GUM, The Guide to the Expression of Uncertainty in Measurement [1]. In fact, MCS propagates the probability density functions, instead of just the variances of the input quantities, so that an estimate of the pdf of the output quantity is provided rather than a single statistical parameter such as the output standard deviation. Thus any required statistic, including estimates of the measurement result, the associated standard uncertainty and confidence intervals, can be obtained from this distribution. Other important advantages of MCS are its applicability regardless of the nature of the model (e.g. strongly non-linear), and the capability of handling multi-stage models.

In recent years, as the tolerances applied in industrial production became more stringent requiring higher accuracies, the role of measurement uncertainty has become more important when assessing conformance with these tolerances. Indeed, the evaluation of measurement uncertainty is increasingly seen as the backbone of quality assurance. This inevitably leads to the necessity of having adequate expressions of uncertainty in measurements to ultimately ensure quality control. Since the mathematical models in metrology have different input quantities, which can be related with different types of probability functions adopted, it becomes also of interest to study the way these functions combine themselves under MCS. The study of such cases can increase the understanding of the influence that these types of input quantities have in the evaluation of measurement uncertainties and can, also, provide relevant information concerning its characteristics and behaviour when combined with other specific probability function types under MCS.

In particular, this paper will concentrate on approaches that are free from the assumptions inherent in the GUM-based procedures that are conventionally used. Those procedures are at the moment "taken as read" by many laboratories when, in fact, the conditions for their application do not necessarily apply (e.g. normality of distributions involved, input quantities uncorrelated). Thus, simulations will be carried out based on a U-shape probability distribution function, to investigate the validity of the GUM approach using the MCS technique as the validation tool.

2. MONTE CARLO SIMULATION

Most of the performed uncertainty evaluations in metrology laboratories are based on models that relate the input quantities to the measurand in a simple additive formulation:

$$Y = a_1 X_1 + a_2 X_2 + \cdots + a_n X_n \qquad (1)$$

The Guide to the Expression of Uncertainty in Measurement (GUM) is particularly suitable to linear models but it requires that the input quantities X_i have independent Gaussian distributions. Any departure from this ideal condition and GUM will only provide an approximate solution. The quality of the approximation will depend on the number of input quantities, the degree of model non-linearity, the departure from normality of each input quantity and the order of magnitude between uncertainties, knowing that the resulting convoluted distribution for Y converges towards the normal distribution as the number of input quantities increases and the closer the values of their uncertainties are to each other. In many circumstances, though, the first order Taylor expansion used by the mainstream GUM approach is not an acceptable simplification and thus the distribution of Y cannot be expressed as a convolution, in which case GUM suggests the application of numerical methods such as Monte Carlo to adequately evaluate measurement uncertainties.

A common example where mainstream GUM can produce an incorrect result is in the sum of two input quantities having a uniform (or rectangular) distribution with the same semi-widths. In such a situation it can easily be shown, either analytically or using MCS, that the resulting output pdf is not Gaussian but triangular instead (or trapezoidal for arbitrary semi-widths) [2]. The approximation to a Gaussian distribution is significantly improved when the sum of input quantities having a uniform pdf increases from two to three, underlying the importance of the number of input quantities in mainstream GUM applications. This also illustrates an important shortcoming of GUM: all it produces is a statistical parameter, the standard deviation, giving no information regarding the shape of the output pdf which is always assumed to be Gaussian, an assumption not valid in all situations.

The U-shaped distribution is not uncommon in current metrology applications. It is especially used in electrical metrology [3] but its distribution is also commonly assigned to variables in temperature monitoring in enclosed spaces. The corresponding probability density function (pdf), for a U-shaped function with limits *a* and *b*, is given by

$$g(x) = \begin{cases} 0, & x < a \\ \dfrac{1}{\pi \sqrt{w^2 - (x-h)^2}}, & a \le x \le b \\ 0, & b < x \end{cases} \qquad (2)$$

where parameters w denotes (*b*-*a*)/2 and h denotes (*b*+*a*)/2 [4]. In the approach followed in mainstream GUM the mean and standard deviation would be extracted from the pdf and used. For the above function the mean x_i is equal to *h*, whereas the standard deviation u_i is given by $w/\sqrt{2}$. The Monte Carlo approach uses the pdf directly. Consider the model function $Y = f(X)$. If the pdf of the input quantity *X* is *g(X)* and the pdf of *Y* is *g(Y)* then the distribution function corresponding to *g* is obtained by integration between *a* and *x*,

$$G(Y) = \int_a^x \frac{1}{\pi \sqrt{w^2 - (x-h)^2}} dx \qquad (3)$$

Adequate estimation of *G(Y)* will permit all the required statistics associated with Y to be determined. The above integral yields an *arc sin* function thus through a simple inversion a *sin* function will be obtained relating *X* to a U uniform function [0,1]. The use of the inversion method applied to a given probability function $F_X(x) = \mathrm{u}$ makes it possible to obtain the relation between that variable and a uniform random variable $x = F_X^{-1}(\mathrm{u})$ which, in the present case, leads to equation (4),

$$x_i = h + w \sin(\pi(\mathrm{u}_i - 1/2)),\ i = 1, \cdots, M \qquad (4)$$

where u_i is generated by the Hill–Wichmann pseudo–number generator [5]. The generated sequences were tested in order to verify uniformity and independence criteria, namely using kolmogorov--smirnov test and empirical tests as described in [6].

MCS is a sampling technique that tends to the exact solution, depending on the number of MC trials simulated (*M* value above), with its accuracy increasing with the number of trials taken. There are processes to estimate the adequate number of MC trials for a specific problem, knowing that the correct number of MC trials will depend on the shape of the pdf and the level of probability required. A value of 60,000 trials has been adequate for a 95% coverage interval in a significant number of tested situations, but it should always be checked using the length of the corresponding 95 % confidence intervals around the

2.5 and 97.5 percentiles against the number of significant digits in the measurand as the convergence criteria [2], to deliver the required accuracy in the output uncertainty. Thus assuming a value of 60,000 trials to be simulated the main steps of MCS would include:

(a) Generate M samples x_i of the input quantities X;

(b) Evaluate the model y_i based on the functional relationship, e.g. $y_i = x_{1,i} + x_{2,i}$ $\quad i = 1,\ldots,M$, to obtain the output quantity;

(c) Sort the values of y_i into non-decreasing order and assemble them into a histogram so that an estimate of the pdf of Y is obtained;

(d) Take the interval $(y_{(\alpha/2)\,M}\ ,\ y_{(1-\,\alpha/2)\,M})$ as a $(1\text{-}\alpha)$ coverage interval for the output;

(e) Perform a specific test to validate the procedure to a required level of accuracy.

The mean value of the y_i values is taken as the measurement result y, whereas the combined standard uncertainty of y – $u(y)$ – is the standard deviation of the y_i values.

3. UNCERTAINTY EVALUATION

To illustrate the use of MCS to U-shaped functions and the corresponding comparison with the conventional procedure stated in the GUM, a number of different situations will be tested in this section.

3.1. Sum of U-shaped distributions

Assume the model $Y = X_1 + \cdots + X_i\ ,\ i \le 4$, with each input quantity having a U-shaped pdf with zero mean and limits $a = -0.08$, $b = 0.08$. Sampling from just one of the input quantities pdf using 60,000 trials and following the steps described above will produce an output pdf having a clear U shape as expected. However, if the functional relationship is applied, summing up two, three or four U-shaped distributions, a completely different output pdf may arise as a result. The shape of the output pdf

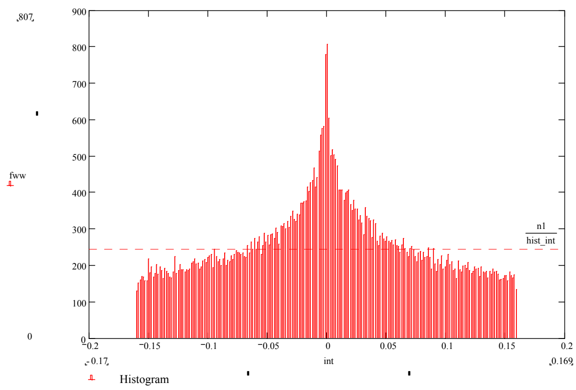

Fig. 1. Sum of two U–Shaped distributions

in Fig. 1 above, resulting from a simple model of a sum of 2 identical input quantities, both having a ± 0.08 U-shaped pdf, clearly shows that assuming a Gaussian distribution for the output function in this case is not reasonable. The 95% confidence interval obtained from the above distribution is [-0.1474, 0.1474], whereas the application of the GUM methodology would produce a standard uncertainty of 0.08 thus an expanded uncertainty of 0.16 for a 95% confidence level. This represents a difference of 8.5% between the two results, which can be significant in certain circumstances. What would happen if the number of input quantities increases from two to three? The output pdf is transformed into the shape displayed in Fig. 2 below.

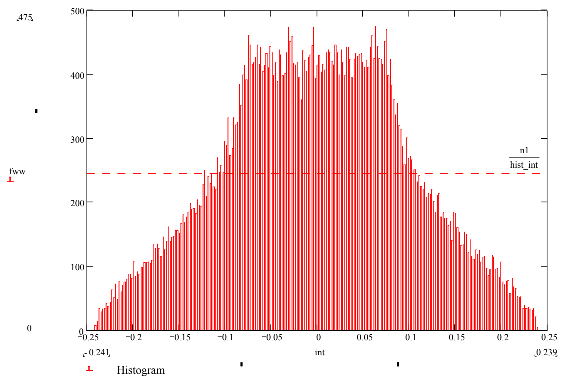

Fig. 2. Sum of three U–Shaped distributions

The assumption of a Gaussian distribution is again far from being accurate. The 95% confidence interval is now limited by -0.1912 and 0.1903, whereas the conventional approach gives a standard uncertainty of 0.098 or an expanded uncertainty for the same level of confidence of 0.196. The difference between results is approximately 3%. Although the difference in results between the two methods has clearly been reduced to reasonable values the question of tendency remains. Would the situation improve if another input quantity is added, supporting the principle that the Gaussian assumption is improved for an increasing number of input quantities? Fig. 3 answers the question in an emphatic way.

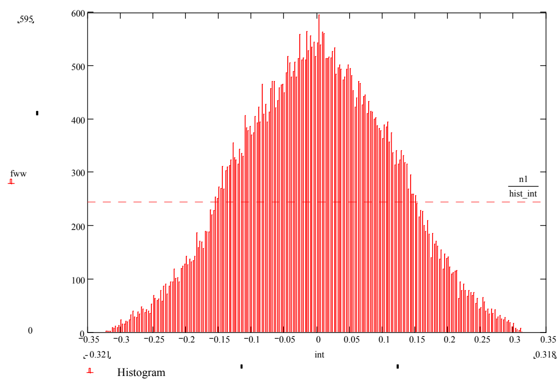

Fig. 3. Sum of four U–Shaped distributions

The output pdf has now a clear Gaussian shape which should be replicable into the results. The 95% confidence interval from MCS has limits – 0.2201 and 0.221 whereas the GUM yields a standard uncertainty of 0.1131 equivalent to an expanded uncertainty $U_{95\%} = \pm 0.2262$. The difference between results has now been reduced to less than 2.5% and the evolution of shapes of the graphs clearly indicates that the Gaussian assumption is a sound approximation when summing up 4 U-shaped input quantities. An example of such a situation can be found in certain calibrations in electrical metrology [3]. The tests results are summarized in Table 1 where a comparison between MCS and mainstream GUM is established for the three tested cases regarding the 95 % coverage interval determined by the two methods, bearing in mind that the expanded uncertainty to a 95 % level of confidence is the key parameter given in calibration certificates, qualifying the measurements taken.

TABLE I – Sum of U-shaped distributions

95 % coverage interval magnitudes			
	2 U	**3 U**	**4 U**
GUM	0.320	0.392	0.452
MCS	0.295	0.382	0.441
% diff	8.5	3.0	2.5

Examples of mathematical models having only three or four input quantities considered abound in current metrology calculations especially when performed by testing laboratories. It is quite common for those to just consider the uncertainties related to the standard, drift and resolution, or these three plus repeatability. In the next section an insight towards that situation will be provided.

3.2. Combinations of U-shaped distributions with other distributions

It is important to discuss the practical effects of summing up a U-shaped distribution with a Gaussian, a triangular or a uniform distribution or a combination of these, in uncertainty models with application to metrology. Let us look first to the consequences of adding up Gaussian and U-shaped distributions. The simulations carried out led to the conclusion that the Gaussian function is clearly dominant for situations where its standard deviation is more than half the U–shaped semi-width. In the transition case, where the Gaussian distribution has a standard deviation with half the value of the U–shaped distribution semi–width, the shape of the output pdf has a Gaussian general contour but the area below the graph is considerably larger, as in Fig. 4.

The difference in the estimation of the standard deviation using MCS or the GUM approach is about 9%. However, for situations where the scale of the U–shaped semi–width is several times that of the

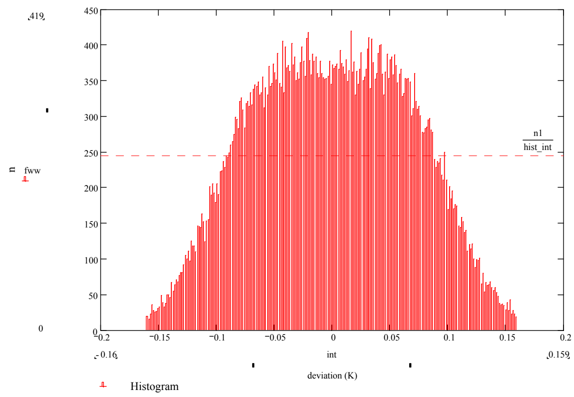

Fig. 4. Sum of a U–shaped with a Gaussian distribution having half the “magnitude”

normal distribution standard deviation, the U shape is quite apparent in the graph of the output pdf (Fig. 5) and the error committed by using the conventional GUM approach in these situations can be as high as 37% when estimating 95% confidence limits. It should be emphasized that these large errors are related to a very simple linear model with two input quantities. Surprises such as these can always be present if care is not taken considering the assumptions upon which the GUM method is based, to decide on the reasonability of its use in each particular case.

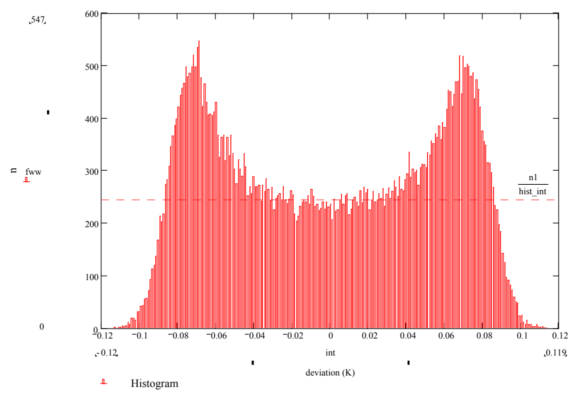

Fig. 5. Sum of a U–shaped with a Gaussian distribution having “magnitude” 8 times smaller

When the U–shaped distribution is combined with uniform or triangular distributions its influence is more pronounced, prevailing in situations where the limits of the U function are higher than those of the other distribution function. Fig. 6 and 7 illustrate the situation of a linear combination between a U distribution and a uniform distribution for cases where the order of magnitude of the limits in the uniform distributions are half and double those of the U distribution, respectively. Comparing with the previous case of the Gaussian distribution, it is obvious that the U distribution prevails now, for the same conditions, as shown in Fig. 4 and 6. The difference in estimating 95% confidence intervals between MCS and GUM is about 15.9 % and 6.7 %, respectively, which stresses the idea that errors increase for larger U distribution presence in the output pdf.

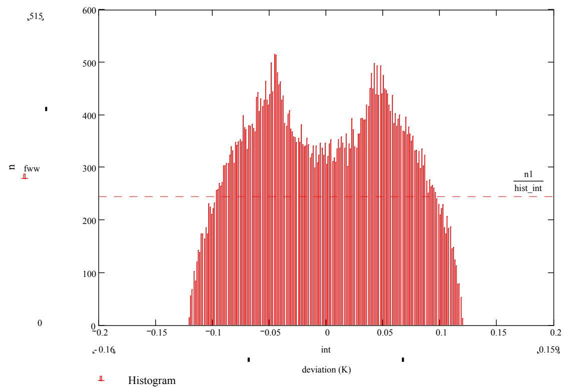

Fig. 6. Sum of a U−shaped with a uniform distribution having half the magnitude

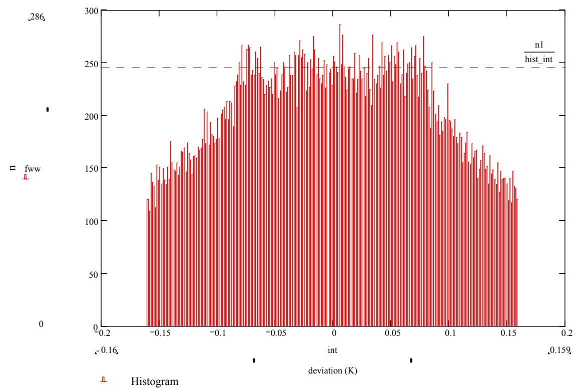

Fig. 7. Sum of a U−shaped with a uniform distribution having double the magnitude

Similar simulations were carried out for combinations between a U distribution and a triangular distribution, with results following the same pattern. For a situation where the triangular distribution has a magnitude 4 times smaller than the U distribution, the difference in estimating a 95% confidence interval by MCS or GUM is 33.5 %. In the case where the sizes of both distributions are identical the difference of using MCS and GUM is accounted to 10.8 %, see Fig. 8, which is in line with previous examples, where if the output pdf approximates a Gaussian distribution the errors are about 10 % or less, and if the U shape is apparent in the output pdf, then the errors can be very significant, perhaps above 30 %.

Lets now consider the case where a U distribution is combined with more than one other distribution, a uniform and a Gaussian distribution, say. Simulations will again focus on the relative order of magnitude of the limits of each distribution involved, to discuss in which conditions is adequate to assume a Gaussian distribution for the output distribution. Increasing the number of input quantities to three and assigning the same order of "magnitude" to the three distributions yields an almost perfect Gaussian distribution. Also calculation of 95 % confidence intervals by both MCS

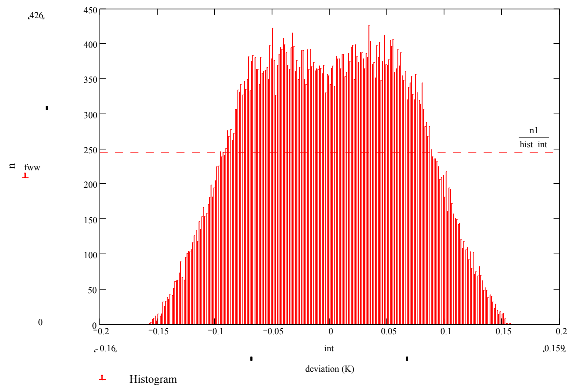

Fig. 8. Sum of a U−shaped with a triangular distribution having the same magnitude

and GUM produces a figure that coincides within 3 %.

Reducing the relative order of "magnitude" of either the Gaussian or the uniform distributions in relation to the U distribution, will induce a departure from Gaussian shape of the output pdf, increasing the error in the calculation of 95 % confidence limits when using the conventional GUM procedure used by the majority of calibration and testing laboratories, in some circumstances without careful validation. Fig. 9 illustrates a case where the U distribution has a semi-width 8.5 times larger than the standard deviation of the Gaussian distribution and 1.7 times larger than the uniform distribution semi-width. The error of using the conventional approach to calculate the output standard deviation is increased to about 13 %. If the limits of the uniform distribution are reduced to just twice those of the Gaussian distribution standard deviation that error increases further about 25 %.

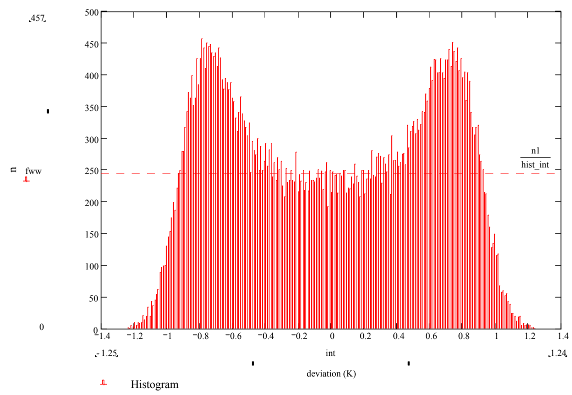

Fig. 9. Sum of a U−shaped with uniform and Gaussian distributions

3.3. U-shaped distribution in a non-linear model

The linear combination in measurement uncertainty models is not always representative of the physical process under analysis. Circumstances exist where that model is non-linear and in those cases the application of mainstream GUM can hardly be justified. To exemplify with a relatively simple model, the study will assume the model $Y = X^2$, where the input quantity has a U-shaped pdf with centre in 0.5 and limits ± 1.2. The output function is always positive which induces an asymmetry around zero as the function is centred on zero with a negative branch in the input set of values. The values here simulated are centred in a non-negative value with a negative branch of values.

The output pdf is shown in Fig. 10 where the shape displayed has no similarities with any of the previous examples.

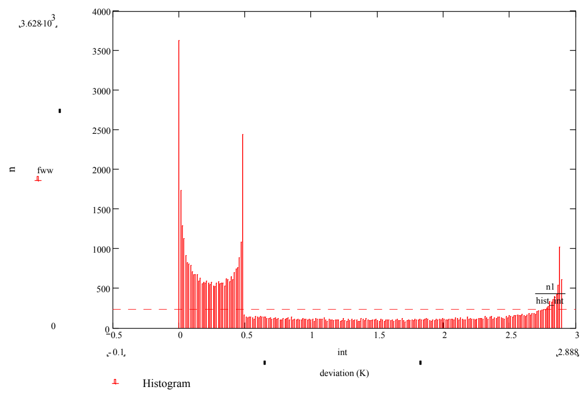

Fig. 10. U–shaped quadratic model centred in 0.5 with limits ± 1.2

What is apparent in the graph is the existence of three local maximums, and the concentration of values from zero to about 0.5. These arise as a consequence of values being squared, which aggregates negative and positive values, and that the zero is placed in the left part of the curve, so that the values in the far left of the curve (high frequency in a U distribution) are aggregated with their symmetrical, the values around zero are all duplicated and the values to the far right of the distribution have a high frequency (but are not aggregated with any other values). Any attempt of using the Central Limit Theorem, which is the theoretical basis of GUM, only by pure chance would not produce erroneous results, since the output pdf has no resemblance with a Gaussian shape. Also it is questionable that in this case the mean value is the best estimate for the measurand. In this particular case there is an error associated with the use of conventional GUM that accounts for about 18 %. This last case is of course an example where the application of mainstream GUM was clearly unjustified, the terms of higher order of the Taylor expansion had to be included, but has the purpose of underlying the mistakes that arise from the misuse of GUM.

4. CONCLUSIONS

The purpose of this study was to investigate the applicability of the mostly used technique for the calculation of measurement uncertainty, as described in GUM [1] and other similar documents, and adopted by the majority of testing and calibration laboratories. The validation tool is a numerical method – Monte Carlo – briefly referred in [1] as an alternative method when conditions for the application of conventional GUM were not met.

The simulations carried out included a sum of U–shaped distributions, a sum of these with uniform, Gaussian and triangular distributions, and an application of a U distribution to a non-linear model. The main conclusions to draw from this study are:

- The number of input quantities is an important factor among the required conditions for GUM application, with increasing number of input quantities favouring GUM adequacy;
- When combining a U–shaped distribution with a Gaussian, uniform or triangular distribution, or a combination of these, the relative size of the Gaussian distribution is more important than the other ones, with the output pdf moving towards normality as that factor increases;
- If the U–shaped distribution prevails the errors incurred by the use of mainstream GUM can be very significant;
- The GUM approach is not adequate to applications of non-linear models, where numerical methods should be used instead.

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