VI CONGRESSO NACIONAL DE ENGENHARIA MECÂNICA
VI NATIONAL CONGRESS OF MECHANICAL ENGINEERING
18 a 21 de agosto de 2010 – Campina Grande – Paraíba - Brasil
August 18 – 21, 2010 – Campina Grande – Paraíba – Brazil

PROPAGATION OF DISTRIBUTIONS USING A MONTE CARLO METHOD: AN ALTERNATIVE APPROACH

Jorge Luis Suzuki, jluissuzuki@gmail.com[1]
Luiz V.O. Dalla Valentina, dalla@joinville.udesc.br[1]
Júlio Miranda Pureza, pureza@joinville.udesc.br[1]

[1] Universidade do Estado de Santa Catarina, Campus Avelino Marcante, Joinville

Abstract. *This article presents an alternative approach of the supplement I to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method (BIPM et.al, 2008). The propagation of distributions is generated by a Markov chain that compares transition probabilities for subsequent states, generated by two different procedures. The first one uses, for all probability distributions, small displacements generated by rectangular distribution, while the second one uses random numbers from specific (uniform or non-uniform) probability distributions, allowing greater displacements, and hence larger variations from one state to another. Both procedures generate a Markov chain with non-uniform transition probabilities that can be analyzed at each step. Two specific calibration examples presented in BIPM* et.al, *(2008) were tested for validation purposes: one regarding a mass calibration and another regarding a gauge block calibration. The simulations carried out 10^7 trials, on which both procedures were in good agreement with the reference for the mass calibration problem, but only the first procedure achieved good results for the gauge block calibration.*

Keywords: *Metrology, Monte Carlo method, Markov chains.*

1. INTRODUCTION

According to Kessel (1997) and Mathiesen (1997), the measure of a physical quantity is only complete when accompanied by its correspondent uncertainty value, usually constituted by several elements, which are identified and assembled to get its numerical value. The Guide to the Expression of Uncertainty in Measurement – GUM, quoted by ISO/GUM, (1995) and INMETRO/ABNT (2003), presents a general procedure called GUM Uncertainty Framework - GUF, that proposes a "law of propagation of uncertainties", using analytic methods. It evaluates the standard uncertainty associated with an estimate of the output quantity, given by:

- Best estimates of the elements that generate the physical quantity;
- Standard uncertainties associated with these estimates;
- Degrees of freedom associated with these standard uncertainties;
- Any non-zero covariance associated with each pair of these estimates.

Despite the GUF usefulness and potential, there are some limitations that justify the analysis of alternative approaches for the problem of the propagation of distributions in complex systems (BIPM *et.al*, 2008). In conventional GUF, the partial derivatives of the stage of propagation of uncertainties concerns the linear terms of a Taylor series. Higher precision models could be evaluated, by performing higher order derivatives (ISO/GUM, 1995). However, this step is sometimes too complex and even impossible to be performed analytically, requiring a more practical procedure.

The Monte Carlo method – MCM, as stated by Jain (1995), is a numerical procedure for the solution of mathematical problems by the simulation of random variables. It generates a complete Probability Distribution Function - PDF, allowing a discrete representation, while GUF makes the propagation of the input quantities. In fact, according to Al-Hujaj and Harney (2006), Monte Carlo is a "Bayesian statistics" method, since prior observation is required in order to make theoretical predictions before observing the phenomenon itself. After empirical observations, prior predictions can be at last compared to the final results, showing the discrepancies between them. This condition allows subsequent experiments to make better predictions of the phenomenon through time.

As quoted by BIPM *et.al* (2008), a Monte Carlo method is a good alternative to the GUF when:

- The linearization of the model provides an inadequate representation for the problem;
- The PDF of the output quantity differs appreciably from a Gaussian distribution or a scaled and shifted t-distribution.

In fact, several model representations used in metrology result in non-symmetrical PDF's, like a log-normal distribution. In this case, it is not possible to assume an equal multiplication of the standard deviation to both sides of

the final probability distribution. With the application of a Monte Carlo method, it is possible to determine the characteristics of the final PDF, and even its nature, using tests of Goodness-of-fit. The expectation and standard deviation can be obtained and, according to the coverage probability, it is possible to evaluate the desired coverage interval, after an adequate number of iterations, as described by Cox and Harris (2001).

.

2. OBJECTIVES

The main objective of this article is to perform an alternative method to the Supplement 1 for the GUM (S1) using a Monte Carlo simulation according to two different procedures and validate it. This validation procedure applies to the two examples presented in S1 and takes into account the statistical parameters, the number of iterations and the numeric stability of the process to indicate which procedure is more effective and reliable.

3. THE METHOD

According to Degroot (1989), a Markov chain is a stochastic process based on conditional probabilities, where each state depends only on the previous state.

The product of a Monte Carlo simulation is a Markov chain composed by states of the system under consideration. Hence, for a given state, random modifications generate a new state. Then the comparison of the probability transitions between these states and a random number generated by the algorithm indicates if the new state substitutes the previous one in the chain. Then, after large number of iterations the system converges to a limiting distribution and the states of the chain are the input data for the Metropolis-Hastings algorithm, as presented by Hastings (1970).

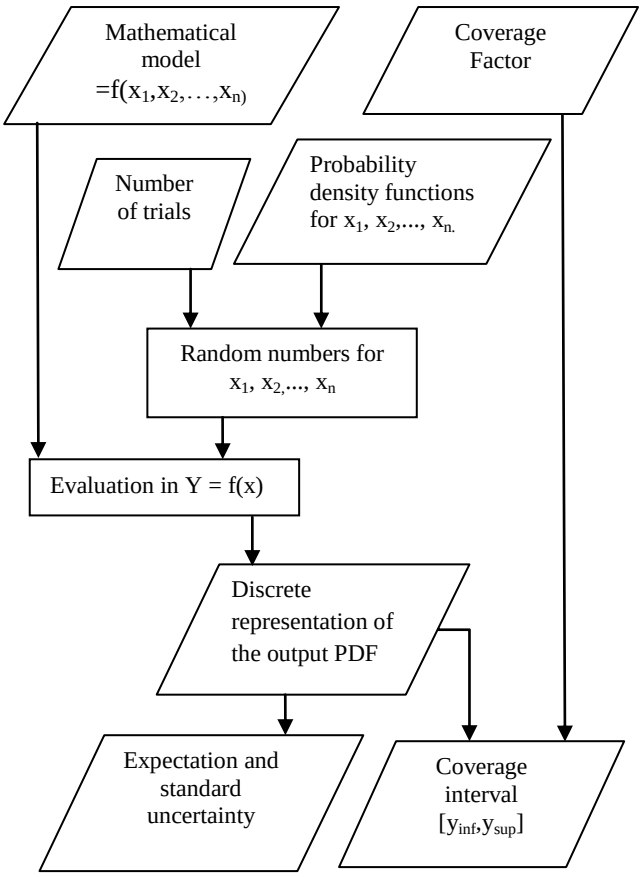

Figure 1: Main steps of a Monte Carlo simulation

Figure 1 presents the main concepts of a Monte Carlo simulation. It is divided in four main steps: (a) Input data, where each probability distribution is assigned; (b) Propagation of the distributions, where the random numbers are evaluated; (c) Output data, where a discrete representation of the final PDF is obtained; (d) and summarization, where a coverage interval is obtained according to the coverage probability selected at the first procedure.

3.1 Input data

At this step, information regarding the variables is set: expectation values, standard deviations, width, depending of the PDF. The number of iterations is set depending on the desired coverage interval. A good estimate is presented by BIPM *et.al* (2008):

$$M \geq 10^4 \times \frac{1}{1-p} \tag{1}$$

Where:

M = Number of iterations;
P = Coverage probability;

3.2 Propagation of distributions

At this step, random numbers are generated, regarding the PDF assigned at the previous step, in order to produce each configuration of the Markov chain. However, after this evaluation, using the mathematical model, the elements of the final PDF are obtained. Depending on the different stochastic nature of the distributions, uniform or non-uniform, different ways of generation are required.

3.2.1 Uniform distributions

For these distributions, each sample was taken with a probability selection of 50%, in order to eliminate tendentious elements. Hence, to establish a new configuration $x_{i(n)}$, a random number from the rectangular distribution, ranging from 0 to 1 is generated. If the axiom r(0,1) > 0.5 is true, the new configuration is accepted. Case sensitive, the previous configuration $x_{i(n-1)}$ is taken.

3.2.2 Non-uniform distributions

A different procedure is required for non-uniform distributions, once the shape of these curves may differ, with or without greater probabilities at the central limit. Hence, it is important to assure that the configurations do not converge completely for low or high probability zones. The Metropolis-Hastings algorithm is used for this propose, and performs a comparison between probability densities for subsequent states of a Markov chain.

Two procedures for the generation of configurations in non-uniform distributions were formulated, conveniently called A and B. At procedure A, the random numbers are generated from rectangular distributions, in spite of the stochastic nature of the phenomenon. Otherwise, at procedure B the random numbers are generated from the specific probability distributions that characterize the system. Both procedures generate a Markov chain with non-uniform transition probabilities, by comparing the values of probability distribution functions.

Procedure A was formulated to simplify the random number generation, as well as to reduce the average computing time, allowing good results with greater performance in applications with more complex mathematical models. X_i corresponds to a hypothetical input quantity, and could be of any non-uniform probability nature:

$$X_{i(n)} = X_{i(n\text{-}1)} + \; r(0,1) - 0.5 \; \times \frac{\sigma}{\alpha} \tag{2}$$

Where:

$X_{i(n)}$ = Current configuration;
$X_{i(n-1)}$ = Previous configuration;
r(0,1) = Random number generated from a rectangular distribution;
σ = Standard deviation of the distribution;
α = Constant number that divides the standard deviation.

The constant α and a 0.5 maximum displacement from the rectangular distribution allow small displacements between each configuration. It is expected that the probability density functions, along with the Metropolis-Hastings algorithm, would achieve the desired results by assembling a Markov chain with non-stationary probabilities.

Procedure B was formulated after the premise that random numbers ought to be generated by specific non-uniform distributions, and along with the Metropolis-Hastings algorithm, build a Markov chain with non-stationary probabilities, and possibly achieve better results than procedure A:

$$X_{i(n)} = X_{i(n-1)} + \gamma \times \frac{\sigma}{\alpha} \quad (3)$$

Where:

$X_{i(n)}$ = Current configuration;
$X_{i(n-1)}$ = Previous configuration;
γ = Random number generated from a specific distribution;
σ = Standard deviation of the distribution;
α = Constant number that divides the standard deviation

This procedure allows greater displacements between the configurations, depending of the random number generated from a specific distribution.

3.3 Output data

This is the stage where a M-element vector is taken as a discrete representation of the final PDF. This PDF would be precisely defined with adherence tests, once in many practical situations, it would be a Gaussian or a scale and shifted t-distribution. Once the shape of the curve is known, the mean, standard uncertainty, y_{low} and y_{high} can be obtained. If only the final parameters are of interest, the model values doesn't need to be allocated.

3.4 Summarization

This is the final stage of the Monte Carlo simulation, and consists of the calculation of the desired parameters from the final PDF. These parameters are the expectation μ, standard deviation σ, and the components of the coverage interval, y_{low} and y_{high}. The length of this coverage interval depends of the coverage factor defined in the step of input data.

4. RESULTS

Two examples were used for validation purposes and, in both of them, the simulations carried out 10^7 trials, and a sample was taken at every ten iterations to assemble the Markov chain, avoiding the strong correlations that characterize the Metropolis-Hastings algorithm. This selection totalizes a final array with 10^6 elements, which guarantees a coverage probability of 99% and retains the statistical properties of the final PDF, according to equation 1.

Ten simulations were performed with different values for α in equations (2) and (3) in order to compare the results with BIPM *et.al* (2008), and to evaluate the convergence with different displacements, as previously described in section 3.2.2. These tests were made for α equal to 1.15 and 1.00 for the mass calibration, and 7.5 and 3.5 for the gauge block calibration.

4.1 Mass calibration

A mass calibration can be evaluated by the following equation, after the application of Arquimedes principle:

$$\delta m = \left(m_{R,c} + \delta m_{R,c}\right)\left[1 + \left(\rho_a - \rho_{a0}\right)\left(\frac{1}{\rho_w} - \frac{1}{\rho_R}\right)\right] - m_{nom} \quad (4)$$

Where:

δm = Associated uncertainty of the mass calibration;
$m_{R,c}$ = Conventional mass of the reference weight;
$\delta m_{R,c}$ = Uncertainty of the reference weight;
ρ_a = Air density;
ρ_{a0} = Air density, without associated uncertainties;
ρ_w = Density of the weight W;
ρ_R = Density of the reference weight R;
m_{nom} = nominal mass of both weights.

Table 1 shows the input parameters for the mass calibration model:

Table 1. Input parameters for the mass calibration problem, with gaussian and rectangular distributions.

Xi	Distribution	Parameters			
		Expectation μ	Standard Deviation σ	Expectation x = (a + b) / 2	Semi-width (b – a) / 2
$m_{R,c}$	N(μ , σ^2)	100000.000 mg	0.050 mg		
$\delta m_{R,c}$	N(μ , σ^2)	1.234 mg	0.020 mg		
ρ_a	R(a , b)			1.20 kg/m³	0.10 kg/m³
ρ_W	R(a , b)			8x10³ kg/m³	1x10³ kg/m³
ρ_R	R(a , b)			8.00x10³ kg/m³	0.05x10³ kg/m³

Figure 2 presents the results for the expectation, with the y-axis in [mg] units, and the x-axis representing the procedure with the respective value of τ. The red dash-dotted line represents the reference value (BIPM *et.al*, 2008) for the MCM, and the blue dash-dotted line for the GUF (BIPM *et.al*, 2008). It is clear that procedure B presented more fluctuation along the simulations, and generally, the results were coherent with GUF.

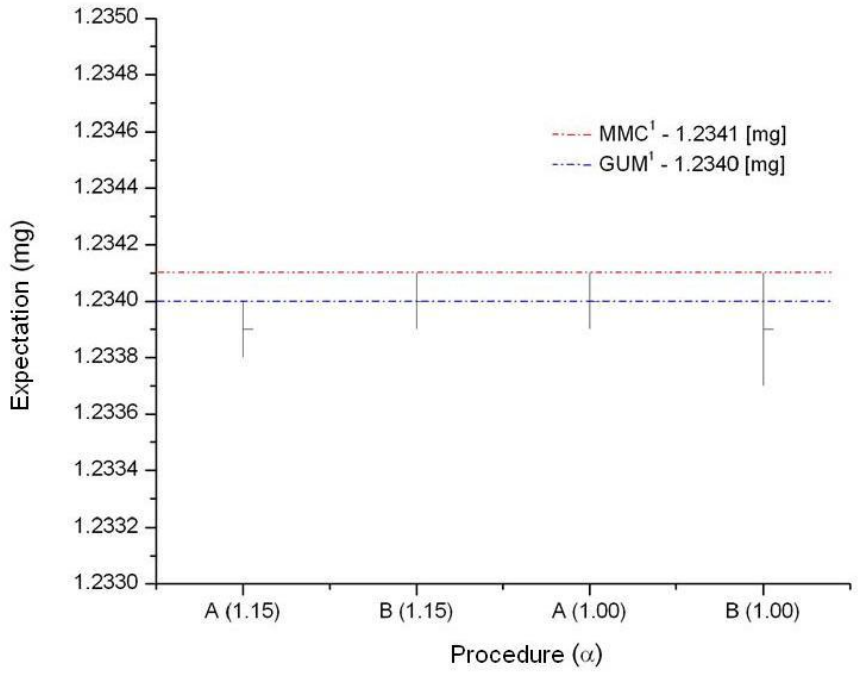

Figure 2. Expectations for the mass calibration.

The results for the standard uncertainty are shown in figure 3. Again, The red dash-dotted line represents the reference value for MCM, and the blue dash-dotted line for the GUF, obtained by BIPM *et.al* (2008). The results for both methods were slightly more conservative than the reference.

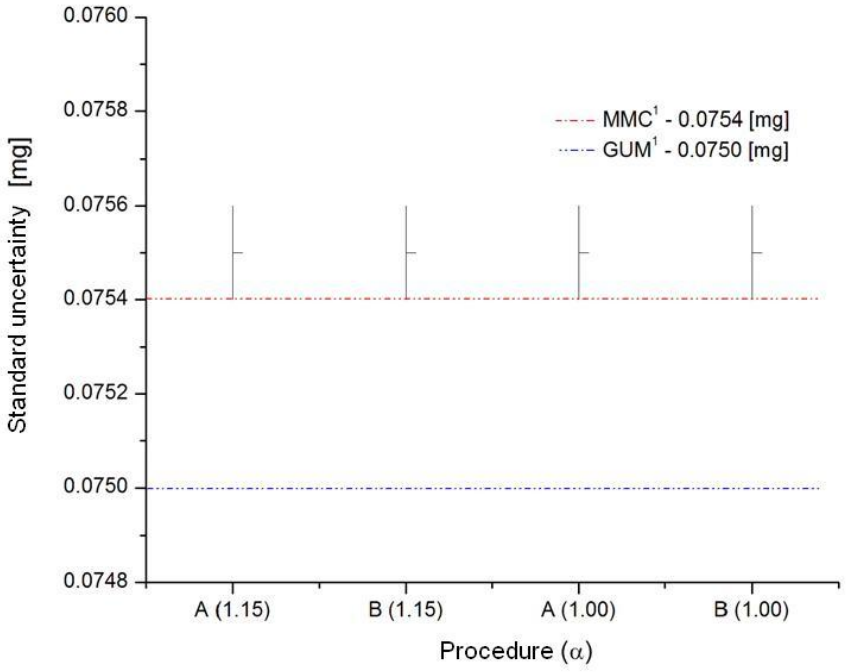

Figure 3. Standard uncertainties for the mass calibration.

4.2 Gauge block calibration

The mathematical model of a gauge block calibration can be described by the following equation:

$$\delta L = L_s + D + d_1 + d_2 - L_s[\delta\alpha(\theta_0 + \Delta) + \alpha_s\delta\theta] - L_{nom} \quad (5)$$

Where:

δL = Uncertainty of the gauge block;
L_s = Length of the reference standard at 20°C;
D = Quantity of which the average of the five indications is a realization;
d_1 = Random effects of the comparator;
d_2 = Systematic effects of the comparator;
$\delta\alpha$ = Difference between thermal expansion coefficients;
θ_o = Average temperature deviation of the gauge block from 20°C;
Δ = Cyclic variation of the temperature deviation from θ_o;
α_s = Thermal expansion coefficient of the reference standard;
$\delta\theta$ = Difference in temperature between the gauge block being calibrated and the reference standard;
L_{nom} = Nominal length of the gauge block.

Table 2. Input parameters for the gauge block calibration problem.

Quantity	PDF	Parameters					
		μ	σ	ν	a	b	d
L_s	$t_\nu(\mu,\sigma^2)$	50000623 nm	25 nm	18			
D	$t_\nu(\mu,\sigma^2)$	215 nm	6 nm	24			
d_1	$t_\nu(\mu,\sigma^2)$	0 nm	4 nm	5			
d_2	$t_\nu(\mu,\sigma^2)$	0 nm	7 nm	8			
α_s	R (a,b)				9.5×10^{-6} °C^{-1}	13.5×10^{-6} °C^{-1}	
θ_o	N (μ,σ^2)	-0.1°C	0.2°C				
Δ	U (a,b)				-0.5 °C	0.5 °C	
$\delta\alpha$	CTrap (a,b,d)				-1.0×10^{-6} °C^{-1}	1.0×10^{-6} °C^{-1}	0.1×10^{-6} °C^{-1}
$\delta\theta$	CTrap (a,b,d)				-0.050 °C	0.050 °C	0.025 °C

Figure 4 presents the results obtained by the simulations for this calibration problem. The y-axis represents the expectation in [nm], and the x-axis, the procedures and correspondent values for τ. The results for procedure A are in good agreement with BIPM *et.al* (2008) for small fluctuations, different from procedure B, which is unstable.

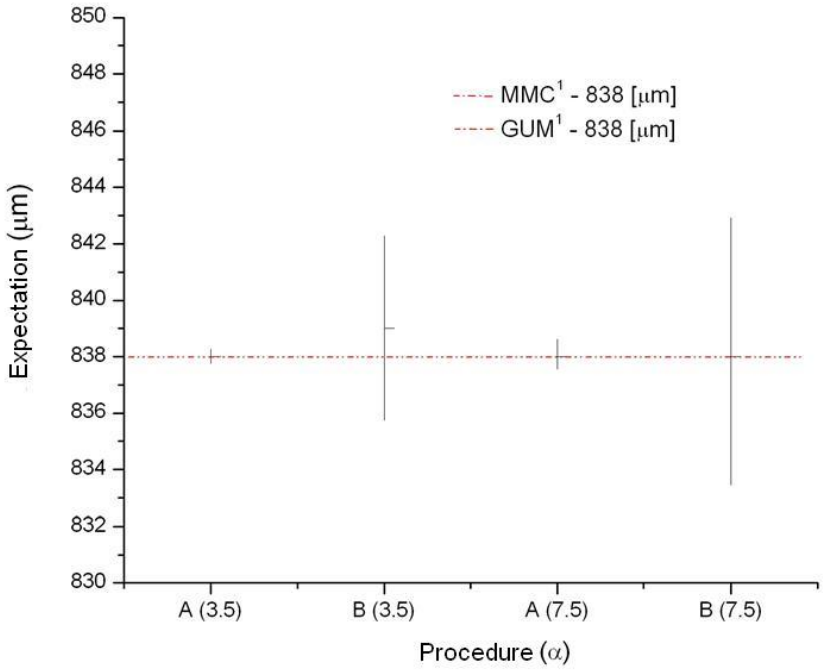

Figure 4. Expectations for the gauge block calibration.

For the standard uncertainty, as shown in figure 5, there is a good agreement with BIPM *et.al* (2008) for procedure A, and high instability for procedure B. The red line represents the results from BIPM *et.al* (2008) for MCM, and the blue and green lines the results for the GUF, also obtained by BIPM *et.al* (2008) with first and second order terms, respectively.

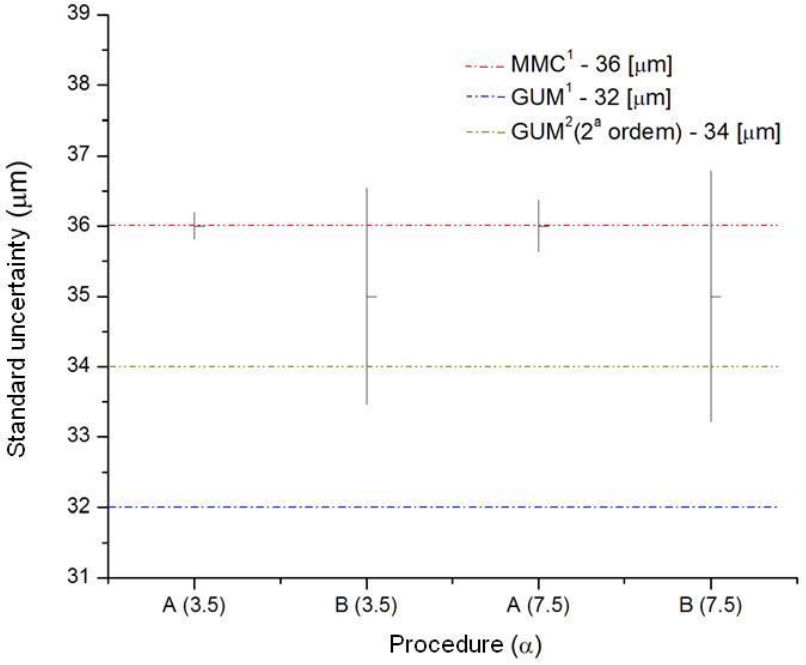

Figure 5. Standard uncertainties for the gauge block calibration.

5. CONCLUSIONS

There is little discrepancy between the results presented by BIPM *et.al* (2008) and the values obtained in this work. The simulation performed in this work is less conservative for the mass calibration but more conservative for the gauge block calibration. However, these differences don't affect the final results, once they are rounded to the number of significant decimal digits.

The gauge block calibration problem yields good results for procedure A, mainly when $\alpha = 3.5$, which presented more stability. Procedure B doesn't seem reliable, since its results are highly unstable.

Another point regards the samples that were taken at each ten iterations to generate the Markov chain. The results showed that this procedure achieved good estimates, but it is still necessary to do tests of goodness-of-fit and to analyse the results.

The next step for this work is to perform adaptive Monte Carlo tests, in order to do a sensibility analysis of the constant α and determine its optimal value.

6. REFERENCES

AL-HUJAJ, H.L; HARNEY. Objective Bayesian statistics. MPI für Kernphysik, Postfach. Heidelberg, Germany, 2006.

BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, OIML 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* Joint Committee for Guides in Metrology, Bureau International des Poids et Mesures, JCGM 101:2008.

COX, M.G and HARRIS, P.M. GUM Supplements. CIE Expert Symposium on Uncertainty Evaluation, method for analysis of uncertainties in optical radiation measurement, Vienna, 2001.G.

DEGROOT, M. Probability and Statistics. Second Edition. Massachusetts, Addison Wesley, 1989.

HASTINGS, W.K. Monte Carlo sampling methods using Markov chains and their applications. Biometrika, 1970.

INMETRO/ABNT. Guia para a Expressão da Incerteza de Medição. INMETRO/ABNT, 2003.

ISO/GUM. Guide to the Expression of Uncertainty in Measurement, International Organization for Standardization, Geneva, Switzerland, 1995.

JAIN, R. The Art of Computer Systems Performance Analysis. New York: Wiley & Sons, 1995.

KESSEL, W. Uncertainty of Measurements: Statement of Physical Ignorance. Advanced School of Metrology: Evaluation of Uncertainty in Measurement. Programa RH-Metrologia, Brasil, 1997.

MATHIESEN, O. Uncertainty of Measurement – understanding the GUM. Advanced School of Metrology: Evaluation of uncertainty in measurement, Programa RH - Metrologia, Brasil, 1997.

7. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.