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Deterministic Sampling for Uncertainty Quantification in Complex Algorithm-Based Measurements

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***Abstract* – The paper deals with the problem of estimating measured values in indirect measurements based on complex processing algorithm. To this aim, deterministic sampling of the random variables (modeling the input quantities) is suggested to efficiently estimate expectation and standard uncertainty of algorithm outputs. In particular, the authors propose an enhanced version of the traditional unscented transform to propagate a defined set of statistical moments of the input quantities through the algorithms (even in the presence of non-analytical formulation). This way, it is possible to assure estimates of output expectation and standard uncertainty as good as those achieved by means of the very large ensemble of random variates typically exploited in brute force Monte Carlo method.**

I. INTRODUCTION

Measuring and expressing the value of a quantity of interest is the main concern in measurements science; in last decades, several proposals have been presented in the literature to the purpose [1]-[5]. Except for the original definition of measurement error, most of the considered proposals relies on statistical fundamentals in order to express the measurement result in terms of the estimates both of expectation and standard uncertainty (i.e. deviation) of the random variable adopted to model the quantity itself . The statistical-based approach has been formalized in the so-called "Guide to the Expression of Uncertainty" (GUM) [4]; in the presence of indirect measurements, the GUM establish a default estimation method based on approximation with linearization of the measurement model (i.e. the relationship between the input and output quantities).

The GUM has recently been amended in order to overcome some limitations evidenced when it was applied on indirect measurements characterized by non-linear evolution of the quantity of interest versus the measurable quantities. The considered amendment, referred to as the "Supplement 1" [5], defines a statistical approach based on random sampling of the input quantities and, presently, represents the indisputable reference method for the propagation of their statistics and distribution through non-linear measurement models. It is worth noting that several interesting papers [1]-[3] have recently been presented with the aim of highlighting some inherent limitations of the GUM and Supplement 1. Nevertheless, the GUM framework still holds and the authors move their analysis and proposal inside the considered framework.

The main advantage associated with Monte Carlo-based methods is the final availability of an estimate of output probability density function as accurate as needed; all the information of interest, in terms of output statistics, can straightforwardly be gained. Unfortunately, all of them suffer from a very slow convergence, i.e. a huge number of random variates (forming the so-called ensemble) for each input quantities is required to accurate and reliable estimate of the measurement result. This way, their exploitation for demanding measurement models turns out to be unfeasible, even though some refinements of Monte Carlo method as response surface methodology or latin hypercube sampling are taken into account [6],[7].

This is particularly true when measurements based on complex algorithms are taken into account. Long sequence of acquired samples (acting a input quantities) have, in fact, to be processed by means of procedures usually expressed in terms of non-analytical formulation. On the one hand, complex algorithms make the application of GUM approach easily error-prone; on the other hand, techniques based on random sampling can rapidly become unmanageable when the number of acquired samples increases.

To overcome the considered limitations, the demand for sampling approaches characterized by limited ensemble size rapidly became of interest [7]. In particular, the traditional pseudo-random generators adopted by Monte Carlo (MC) methods were substituted by defined rules

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capable of deterministically selecting a reduced number of random variates of the input quantities. This way, accurate estimates of the measurement result can be gained also by means of small ensemble of definite size.

Stemming from their past experience on the application of deterministic sampling in indirect measurements [8],[9], the authors investigate hereinafter the suitability of the deterministic sampling for the estimation of output expectation and standard uncertainty in measurements based on complex algorithms (i.e. any algorithm characterized by an amount of digital signal processing, [10]-[16]). As a matter of practice, the rule adopted for the selection of the ensemble of the unscented transform is the conservation of the central moments up to the 8^{th} order for input quantities modeled as random variables with symmetric pdf, 4^{th} order otherwise. The limited number of deterministic samples can, thus, straightforwardly be gained by solving an equations system. With regard to the input quantities, the authors focus their attention on the whole metrological chain from the sensor down to analog-to-digital converter; this way, all the uncertainty contributions should be considered.

The paper is organized as follows: after a brief presentation about techniques based either on random or deterministic sampling, the theoretical background of the proposed approach along with the fundamental steps of its application to complex algorithms-based measurements are described in details. Preliminary results obtained in some numerical tests involving different algorithms are finally presented; to assess the performance of the proposed approach, the obtained estimates are compared to those provided by MC simulations, taken as reference.

II. RANDOM VERSUS DETERMINISTIC SAMPLING

Let us consider a vector $\underline{\boldsymbol{X}} = [X_1, X_2, \ldots, X_N]$ of measurable quantities of an indirect measurement $Y = f(X_1, X_2, \ldots, X_N)$; each quantity is modeled as random variable characterized by its own pdf and sample space. Random sampling, originally referred to as statistical sampling [6], has recently been chosen as the key method for the quantification of the measurement uncertainty in indirect measurements characterized by non-linear evolution versus the input quantities. In particular, brute force MC method is suggested in the amendment “Supplement 1” to the GUM as the suitable solution to overcome its deficiencies in the presence of non-linear measurement models.

Two main advantages are associated with MC methods: (i) its inherent practical simplicity and (ii) the offered opportunity of gaining an estimate of the output quantity pdf. Brute force MC method is, in fact, based on the application of the considered measurement equation on different ensembles (i.e. realizations of the input N-tuple) in order to gain the corresponding output values; to this aim, traditional and well-settled random generators can be adopted to realize the observed values of each quantity from the associated pdf (whatever its shape).

Collecting the output corresponding to each ensemble, the empirical distribution function can be estimated, thus making it possible to gain not only expectation and standard uncertainty but also the confidence intervals and other order statistical moments. However, as stated above, the convergence to the actual statistics is usually very slow, thus requiring several samples to achieve the desired result and making the method unfeasible when a large number of input quantities are involved (as for algorithm-based measurements).

To reduce the dimension of the ensembles and improve its efficiency, MC method have successively been refined. As an example, in Latin hypercube sampling [6], the stratification is exploited to hardly reduce the number of realizations required to match as close as needed the assigned statistics of each input quantity. In particular, the sample space is divided into intervals (usually referred to as stratas) characterized by the same probability and only one sample is realized for each interval. This way, it is possible to propagate several statistics of the input quantities without requiring large ensembles; however, assure suitable convergence on higher order moments usually still require unmanageable ensemble.

Deterministic sampling is a recent approach that turned out to be a valuable alternative to the random sampling in estimating output statistics of indirect measurements. Differently from the random realizations adopted by MC methods, the ensembles of deterministic sampling are selected according to a defined set of rules (principally the conservation of the moments of the input random variables up to a determined order). The first noticeable example of deterministic sampling was presented by Julier and Ulhmann in [17] to propagate the covariance in the unscented Kalman filter. The approach is based on the so-called unscented transform, i.e. a technique capable of simultaneously propagating random variable across a non-linear equation and reducing as low as possible the so-called scent γ, define as

$$\gamma = \mathrm{E}[Y] - f(\mathrm{E}[\underline{\boldsymbol{X}}]) \qquad (1)$$

where $\mathrm{E}[\cdot]$ is the traditional expectation operator. Thanks to a simple set of rules, the unscented approach defines a limited number of ensembles ($2N$ in its original version [11]) to correctly propagate expectation and standard uncertainty of the input quantities through the measurement model. This is particularly interesting, since it can be easily demonstrate that the first order term of the scent can be attained by the combination of the input covariance matrix and the sensitivity coefficients of the considered measurement model.

To assure a correct conservation of high order moments, several approaches have been presented; the most valuable is presented in [Hessling]; in particular, the proposed binary ensemble allowed to obtained as good estimates as those obtained through 10^6 MC simulation with only 128 samples per random variable. Unfortunately, as stated by Hessling in [7], the binary ensemble can be applied only to moderately sized models.

III. PROPOSED APPROACH

The authors proposed in [8] and [9] an innovative approach for deterministic sampling based on an enhanced version of the unscented transform. Thanks to a suitable definition of a set of rules, it has been possible to generate limited dimension ensembles capable of correctly conserving central moments up to 8th and 4th order for symmetrically and asymmetrically shaped pdfs, respectively. For the sake of the clarity, the theoretical background and the proposed application of DS to measurements based on complex algorithms will be presented in the following with reference to input quantities modeled as uncorrelated random variables characterized by symmetrically shaped pdfs.

A. Theoretical background

According to the deterministic sampling approach, for each input quantity X_i (i=1,..,N), expectation and a suitable collection of central moments have firstly to be estimated. This step is similar in terms of required information to the knowledge of the pdf of the input quantities of the Monte Carlo methods and can easily be accomplished either through repeated measurements or already available information and/or user knowledge and experience.

According to UT theory, the desired ensembles are organized in terms of matrix $\boldsymbol{\chi}$; in particular, each ensemble consists of a column of the matrix $\boldsymbol{\chi}$ and is usually referred to as sigma point:

$$\boldsymbol{\chi} = \begin{bmatrix} \mathbf{X}+\boldsymbol{\Sigma}_1 & \mathbf{X}+\boldsymbol{\Sigma}_2 & .. & \mathbf{X}+\boldsymbol{\Sigma}_G & \overline{\mathbf{x}}^T \end{bmatrix} \quad (2)$$

Generally speaking, $\boldsymbol{\chi}$ is characterized by N rows and $G{\cdot}N{+}1$ columns, where G is the maximum order central moments that has to be conserved. The elements of the vector $\overline{\mathbf{x}}$, last column of $\boldsymbol{\chi}$, are the expectation best estimates (x_i, i=1,..,N) of each variables X_i. With regard to $\mathbf{X}$ and $\boldsymbol{\Sigma}_j$ (j=1,..,G), they are N-dimensional, square matrices expressed respectively as

$$\mathbf{X}=\begin{pmatrix} x_1 & \cdots & x_1 \\ \vdots & \ddots & \vdots \\ x_N & \cdots & x_N \end{pmatrix} \text{ and } \boldsymbol{\Sigma}_j=\begin{pmatrix} s_{j1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & s_{jN} \end{pmatrix} \quad (3)$$

The matrices $\boldsymbol{\Sigma}_j$ are obtained by solving the following nonlinear equation system:

$$\begin{cases} 1 = W_0 + N(W_1 + W_2 + .. + W_G) \\ \mathbf{0} = W_1\boldsymbol{\Sigma}_1 + W_2\boldsymbol{\Sigma}_2 + .. + W_G\boldsymbol{\Sigma}_G \\ \boldsymbol{\mu}^2 = W_1\boldsymbol{\Sigma}_1^2 + W_2\boldsymbol{\Sigma}_2^2 + .. + W_G\boldsymbol{\Sigma}_G^2 \\ \ldots \\ \boldsymbol{\mu}^G = W_1\boldsymbol{\Sigma}_1^G + W_2\boldsymbol{\Sigma}_2^G + .. + W_G\boldsymbol{\Sigma}_G^G \end{cases} \quad (4)$$

and assure that the considered ensemble conserve the central moments of the input quantities.

$\boldsymbol{\mu}^k$ are, in fact, NxN diagonal matrices, the generic entry of which, μ_{ii}^k, is equal to the k^{th} central moment of the i^{th} input random variable. Even though the weights W_i can, in principle, be arbitrarily fixed, their values that makes easier the solution of the equations system (4) have to be preferred. As stated above, statistics of the resulting ensembles are inherently equal to those characterizing the vector $\boldsymbol{X}$.

The function f is then applied to each sigma point: $\psi_j = f\left(\boldsymbol{\chi}|_j\right)$, $j=1,..,GN+1$. $\boldsymbol{\chi}|_j$ stands for the j^{th} column of the matrix $\boldsymbol{\chi}$. To estimate the output quantity expectation and standard uncertainty, the obtained values, ψ_j, have to be processed according to the following expressions:

$$\overline{y} = \sum_{j=1}^{G}\sum_{i=1}^{N} W_j\psi_{ji} + W_0\psi_{GN+1} \quad (5)$$

$$\mu_{\overline{y}} = \sqrt{\sum_{j=1}^{G}\sum_{j=1}^{N} W_j\left(\psi_{ji}-\overline{y}\right)^2 + W_0\left(\psi_{GN+1}-\overline{y}\right)^2} \quad (6)$$

Equations system (4) can be simplified if the input quantities modeling by random variables are characterized by symmetric pdf's; if this is the case, the following choices can be made to solve the system (4):

$$\underline{\underline{\Sigma}}_{2k} = -\underline{\underline{\Sigma}}_{2k-1},\ W_{2k} = -W_{2k-1},\ k=1,..,\frac{G}{2} \quad (7)$$

This way, only $\frac{G}{2}$ equations along with related weights W_i and unknown matrices $\underline{\underline{\Sigma}}_i$ are necessary to assure that (i) even central moments, up to the G^{th} order, of resulting sigma points are equal to the corresponding ones of input variables and (ii) odd central moments are null according to the assumption of input random variables characterized by symmetric pdf's. Thanks to a proper selection of the values of W_i (W_1=W_3 and W_2=W_4 = -W_1), the authors are able to solve the equation system (4) in explicit form, for central moments up to the 8th order.

It is worth highlighting that the higher the number of considered input central moments, the more accurate the estimates of the output expectation and standard uncertainty [8]. Moreover, results similar to those granted by higher-order Taylor series approximations can be assured with no need of any derivative of f. This is a very attractive feature whenever the analytical form of f is not available, as in the presence of complex digital signal-processing algorithms.

B. Application of deterministic sampling to complex algorithms

For the sake of the clarity, the proposed approach will be presented with reference to an application example considering the ADC as the only uncertainty source. As stated above, from a metrological point of view, a measurement based on complex processing algorithm has to be considered as an indirect measurement. In the presence of algorithm-based measurement, the number N of input quantities X_i, i=1,..,N, could however be high, thus making unacceptable the dimension of the matrix χ containing the sigma points to be transformed. To suitably reduce the number of sigma points needed, it is useful to note that each input sample X_i can be gained by the corresponding code k_i provided by the analog-to-digital section through a straightforward expression:

$$X_i = \frac{k_i + Q_i}{T_i} + O_i \quad (8)$$

Q_i, T_i, and O_i are random variables modeling the analog-to-digital converter quantization, gain and offset; the variates depend only on the considered code k_i; for the sake of the simplicity, other typical factors (as INL, jitter and so on [Giaq]) have been neglected. The measurement model can thus be written:

$$Y = f\left(X_1,..,X_N\right) = g\left(Q_1,T_1,O_1,..,Q_M,T_M,O_M\right) \quad .(9)$$

M stands for the number of actually stimulated ADC codes. The UT approach can successfully be applied to the new function $g(\cdot)$. In the worst case of an input signal capable of stimulating all ADC codes, it is possible to reduce the number of sigma points to a maximum value equal to $3GH$+1, where H, equal to 2^n (n is the ADC resolution) is the number of ADC codes. It is worth noting that we focus only on the effect that the considered ADC parameters have on the estimate of output expectation and standard uncertainty; no other effect has been taken into account.

IV. NUMERICAL RESULTS

A number of tests have been conducted on simulated measurement data. Three typical DSP algorithms have been considered, characterized respectively by scalar, vector, and matrix output. For each DSP algorithm, estimates of the output expectation, y, and standard uncertainty, μ, have been gained both through the proposed approach and Monte Carlo simulations.

For the sake of simplicity, the random variables modeling Q, T, and O have been supposed uniformly distributed; no additional computational burden is required if this assumption is not met. In particular, the quantization Q and offset O have been modeled as zero-mean, uniformly distributed random variables, characterized by the same width equal to $\frac{LSB}{2}$, while the gain T has been modeled as a uniformly distributed random variate with mean and width equal respectively to 1 and 0.01.

As first example, a very common DSP algorithm has been considered. It is mandated to the evaluation of the root mean square value of an acquired waveform, according to the following relation:

$$Y = \sqrt{\frac{1}{N}\sum_{i=1}^{N} X_i^2} \quad . \quad (10)$$

Several tests have been conducted on simulated sinusoidal signals, the samples of which have been obtained in the assumption of an 8-bit, bipolar ideal ADC. All signals have been characterized by a different value both of the effective range ER (i.e. twice the maximum code acquired in the record) and record length N. Moreover, their normalized frequencies have been fixed equal to $\frac{1}{N}$ in order to operate in the hypothesis of coherent sampling. Achieved performance is given as differences Δy and $\Delta \mu$, both expressed in relative percentage terms, between the obtained estimates and those granted by $K=10^5$ Monte Carlo simulations.

Obtained results are given in Tab.I Remarkable concurrence can be noticed; differences never greater then 0.4% have, in fact, been experienced. It is worth noting that such a high value of K is necessary in order to assure reliable output estimates that can, thus, be taken as reference.

The advantage of the approach based on deterministic sampling proposed by the authors is clearly highlighted in Fig.1 which gives the outcomes of 100 different runs of Monte Carlo simulations (blue dots) for different values

Tab.I Results obtained in tests on the considered DSP-based algorithm. Δy and $\Delta \mu$ are expressed in percentage relative terms.

ER / N	128			256		
	M	Δy (%)	$\Delta \mu$ (%)	M	Δy (%)	$\Delta \mu$ (%)
256	102	$1.3\cdot10^{-4}$	0.13	116	$-2.6\cdot10^{-4}$	-0.045
512	128	0.0013	0.027	204	$2.4\cdot10^{-4}$	-0.42
1024	128	$-2.2\cdot10^{-4}$	0.031	256	$-2.4\cdot10^{-4}$	-0.16
2048	128	$-2.8\cdot10^{-4}$	-0.23	256	$-1.6\cdot10^{-4}$	0.017
4096	128	$4.3\cdot10^{-4}$	-0.22	256	$-1.0\cdot10^{-4}$	0.13

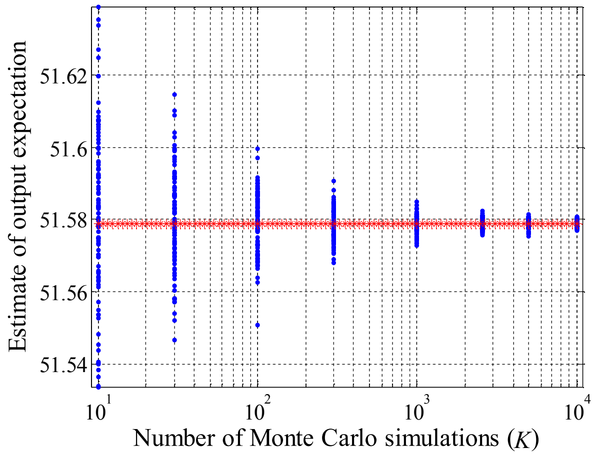

Fig.1 Outcomes provided by the proposed approach (red star) and Monte Carlo simulations (blue dots) in 100 different runs, for different values of *K*.

of K, i.e. 10, 30, 100, 300, 1000, 2544 (equal to $3GM+1$ with G=8 and M=106), 3000, and 10000. For low values of K, expectation estimates provided by Monte Carlo simulations are very poor and scattered about the correspondingly mean values, which are very close to those granted by the proposed approach (red stars). Similar considerations hold for standard uncertainty.

The application of the proposed approach to a DFT (discrete Fourier transform) algorithm is presented in the following [10]. In particular, the evaluation of the magnitude spectrum versus the normalized frequency according to

$$Y(0)=\left|\frac{1}{N}\sum_{n=0}^{N-1}X_n\right|$$
$$Y\left(\frac{i}{N}\right)=\left|\frac{2}{N}\sum_{n=0}^{N-1}X_n e^{-j2\pi\frac{i}{N}n}\right| \quad i=1,..N-1 \qquad (11)$$

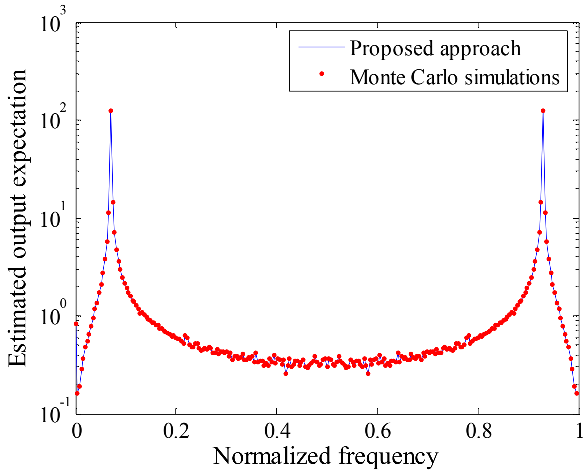

Fig.2. Comparison of expectation estimates provided by the proposed approach to those granted by 10^5 Monte Carlo simulations, for each spectral line.

has been pursued. Several tests have been conducted on simulated sinusoidal signals, characterized by different value both of the effective range *ER* and record length *N*. Achieved performance has been expressed both as RMS and maximum value of the difference vectors, Δy and $\Delta\mu$, between the obtained estimates and those granted by 10^5 Monte Carlo simulations. RMS values has, in particular, been evaluated according to the relations

$$RMS\Delta y=\sqrt{\frac{1}{N}\sum_{i=1}^{N}\Delta y_i}$$
$$RMS\Delta\mu=\sqrt{\frac{1}{N}\sum_{i=1}^{N}\Delta\mu_i} \quad i=1,..,N \qquad (12)$$

A valuable concurrence between the estimates provided by the proposed approach and those granted by Monte Carlo simulations has been encountered also in these tests. RMS values normalized to the signal amplitude never greater than 0.002 and a maximum difference, in percentage relative terms, always lower than 0.2% have been experienced. As an example, Fig.2 shows the results provided by the proposed approach when applied to a sinusoidal signal whose effective range and normalized frequency have been respectively equal to 256 and $1/\sqrt{200}$. Obtained estimates are superimposed to those granted by Monte Carlo simulations. The concurrence is still more evident if the difference vectors Δy and $\Delta\mu$ are also considered (Fig.3).

As a final example, the results obtained when the proposed approach is applied to a standard short time Fourier transform (STFT) are presented. The analyzed signal is the sum of two interfering chirps, both consisting of 4000 samples. In particular, Fig.4 and Fig.5 show the differences, for each point of time-frequency plane, between the expectation and standard uncertainty estimates of STFT coefficients, taken in modulus, provided by the proposed approach and those granted by

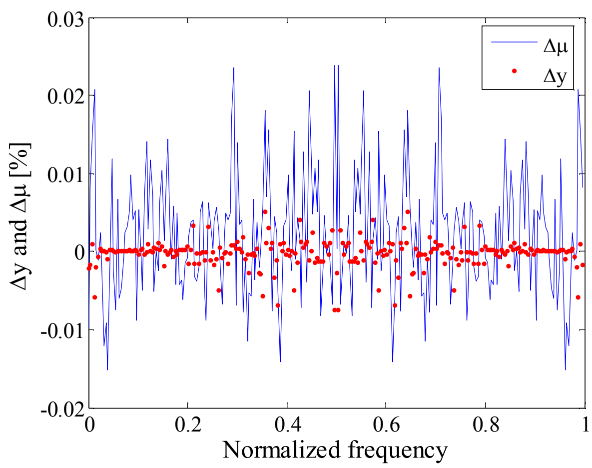

Fig.3. Δy and $\Delta\mu$, expressed in percentage relative terms, versus normalized frequency.

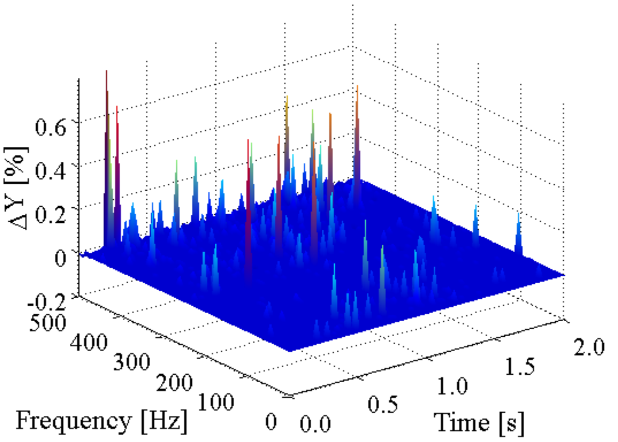

Fig.4. Differences, for each point of the time-frequency plane, between expectation estimates of the STFT coefficients provided by the proposed approach and those granted by 10^4 Monte Carlo simulations.

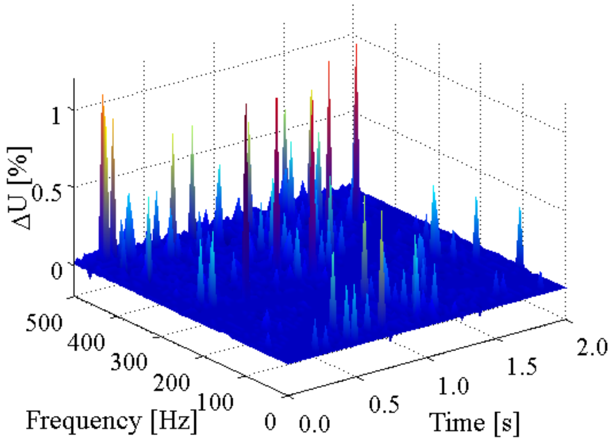

Fig.5. Differences, for each point of the time-frequency plane, between standard uncertainty estimates of the STFT coefficients provided by the proposed approach and those granted by 10^4 Monte Carlo simulations.

10^5 Monte Carlo simulations. Remarkable concurrence can be noticed; percentage relative differences always lower than 1% has, in fact, been experienced. As regards the computational time, the proposed approach provides the desired estimates in 5 s; on the contrary, Monte Carlo simulation takes over 7 minutes.

CONCLUSIONS

The suitability of deterministic sampling for uncertainty quantification in measurements based on complex algorithm has been investigated in the paper. In particular, the authors proposed the unscented transform to provide reliable estimates of the output quantity and focused their attention on the influence of the analog-to-digital conversion section on the final output.

Several tests conducted in the presence of different DSP measurements algorithms have been conducted in order to assess the reliability of the proposed approach. For each test, the results provided by the proposed approach have been compared with those granted by a suitable number of Monte Carlo simulations. Remarkable concurrence has been noticed; differences between obtained estimates and those granted by Monte Carlo simulations have, in fact, been always lower than 0.7%.

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