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Visualization of uncertainty  
associated with classes of  
electrical measurement

By

M G Cox, T J Esward, P M Harris

Centre for Mathematics and

Scientific Computing, NPL

N McCormick

Materials Centre, NPL

N M Ridler, M J Salter

Centre for Electromagnetic and Time

Metrology, NPL

J P R B Walton

NAG Ltd, Oxford, UK

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M G Cox, T J Esward, P M Harris  
Centre for Mathematics and Scientific Computing, NPL  
N McCormick  
Materials Centre, NPL  
N M Ridler, M J Salter  
Centre for Electromagnetic and Time Metrology, NPL  
J P R B Walton  
NAG Ltd, Oxford, UK

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## ABSTRACT

The interpretation of statements of measurement uncertainty can be difficult when there are several input quantities and several output quantities involved in the model of measurement. Appropriate ways of visualizing the uncertainty information can be helpful in this regard. The use of visualization tools is investigated for two problems that occur in electrical metrology and electrical engineering. One problem concerns co-ordinate system transformations, as arise in converting measurements from Cartesian (real and imaginary) co-ordinates to polar (magnitude and phase) co-ordinates. The other concerns microwave power meter calibration, specifically the determination of ‘comparison loss’. The underpinning measurement models also arise in other disciplines. Moreover, the visualization tools considered have aspects that are generically applicable.

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Authorised by Dr Dave Rayner,  
Head of the Centre for Mathematics and Scientific Computing

National Physical Laboratory,  
Queens Road, Teddington, Middlesex, United Kingdom TW11 0LW

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*The reader should refer to section 1.1 before making use of this document electronically. In particular, it is recommended that, before reading the document, the reader confirms that the multimedia objects listed in section 1.1 operate correctly.*

## 1 Background

The first NMS Software Support for Metrology programme, 1998–2001 (SSfM-1), addressed the need for dissemination of information on current visualization techniques [24]. However, some of the case studies presented as part of that work revealed technical problems that needed to be considered separately in the second programme, 2001–2004 (SSfM-2). Two main problems were identified:

- The visualization of uncertainty regions for vector and multi-dimensional data
- The calculation, validation and visualization of uncertainties associated with continuous models.

It was recognized that the solutions to these problems in particular metrology areas needed to be addressed through appropriate studies. Moreover, consideration needed to be given to the ways in which these solutions could be generalized to apply to metrology areas other than those chosen for the case studies. It was also considered that in the third programme, 2004–2007, additional case studies should be considered, to provide clear demonstration of the applicability to other metrology areas.

The importance of tackling the issues of calculation, validation and visualization of uncertainties is that without the consideration of these issues the effectiveness of visualization techniques for metrologists would be limited. Although visualization of data or a model can give the viewer a feeling of understanding, it is impossible to know what level of assurance can be given to that understanding unless a statement or visualization of the associated uncertainty is also available. Indeed, to the unwary, data or model visualization using impressive graphics can be very misleading. It can tempt the viewer to ignore or forget the basic principle that every measurement should have an uncertainty associated with it.

This report considers the visualization of uncertainty regions for vector and multi-dimensional data, viz., for instances of discrete modelling. The work has benefited from that on the visualization of ellipses of uncertainty associated with complex-valued electromagnetic measurements undertaken in NPL's Centre for Electromagnetic and Time Metrology as part of the NMS Electrical programme.

In carrying out the work, account was taken of other activity within SSfM-2, particularly relating to uncertainties and statistical modelling (especially the best-practice guide [10]), visualization (especially the good-practice guide [18]), empirical modelling and discrete modelling, and various awareness presentations and conferences [12]. Relevant work within SSfM-1, especially on visual modelling and data visualization [24], was also considered.

## 1.1 Multimedia objects

This document contains a number of multimedia objects for visualization. They are available by viewing the document electronically using *Acrobat* reader, available from

<http://www.adobe.com/products/acrobat/readstep2.html>

To ensure the objects are visible, appropriate viewers are required to be installed.

Two types of multimedia object are used:

**Movies** provided with the document in the form of AVI movie files (section 3.3.3). The movies can be viewed using a suitable player such as *Windows Media Player*.

**Views** of (three-dimensional) objects that allow also some interaction with the objects displayed (sections 3.4 and 4.3). To interact with these views a web browser, such as Internet Explorer, is used to download a page containing a Java applet from the internet or to open a page<sup>1</sup> provided with the document. To display the view a browser plug-in is required, such as *Cortona* or *Cosmoplayer*, dependent on the computing platform. *Cortona* can be obtained from

<http://www.parallelgraphics.com/products/cortona>

and is available for Windows and Macintosh operating systems. *Cosmoplayer* can be used in Unix environments, and can be obtained from

<http://www.sgi.com/software/cosmo/>

The web pages have been tested using Internet Explorer with the *Cortona* VRML viewer and the Microsoft Java VM. They have also been tested using Netscape 4.x, with the *Cosmoplayer* VRML viewer and the Netscape Java VM in an Irix environment.

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<sup>1</sup>These pages are provided as files with extension '.wrl'.

Links to the multimedia objects provided in this document are given below. The objects may also be accessed from the sections indicated, where information on how to use the objects, and interpret what they show, is also provided.

- Movie 1 for co-ordinate system transformation (section 3.3.3)
- Movie 2 for co-ordinate system transformation (section 3.3.3)
- Movie 3 for co-ordinate system transformation (section 3.3.3)
- Movie 4 for co-ordinate system transformation (section 3.3.3)
- Web page 1 for co-ordinate system transformation (section 3.3.2)
- Web page 2 for co-ordinate system transformation (section 3.3.2)
- Web page 3 for co-ordinate system transformation (section 3.4)
- Web page for comparison loss in microwave power meter calibration (section 4.3).

## 1.2 Units

Throughout this work, no unit is used to express the dimensionless (and complex-valued) voltage reflection coefficients considered when they are represented in terms of their real and imaginary parts. Doing so is consistent with common practice in this area of electrical engineering.<sup>2</sup> Further, when these complex-valued quantities are expressed in polar form, i.e., in terms of magnitude and phase, phase angle is expressed in degrees (rather than radians), and the corresponding magnitude remains dimensionless.

## 2 Uncertainty evaluation in electrical work

This document is concerned with a study of the visualization of uncertainty for two particular discrete models. The end users of these models are electrical engineers and those generally concerned with electrical measurement. In this area, even some of the fundamental concepts are less understood than is desirable. As a consequence, the use of visualization aids to assist with that understanding is especially appropriate.

A complication in electrical work is that the measurements are typically of complex-valued quantities. For some purposes these quantities are represented in terms of

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<sup>2</sup>In contrast, all quantities of dimension one are formally said to have the SI coherent derived unit ‘one’ with the symbol ‘1’ [14, 20].

their real and imaginary parts (Cartesian co-ordinates) and for other purposes in terms of magnitude and phase (polar co-ordinates). Uncertainties are invariably associated with these measurements.

In particular, measurement results frequently have to be transformed from one system of co-ordinates to the other. The associated uncertainties have accordingly to be transformed in a valid manner. The latter problem creates difficulties for some engineers and scientists, and indeed is not trivial.

One of the studies concerns this co-ordinate system transformation problem. The other study concerns comparison loss in microwave power meter calibration, again involving complex-valued quantities. This problem has a number of features, the handling of which cannot reliably be carried out using conventional uncertainty procedures. Visualization is shown to be useful for both problems.

## 2.1 Use of the GUM

Let  $Y = f(X_1, \dots, X_n)$  denote a model of measurement, where the  $X_i$  are the input quantities and  $Y$  is the output quantity. Suppose estimates  $x_i$  of the values of the  $X_i$  are given, and also available are the standard uncertainties  $u(x_i)$  associated with the  $x_i$ .

The law of propagation of uncertainty is defined in the Guide to the Expression of Uncertainty in Measurement (GUM) [5, Clause 5]. It relates to the evaluation of the standard uncertainty associated with  $y$ , the estimate of the value of  $Y$  given by evaluating the model at  $X_i = x_i$ , in terms of the  $u(x_i)$  and the corresponding sensitivity coefficients  $c_i$  [5, Clauses 5.1.2, 5.1.3]. The  $c_i$  are determined by evaluating the partial derivatives of first order of the model as a function of the  $X_i$  at the  $x_i$ . The input quantities may be mutually dependent, in which case the corresponding covariances<sup>3</sup>  $u(x_i, x_j)$  are included as additional terms in the law of propagation of uncertainty [5, Clause 5.2.1]. The values used for the  $c_i$  should also take account of partial derivatives of higher order if their influence is significant [5, Clause 5.1.2].

Following the application of the law of propagation of uncertainty, in order to provide an expanded uncertainty  $U$  and hence a coverage interval [5, Clauses 6 and G] for the value of  $Y$  corresponding to a prescribed coverage probability  $p$ ,  $u(y)$  is multiplied by a coverage factor  $k_p$ . Thus,  $U = k_p u(y)$  and the coverage interval is  $y - U$  to  $y + U$ . The coverage factor  $k_p$  is typically determined by assigning a Gaussian distribution with expectation  $y$  and standard deviation  $u(y)$  to the value of  $Y$ . This assignment is dependent on the applicability of the Central Limit Theorem [5, Clause G.2].<sup>4</sup>

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<sup>3</sup>Sometimes referred to as *mutual uncertainties*.

<sup>4</sup>The coverage factor  $k_p$  is instead determined from a  $t$ -distribution with an appropriate degrees of freedom if the degrees of freedom assigned to the  $u(x_i)$  are not all infinite [5, Clause G.4]. Such

In this document the term LPU is taken as meaning the use of the law of propagation of uncertainty of the GUM, including covariance terms when appropriate, based on the  $c_i$  determined from first-order partial derivatives, together with  $U$  determined on the above Gaussian basis.

## 2.2 The two phases of uncertainty evaluation

The problem of uncertainty evaluation can be divided into two phases: formulation and calculation [4, 10].

The *formulation* phase of uncertainty evaluation comprises the stages:

1. Develop a model for the measurement relating the input quantities  $X_i$ ,  $i = 1, \dots, n$ , to the output quantity  $Y$  [5, Clause 4.1].
2. Assign probability density functions (PDFs) [5, Clause C.2.5]—Gaussian (normal), rectangular (uniform), etc.—to the values of the  $X_i$ .<sup>5</sup>

Using the information provided by the formulation phase, the *calculation* phase of uncertainty evaluation then comprises the stages:

1. *Propagate* the PDFs for the values of the  $X_i$  through the model to obtain the PDF for the value of  $Y$ .
2. Obtain from the PDF for the value of  $Y$ :
  - (a) Its expectation, taken as the estimate  $y$  of the value of  $Y$ .<sup>6</sup>
  - (b) Its standard deviation, taken as the standard uncertainty associated with  $y$  [5, Clause E.3.2].<sup>7</sup>
  - (c) An interval (the coverage interval) containing the output quantity value with a specified probability (the coverage probability  $p$ ).

## 2.3 The calculation phase of uncertainty evaluation

LPU (section 2.1) provides one approach to the calculation phase of uncertainty evaluation. It operates with the expectations and standard deviations of the PDFs assigned to the values of the input quantities, rather than the PDFs *per se*.

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instances are not treated here.

<sup>5</sup>Assign instead a joint probability density function to the values of those  $X_i$  that are mutually dependent.

<sup>6</sup>The  $y$  determined by LPU (section 2.1) is an approximation in general to the  $y$  considered here.

<sup>7</sup>Similarly, the  $u(y)$  determined by LPU (section 2.1) is an approximation to the standard deviation considered here, although for a linear model  $u(y)$  is correct.

Monte Carlo simulation (MCS) is an approach that is more general than LPU and is the subject matter of the first supplemental guide to the GUM, which is in an advanced stage of preparation [4]. It is consistent with the GUM in that it falls into the category of ‘other analytical or numerical methods’ permitted by it [5, Clause G.1.5]. The approach is based on the *propagation of distributions*.

MCS is computationally more intensive but conceptually simpler than LPU. It involves generating a large number of values of the output quantity by, repeatedly, sampling randomly from the PDFs assigned to the values of the input quantities and evaluating the model for these samples. The large number of values of the output quantity so obtained is used to approximate the distribution function, viz., the indefinite integral of the PDF, for the value of the output quantity, from which the quantities of interest (expectation, standard deviation and a coverage interval for the value of the output quantity) can be formed.

The propagation of distributions, and an implementation of it based on Monte Carlo simulation, is summarized in appendix A.

## 2.4 The context for the studies

The GUM provides invaluable advice on the treatment of uncertainties associated with the input and output quantities of models of measurement. However, the GUM is a large and sophisticated document (over 100 pages), and as a consequence organizations such as the United Kingdom Accreditation Service (UKAS) [36] and EURACHEM [17] have adopted principally those parts of the GUM specifically concerned with LPU, and predominantly applied only LPU (section 2.1) in a wide range of circumstances. The European co-operation for Accreditation (EA) has taken matters somewhat further and provides examples in which non-normality of the distribution for the value of  $Y$  is treated, at least approximately [15]. However, there are classes of problems for which LPU (and the treatment by EA) does not provide completely adequate solutions. Both the co-ordinate system transformation problem and the comparison loss application fall into this category.

Even if the real and imaginary parts in the Cartesian representation of a complex-valued measurement are uncorrelated, following transformation the magnitude and phase components of the polar representation will generally not be so. A similar statement applies when performing the inverse transformation. If correlations already exist, such interdependencies will be present following transformation, but in a different form. The GUM does not treat generically cases of more than one output quantity, although two examples are given of models with two output quantities [5, Clauses H.2, H.3].

If expanded uncertainties are required, as they are for many calibrations, it is necessary to have knowledge of the probability distributions for the values of the quan-

tities concerned. Applying the counterpart of LPU for two output quantities, in which a bivariate Gaussian distribution would be assigned to the values of the output quantities, may lead to invalid results. One reason is that generally the Central Limit Theorem (section 2.1), on which the assignment depends, strictly applies asymptotically, i.e., for sufficiently large  $n$ , and yet only two input quantities to the co-ordinate system transformation problem are involved. Similarly, for the special case of the comparison loss problem considered here, again only two input quantities are involved.

## 2.5 The studies

The studies both have the purpose of understanding better the uncertainties associated with electrical measurements, the first when co-ordinate system transformations are made, and the second when microwave power meters are calibrated, and the extent to which ‘uncertainty visualization’ can assist in this regard.

For the second study, an additional purpose is to examine visually the uncertainties provided by LPU and MCS as an implementation of the propagation of distributions, especially in situations where the straightforward use of LPU over the whole domain of concern might be misleading. For parts of the studies, use is made of some analytical results, since they provide definitive solutions for comparison purposes.

In summary, the studies, treated in detail in sections 3 and 4, respectively, are as follows.

- 1. Transformation from Cartesian to polar co-ordinates.** Given a bivariate Gaussian distribution assigned to the values of  $X$  and  $Y$ , provide visualizations of coverage regions for the values of the quantities  $(R, \Theta)^T$ , where  $R^2 = X^2 + Y^2$  and  $\tan \Theta = Y/X$ .<sup>8</sup>
- 2. Comparison loss in microwave power meter calibration.** For the reflection-less case of comparison loss in microwave power meter calibration, expressed in terms of the model  $M = 1 - X^2 - Y^2$ , quantify the dependence of the standard uncertainty  $u(m)$  associated with an estimate  $m$  of the value of  $M$  on values  $x$  and  $y$  (of  $X$  and  $Y$ ) and the standard uncertainties  $u(x)$  and  $u(y)$  and covariance  $u(x, y)$  associated with  $x$  and  $y$ . For the case that  $x$  and  $y$  are given, this corresponds to providing visualizations of a relation-

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<sup>8</sup>A second problem is the inverse problem, viz., given a bivariate Gaussian distribution assigned to the values of  $R$  and  $\Theta$ , provide visualizations of coverage regions for the values of the quantities  $(X, Y)^T$ , where  $X = R \cos \Theta$  and  $Y = R \sin \Theta$ . Only the former problem is addressed here because of its greater appropriateness in electrical engineering as a starting point for uncertainty evaluations.

ship between four variables. Specifically, appropriate visual images of the ‘hypersurface’  $u(m)$  as a function of  $u(x)$ ,  $u(y)$  and  $u(x, y)$  are required.

## 2.6 Frequency dependence

An aspect of concern to electrical engineers is that their models are required to apply more broadly than the models in some other areas. The extra dimension relates to the fact that the models have a frequency dependence. For any particular frequency such a model can be regarded as a discrete model. However, the engineer requires knowledge of behaviour and performance throughout a *range* of frequencies. It may be the case that the application of LPU will be valid for part of the frequency range, but invalid elsewhere.

Moreover, the models often have to apply for different values of the input quantities. Again, as a consequence, the degree of validity of the uncertainties associated with the measurement results may be influenced by these values.

Suitable visualization can be used to help gain insight into the nature of the regions of validity, as well as providing a mechanism to aid understanding of the behaviour in general.

## 2.7 Further remarks

A specific benefit to the electrical engineer in using appropriate visualizations for problems such as those presented here can be an improved ability to interpret complicated or multiple sets of measurement data. In particular, a better understanding should be possible of the uncertainties associated with frequency-dependent measurements that may include features such as strong non-linearities, cusps, etc. Such features would not be so apparent in tables of values alone.

It has been recommended [30] that the analysis of the complex-valued quantities encountered in electrical engineering should be performed on the real and imaginary components of the complex-valued quantities (i.e., in Cartesian form). Such an analysis includes the assignment of PDFs to the values of the quantities concerned. However, as also stated [30], the subsequent use of such complex-valued quantities is often more convenient when they are expressed in magnitude and phase format (i.e., in polar form). The PDFs for the values of the polar quantities then need to be derived from the PDFs for those of the quantities in Cartesian form.

The validation of visualizations is not the main consideration of this work. However, just as the numerical correctness of mathematical and statistical software [2, 7, 9] is important to metrologists, who need to have confidence in the software they

use, so is the faithful visual representation of objects, functions and relationships, in order that the metrologist is not unwittingly misled. Appendix B discusses this aspect.

### 3 Co-ordinate system transformation

This section is concerned with the transformation from the Cartesian representation (real and imaginary parts) of complex-valued quantities to the polar representation (magnitude and phase) of those quantities. As stated in section 2.5 this (forward) transformation is more appropriate in electrical engineering than the inverse transformation used in some other disciplines (an instance is indicated below). The uncertainties associated with such a transformation are evaluated using (a) LPU, (b) MCS, and (c) (in special circumstances) an analytical treatment.

#### 3.1 Formulation phase

The model of measurement relating input quantities  $(X, Y)^T$  to output quantities  $(R, \Theta)^T$  is<sup>9</sup>

$$R^2 = X^2 + Y^2, \quad \tan \Theta = Y/X. \quad (1)$$

Estimates  $(x, y)^T$  of the values of Cartesian co-ordinates  $(X, Y)^T$  are available. The uncertainty matrix (covariance matrix)

$$V_{x,y} = \begin{bmatrix} u^2(x) & u(x, y) \\ u(x, y) & u^2(y) \end{bmatrix} \equiv \begin{bmatrix} u^2(x) & \rho(x, y)u(x)u(y) \\ \rho(x, y)u(x)u(y) & u^2(y) \end{bmatrix}, \quad (2)$$

where  $u(x)$ ,  $u(y)$  and  $u(x, y)$  denote the standard uncertainties and covariance associated with  $x$  and  $y$ , and  $\rho(x, y)$  the corresponding correlation coefficient, is assumed to be available. A bivariate Gaussian distribution with expectation

$$(\mu_x, \mu_y)^T = (x, y)^T$$

and uncertainty matrix  $V_{x,y}$  is assigned to the values of  $(X, Y)^T$ , e.g., on the basis of maximum entropy considerations [10, 40, 41].<sup>10</sup>

<sup>9</sup>This is an *implicit* model for  $R$  and  $\Theta$  [10]. Since  $R$  is a magnitude, and is known to be non-negative, it is determined uniquely by considering the positive square root of  $R^2$ . By using a ‘four quadrant inverse tangent function’ (often denoted by ‘atan2’),  $\Theta$  is determined uniquely from the model to satisfy  $-180^\circ < \Theta \leq 180^\circ$ ,

<sup>10</sup>In the following, the notation  $x$  (and  $y$ , etc.) will be used in the application of LPU and MCS to the formulated problem, whereas  $\mu_x$  (and  $\mu_y$ , etc.) will be used in the analytical treatment. The former is a notation that is consistent with the GUM and the forthcoming supplemental guide on the propagation of distributions; the latter is (perhaps) a more natural notation for the parameters of the distributions that are assigned (to the values of the input quantities) and derived (for the values of

Required is the bivariate distribution for the values of the polar co-ordinates  $(R, \Theta)^T$ . From this distribution the expectation  $(\mu_r, \mu_\theta)^T = (r, \theta)^T$  of the values of  $(R, \Theta)^T$ , the uncertainty matrix  $V_{r,\theta}$  associated with  $(r, \theta)^T$ , and a coverage region for the values of  $(R, \Theta)^T$ , corresponding to a stipulated coverage probability, can then be determined (section 2.2).

### 3.2 Calculation phase

The purpose of this section is to determine the distributions for the values of the output quantities  $(R, \Theta)^T$  obtained from the application of the LPU and MCS approaches to uncertainty evaluation, and given by an analytical treatment of the problem formulated in section 3.1. From the application of LPU, values are obtained for the parameters (expectations, variances, etc.) of a bivariate Gaussian distribution *assigned* to the values of  $(R, \Theta)^T$ . From MCS, the distribution is represented by a *sample* of values of  $(R, \Theta)^T$ .

Results are given in the particular case that the input quantities  $X$  and  $Y$  are mutually independent and have equal variance. LPU and MCS may be applied more generally, but an analytical treatment is only provided when these conditions are assumed to hold.

#### 3.2.1 Law of propagation of uncertainty

In order to implement the counterpart of LPU for two output quantities, the Jacobian of the model, viz., the matrix of partial derivatives of first order of the output quantities with respect to the input quantities, is required [10, 11]:

$$J = \begin{bmatrix} \partial R / \partial X & \partial R / \partial Y \\ \partial \Theta / \partial X & \partial \Theta / \partial Y \end{bmatrix}.$$

Forming these partial derivatives and evaluating them at  $(x, y)^T$  gives

$$J = \begin{bmatrix} x/r & y/r \\ -y/r^2 & x/r^2 \end{bmatrix} = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta / r & \cos \theta / r \end{bmatrix}, \quad (3)$$

where

$$r^2 = x^2 + y^2, \quad \tan \theta = y/x.$$

The uncertainty matrix associated with  $r$  and  $\theta$  is then evaluated from

$$V_{r,\theta} = J V_{x,y} J^T. \quad (4)$$

the output quantities) in the analytical treatment. Similarly,  $u(x)$  (and  $u(y)$ , etc.) will be used in LPU and MCS to denote the standard uncertainty associated with  $x$  (and  $y$ , etc.), whereas  $\sigma$  (perhaps subscripted by  $x$ , etc.) will be used in the analytical treatment for the standard deviation parameter of a probability distribution.

where  $V_{x,y}$  is given by expression (2) and  $J$  by expression (3) [8, 10].<sup>11</sup> Finally, the result of applying LPU to the problem formulated in section 3.1 is to assign a bivariate Gaussian distribution, with expectation  $(r, \theta)^T$  and uncertainty matrix  $V_{r,\theta}$ , to the value of  $(R, \Theta)^T$ .

When  $\rho(x, y) = 0$ , the case of mutually independent input quantities,

$$V_{r,\theta} = \begin{bmatrix} \cos^2 \theta u^2(x) + \sin^2 \theta u^2(y) & (\cos \theta \sin \theta / r)(u^2(y) - u^2(x)) \\ (\cos \theta \sin \theta / r)(u^2(y) - u^2(x)) & (\sin^2 \theta / r^2)u^2(x) + (\cos^2 \theta / r^2)u^2(y) \end{bmatrix}.$$

Furthermore, when  $\rho(x, y) = 0$  and  $u(x) = u(y)$ , it follows that  $R$  and  $\Theta$  are uncorrelated. In this special circumstance, of uncorrelated quantities assigned a bivariate Gaussian distribution, it follows that  $R$  and  $\Theta$  are mutually independent [25, Theorem 3.1.3].<sup>12</sup> Consequently, the result of applying LPU to the problem formulated in section 3.1 is to assign Gaussian distributions<sup>13</sup>  $N(r, u^2(r))$  and  $N(\theta, u^2(\theta))$  to the values of  $R$  and  $\Theta$ , where

$$u^2(r) = \cos^2 \theta u^2(x) + \sin^2 \theta u^2(y)$$

and

$$u^2(\theta) = (\sin^2 \theta / r^2)u^2(x) + (\cos^2 \theta / r^2)u^2(y).$$

There are clearly some anomalies that arise from the application of LPU to the co-ordinate system transformation problem.

Firstly, in the special circumstance indicated above, mutually independent Gaussian distributions are assigned to the values of  $R$  and  $\Theta$ , with parameters given above, *irrespective* of the values of  $x$ ,  $y$  and  $u(x) = u(y)$ . For an estimate  $(x, y)^T$  of the value of the quantity close to the origin this can be expected to give a distribution for the value of the magnitude  $R$  of the quantity that includes negative (infeasible) values.

Secondly, it is not clear how to apply LPU in the case that  $x = y = 0$ , i.e., the estimate of the value of the quantity is at the origin. In this case,  $\theta$ , the corresponding

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<sup>11</sup>The reverse transformation is basic in surveying [32, p329], distance and angle measurements being converted to (Cartesian) spatial locations. Information is available concerning  $R$  and  $\Theta$  and it is required to provide information concerning  $X$  and  $Y$ . Covariance propagation is then effected by inverting expression (4):

$$V_{x,y} = J^{-1} V_{r,\theta} J^{-T}.$$

<sup>12</sup>In contrast, in the analytical treatment (section 3.2.3), where a bivariate Gaussian distribution is *not* assigned to the value of  $(R, \Theta)^T$ , the conditions  $\rho(x, y) = 0$  and  $u(x) = u(y)$  are *not* sufficient to ensure that  $R$  and  $\Theta$  are mutually independent. An additional condition, viz.,  $x = y = 0$ , is required.

<sup>13</sup>The notation  $N(\mu, \sigma^2)$  is used to denote a Gaussian distribution with expectation  $\mu$  and variance  $\sigma^2$ .

estimate of the value of phase angle  $\Theta$ , and  $J$ , the Jacobian of the model, are not well-defined.

MCS and the analytical treatment presented in the following sections provide a more robust approach to evaluating uncertainties for the co-ordinate system transformation problem.<sup>14</sup> Visualization of the results obtained using MCS and an analytical treatment are used to expose and illustrate these anomalies.

### 3.2.2 Monte Carlo simulation

A key task in the application of MCS to the problem formulated in section 3.1 is to be able to draw random samples  $(x_k, y_k)^T$ ,  $k = 1, \dots, N$ , where  $N$  is the number of Monte Carlo trials, from a bivariate Gaussian distribution with expectation  $(x, y)^T$  and uncertainty  $V_{x,y}$  given by expression (2). A way in which this task can be carried out is given in appendix C.

For each random sample  $(x_k, y_k)^T$  so obtained, the model (1) is used to determine corresponding values  $(r_k, \theta_k)^T$  of the output quantities, viz.,

$$r_k^2 = x_k^2 + y_k^2, \quad \tan \theta_k = y_k/x_k, \quad k = 1, \dots, N.$$

Visualizations of the joint PDF for the values of  $R$  and  $\Theta$ , where that PDF is represented by the set of points  $(r_k, \theta_k)^T$ ,  $k = 1, \dots, N$ , are provided in section 3.3.

### 3.2.3 Analytical treatment

Consider, as in section 3.2.1, the case of mutually independent input quantities with equal variances. Specifically, assign Gaussian PDFs  $N(\mu_x, \sigma^2)$  and  $N(\mu_y, \sigma^2)$  to, respectively, the values of  $X$  and  $Y$ .

Appendix D provides expressions for the joint PDF for the values of  $R$  and  $\Theta$  (expression (12)) and their respective marginal distributions<sup>15</sup> (expressions (13) and (14)). The marginal distribution for the value of  $R$  is shown to be a Rice distribution [27].

It is also shown in appendix D that when  $\mu_x = \mu_y = 0$ , the output quantities are mutually independent, with the value of  $R$  described by a  $\chi$ -distribution with two

<sup>14</sup>For example, MCS makes no use of the Jacobian of the model and makes no assumption about the PDF for the values of the output quantities [4, 10]. If, in an implementation of MCS, the random sample  $(0, 0)^T$  for the values of the input quantities  $(X, Y)^T$  arises, it is safe to ignore this case (being one out of many), and thus avoid the need to evaluate the model.

<sup>15</sup>A marginal distribution is given by integrating the joint distribution over all values of the other variables.

degrees of freedom,<sup>16</sup> or equivalently a Rayleigh distribution [27] with PDF

$$g(R) = \frac{R}{\sigma^2} \exp\left(\frac{-R^2}{2\sigma^2}\right), \quad R \geq 0,$$

and the value of  $\Theta$  by a rectangular distribution with PDF

$$g(\Theta) = \frac{1}{2\pi}, \quad -\pi < \Theta \leq \pi.$$

Visualizations of the joint PDF for the values of  $R$  and  $\Theta$ , and their respective marginal distributions, for the above special circumstances are provided in sections 3.3 and 3.4.

### 3.3 Non-interactive visualization

Various forms of non-interactive visualization of the PDF for the values of  $R$  and  $\Theta$  are first considered.

#### 3.3.1 Slices

Figure 1 shows the PDFs (13) and (14) given in appendix D corresponding to the marginal distributions for the values of magnitude  $R$  and phase angle  $\Theta$  for particular values of  $\mu_x$ ,  $\mu_y$  and  $\sigma$ .

#### 3.3.2 Elevated surfaces

The stacking (vertically or, here, side-by-side) of a sequence of slices provides a representation of a marginal PDF in the form of a surface for which the ‘independent variables’ are the output quantity (here  $R$  or  $\Theta$ ) and the ‘slice’ variable (here  $\mu_x$ ). It provides a visualization of the marginal PDFs for the values of  $R$  and  $\Theta$  using a two-dimensional display, either as contour plots or as elevated surfaces. Figure 2 shows these marginal PDFs as *elevated surfaces*.

Three-dimensional views of the elevated surfaces shown in figure 2 are provided for the marginal PDFs for the value of  $R$  and those for the value of  $\Theta$ .<sup>17</sup> These views can be examined from different viewpoints using the controls labelled *Plan*, *Pan*, *Turn* and *Roll* in accordance with the type of movement required by the user. Doing so constitutes a simple form of *interaction* but, unlike the interactive visualization

<sup>16</sup>The square root of the sum of the squares of two standard Gaussian variates.

<sup>17</sup>In these views, the axes are labelled with ‘mux’ to denote  $\mu_x$ , ‘r’ the value of the magnitude  $R$ , ‘theta’ the value of the phase angle  $\Theta$ , and ‘PDF’ to denote probability density (dimensionless for magnitude  $R$  and in units of ‘degrees<sup>-1</sup>’ for phase angle  $\Theta$ ).

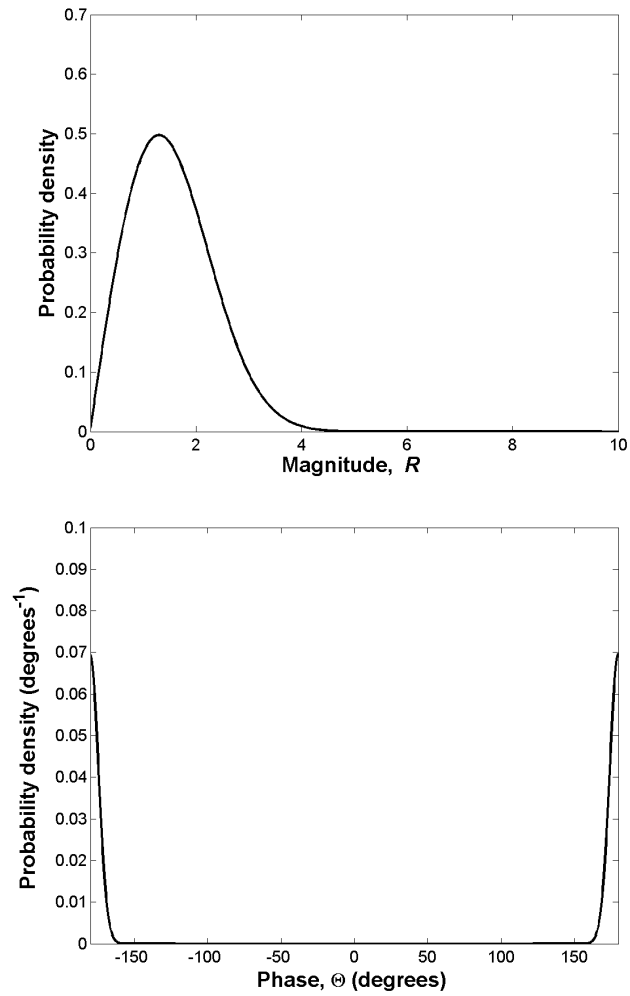


Figure 1: The marginal PDF for the value of magnitude  $R$  corresponding to  $\mu_x = -1$ ,  $\mu_y = 0$  and  $\sigma = 1$ , and (bottom) that for the value of phase angle  $\Theta$ , corresponding to  $\mu_x = -10$ ,  $\mu_y = 0$  and  $\sigma = 1$ .

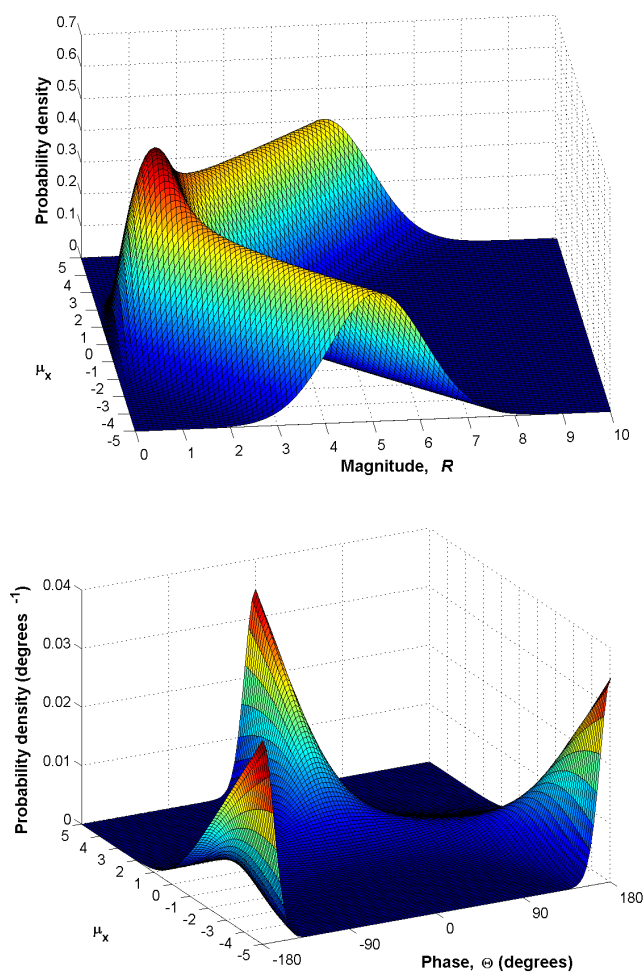


Figure 2: Elevated surfaces showing, as a function of  $\mu_x$ , the marginal PDFs for the value of  $R$  and (bottom) those for for the value of  $\Theta$ .

presented in section 3.4, there is no provision for the values of the parameters  $\mu_y$  and  $\sigma$  that determine the object displayed to be altered.

### 3.3.3 Movies: slices, elevated surfaces and contour plots

The presentation of a succession of slices (in time) as one of the defining parameters changes throughout its permissible range of values constitutes a movie. It provides an alternative to the use of elevated surfaces to portray the marginal PDFs for the values of  $R$  and  $\Theta$  as  $\mu_x$  cycles through a sequence of values.

A movie of the marginal PDFs for the value of  $R$  as given by expression (13) in appendix D with  $\mu_y = 0$  and  $\sigma = 1$ , as  $\mu_x$  ranges from  $-10$  to  $10$  in steps of  $0.5$ , can be viewed, as can the other multimedia objects indicated in this document, through examining on-line the PDF version of this document. A movie of the marginal PDFs for the value of  $\Theta$  as given by expression (14) in appendix D for the same values of  $\mu_y$  and  $\sigma$ , and the same range of values of  $\mu_x$ , can also be viewed.

It is emphasized that each frame of these movies shows the marginal PDF for the value of magnitude or phase angle corresponding to a particular value of  $\mu_x$  (as in figure 1).

Movies may also be used to show the *evolution* of elevated surfaces. A movie of the joint PDFs for the values of  $(X, Y)^T$  and  $(R, \Theta)$  as given by expression (12) with  $\mu_y = 0$  and  $\sigma = 1$ , as  $\mu_x$  ranges from  $-5$  to  $5$  in steps of  $0.5$ , can be viewed. On the left of the movie is shown the evolution of the joint PDF for the value of  $(X, Y)^T$  (a bivariate Gaussian distribution) and on the right that of the corresponding PDF for the value of  $(R, \Theta)^T$ . A movie of the joint PDFs represented as contour plots, in place of elevated surfaces, can also be viewed.

### 3.3.4 Scatter plots

Some surfaces, especially approximations to PDFs generated using MCS, are represented by point clouds (unless further processing is used to provide, usually, continuous approximations). For the problem of concern, it is shown in appendix D that  $R$  and  $\Theta$  are mutually independent when the input quantities are mutually independent, and have zero expectations and equal variances.

Figure 3 shows 10 000 points sampled randomly from a PDF given by the product of two Gaussian PDFs, for the values of  $X$  and  $Y$ , each having mean zero and unit standard deviation, and the corresponding points in the magnitude-phase plane.

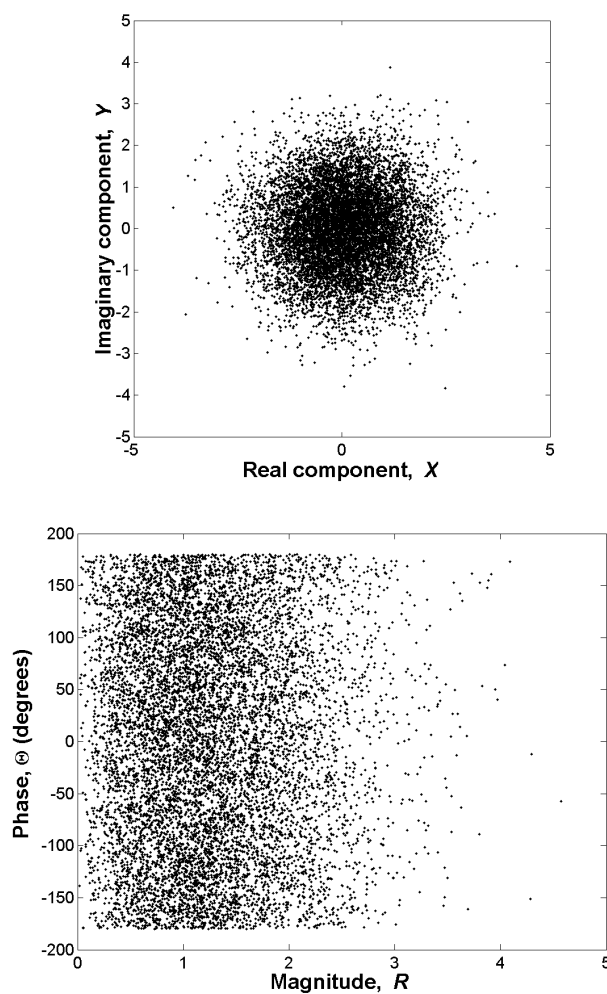


Figure 3: 10 000 points sampled randomly from a PDF given by the product of two Gaussian PDFs, for the values of  $X$  and  $Y$ , each having mean zero and unit standard deviation, and (bottom) the corresponding points in the magnitude-phase plane.

### 3.3.5 Scaled histograms

Because  $R$  and  $\Theta$  are mutually independent in the above instance, the joint PDF for the value of  $R$  and  $\Theta$  can be expressed as the product of the PDF for the value of  $R$  and that for  $\Theta$ . Thus, an approximation to the PDF for the value of  $R$  can be provided by presenting the (10 000)  $R$ -values obtained as a ‘scaled histogram’, with a similar statement for  $\Theta$ .

Figure 4 shows such an approximation to the PDF for the value of  $R$ . The range of  $R$ -values is divided into 20 sub-intervals of equal width. The area of a rectangle of the histogram is proportional to the number of  $R$ -values within the corresponding sub-interval, with the resulting histogram scaled to have an area of unity. The figure also shows the exact PDF, a Rayleigh distribution (section 3.2.3 and appendix D). Figure 4 also shows the counterpart for  $\Theta$ , for which the exact PDF is a rectangular distribution.

## 3.4 Interactive visualization

The above visualizations are not under the direct control of the human observer. Of course, a mild form of interaction is possible through the provision by the user of particular values for  $\mu_x$ , e.g., and the examination of the corresponding display.

This section presents an interactive tool, having several user controls, for visualizing co-ordinate system transformations.

### 3.4.1 Operating the visualization

Figure 5 contains a screen shot from the tool. The screen is subdivided into two parts. The left side of the tool relates to the model input quantities  $X$  and  $Y$ . It depicts a circular coverage region, shown as a red disc, corresponding to a required coverage probability  $p$ , for the values of  $X$  and  $Y$ . It also shows the controls that are used to choose  $\mu_x$ ,  $\mu_y$  and  $\sigma$ .  $\mu_x$  and  $\mu_y$  can be selected using the sliders or entered directly into the appropriate control boxes.  $\sigma$  is also entered using a control box on the lower left side of the tool. Of the two remaining control boxes on the lower left of the tool, ‘coverage probability (%)’ is used for  $p$ , and *Grid size* for the resolution to which the transformation is to be carried out. Higher values of *Grid size* result in more accurate results, but in longer computation times.

The right side of the tool relates to the output quantities  $R$  and  $\Theta$ . It shows a three-dimensional scene in which a  $100p$  % coverage region for the values of  $R$  and  $\Theta$  is displayed in a cylindrical co-ordinate system. This scene can be rotated, transformed, etc., as required, using the standard controls on the right part of the screen. If the cylinder is clicked, it will unroll and show a flat representation of

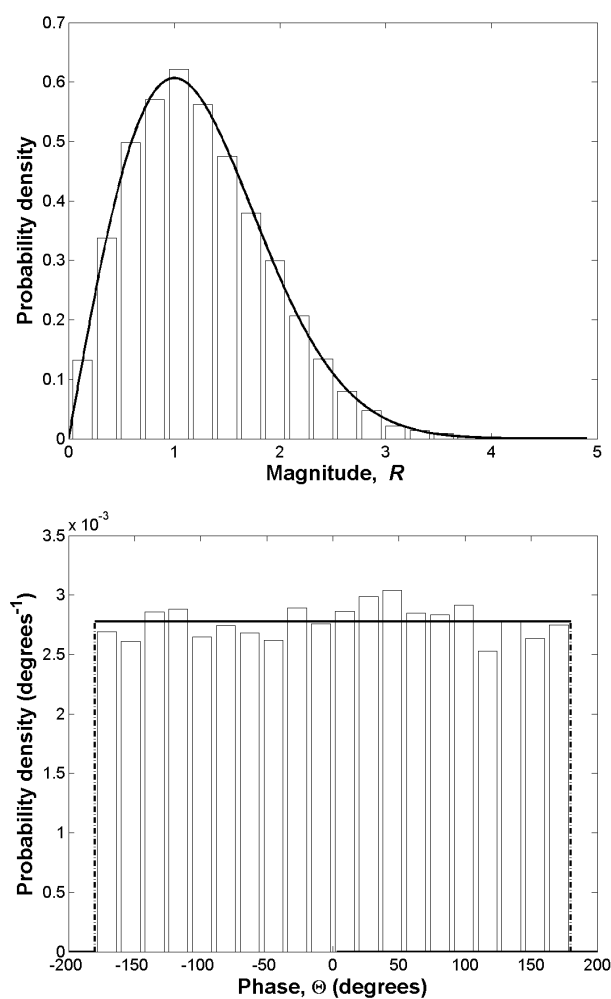


Figure 4: An approximation in the form of a scaled histogram to the PDF for  $R$  and the analytic PDF for  $R$ , a Rayleigh distribution, and (bottom) the corresponding approximation to the PDF for  $\Theta$ , with the exact PDF for  $\Theta$ , a rectangular distribution.

the cylindrical co-ordinate system with  $R$  in the vertical and  $\Theta$  in the horizontal direction. Clicking on this plane will cause it to roll up into a cylinder again.

### 3.4.2 How does the visualization work?

The tool for visualizing co-ordinate system transformations uses expression (12) in appendix D as the basis of the evaluation of a coverage region, corresponding to a required coverage probability  $p$ , for the values of  $R$  and  $\Theta$  in the following way.

Consider a  $100p$  % coverage probability (with  $p = 0.95$  for a 95 % coverage probability). The *smallest coverage region*, i.e., that of smallest area, corresponding to this coverage probability has a boundary curve given by the intersection of a plane parallel to the  $R$ - $\Theta$  plane and the joint PDF for  $R$  and  $\Theta$ . The ‘height’ of the plane is determined such that the integral of the PDF over the region bounded by the curve is equal to  $p$ .<sup>18</sup>

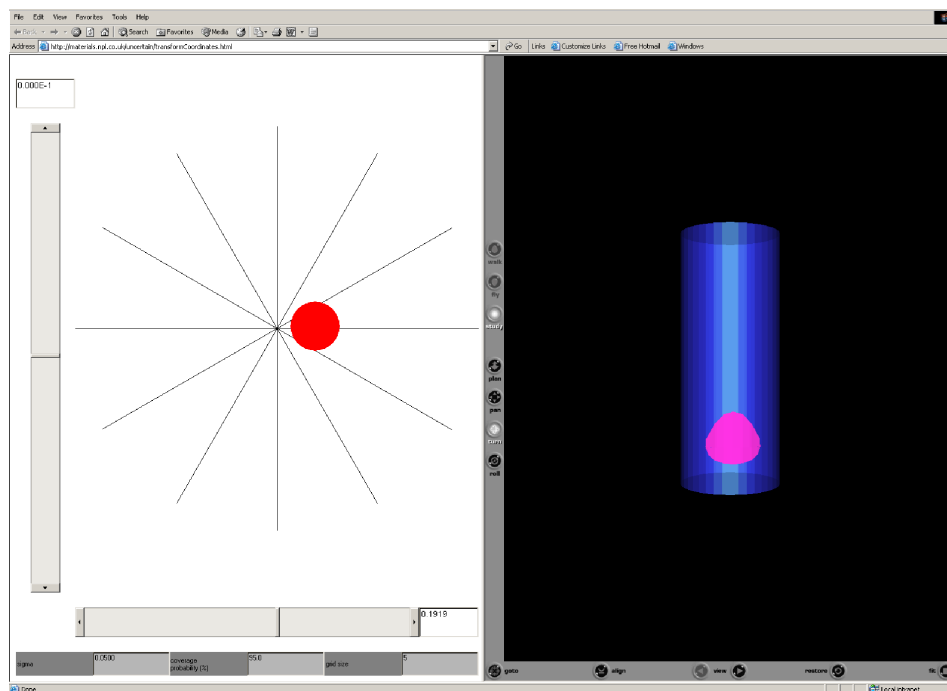


Figure 5: Screen shot of the tool for visualizing co-ordinate system transformations.

<sup>18</sup>By comparison, in the case of a univariate and unimodal PDF for the value of a quantity  $Z$ , say, the shortest coverage interval corresponding to the coverage probability  $p$  has endpoints given by the intersection of a line parallel to the  $Z$  axis and the PDF for  $Z$ . The line is chosen such that the integral of the PDF over the interval defined by the endpoints is equal to  $p$  [4].

### 3.5 Discussion on the various visualizations

Some comments are made on the respective merits of non-interactive and interactive visualization of a function in the context of this co-ordinate system transformation application (and other similar applications).

- A slice of a surface in three dimensions is a plane profile of a section of that surface. There is no distortion in viewing it, but it is literally a ‘snapshot’ of a single section of the surface.
- A movie (in the context considered here) constitutes a sequence of adjacent slices through a surface. Each frame of the movie (corresponding to a slice) displays the actual shape of that slice. To obtain a complete understanding of the surface, however, requires the viewer to ‘remember’ the whole sequence. Unless the variable being animated is time, the association of frames with a changing parameter rather than time can be difficult to appreciate. A movie emphasizes the variation with a particular choice of variable ( $\mu_x$ , e.g., as here). A more complete understanding would be obtained also by an additional movie involving ‘the other variable’. Limited interaction is possible through changing a parameter on which the movie depends, and re-viewing.
- A two-dimensional display such as an elevated display depicts the overall shape of the ‘complete’ function. The height of the surface at any point is proportional to the value of the function depicted by the surface at that point. There are likely to be ‘hidden regions’ (which can sometimes be revealed using a different viewing point). The display may or may not incorporate perspective effects. The consequent influence on the perceived ‘size’ of surface features should be taken into account.
- Contour plots are familiar (Ordnance Survey maps, weather forecasts, etc.) and therefore may be accepted as useful on this basis. They constitute a set of (generally curved) lines corresponding to constant surface height. These lines are sensitive to small fluctuations (compare the formation of puddles on a nominally flat surface), which can be advantageous in terms of highlighting fine features, but ‘annoying’ in that they can be considered too detailed in terms of the ‘overall picture’.
- The above visualizations are not interactive, since they are not under the direct control of the human observer. Of course, a limited form of interaction is possible through the provision by the user of particular values for  $\mu_x$ , e.g., and the examination of the corresponding visualization.
- An interactive visualization has the advantage that the observer has the opportunity to display the ‘object’ in a manner that is deemed appropriate to the application. The use of a limited set of viewpoints may paint an unfaithful

picture of the surface, however. Parts of the scene are likely to be obscured by other parts. For both reasons a detailed exploration using the provided facilities (roll, turn, zoom, etc.) is advised. For purposes of publication of results, one or more of the above forms of display may be more suitable. If, however, the publication is in the form of an electronic document such as the present document when viewed online, interactive visualization through that document is possible.

## 4 Comparison loss in microwave power meter calibration

This section is concerned with the study of comparison loss in microwave power meter calibration. As well as being important in its own right in the area, this problem has a number of features that satisfy the requirement to cover generic aspects and the way in which the understanding gained can be transferred to other areas of metrology.

There are two particular objectives:

1. Assess whether the power meter conforms to specification
2. Compare the use of LPU and MCS for evaluating the uncertainties.

### 4.1 Formulation phase

During the calibration of a microwave power meter, the power meter itself and a standard power meter are connected in turn to a stable signal generator. The power absorbed by each power meter will in general be different because their input voltage reflection coefficients are not identical. The ratio  $M$  of the power  $P_M$  absorbed by the power meter being calibrated and that,  $P_S$ , absorbed by the standard power meter is [29, 30]

$$M = \frac{P_M}{P_S} = \frac{1 - |\Gamma_M|^2}{1 - |\Gamma_S|^2} \times \frac{|1 - \Gamma_S \Gamma_G|^2}{|1 - \Gamma_M \Gamma_G|^2}, \quad (5)$$

where  $\Gamma_G$  is the voltage reflection coefficient of the signal generator,  $\Gamma_M$  that of the power meter being calibrated and  $\Gamma_S$  that of the standard power meter. This power ratio is an instance of ‘comparison loss’ [3, 21]<sup>19</sup>

Consider the simple case where both the standard and the signal generator are reflectionless, i.e.,  $\Gamma_S = \Gamma_G = 0$ , and where measurements are made of the real

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<sup>19</sup>Strictly, because  $M$  is a scalar quantity, it should be referred to as a *quotient*, a ratio being of the form  $a : b$ . The popular term will, however, be used here.

and imaginary parts, viz.,  $X$  and  $Y$ , of  $\Gamma_M = X + jY$ , where  $j = \sqrt{-1}$ . Since  $|\Gamma_M|^2 = X^2 + Y^2$ , the comparison loss in formula (5) becomes

$$M = 1 - |\Gamma_M|^2 = 1 - X^2 - Y^2. \quad (6)$$

The evaluation of uncertainty for this model of comparison loss is treated by applying LPU, and by using the propagation of distributions implemented using MCS.

Given are estimates  $x$  of  $X$  and  $y$  of  $Y$  from measurement. In general, the measurements are such that  $x$  and  $y$  are correlated. Let  $\rho(x, y)$  denote the corresponding correlation coefficient. Equivalently, the covariance associated with  $x$  and  $y$  is  $u(x, y) = \rho(x, y)u(x)u(y)$ . The nature of the measurements is such that  $\Gamma_M$  is assigned a bivariate Gaussian distribution in  $X$  and  $Y$  with mean  $(x, y)^T$  and uncertainty matrix

$$\begin{bmatrix} u^2(x) & \rho(x, y)u(x)u(y) \\ \rho(x, y)u(x)u(y) & u^2(y) \end{bmatrix}. \quad (7)$$

Required is an estimate  $m$  of the value of  $M$  and the associated standard uncertainty  $u(m)$ .

#### 4.1.1 Unquantified correlation

The current state of the art in electrical measurement for the quantities currently under discussion is that it is frequently difficult to quantify the correlation  $\rho(x, y)$  associated with the estimates of  $x$  and  $y$ . Indeed, because  $\rho(x, y)$  can in principle lie anywhere in the interval  $-1$  to  $+1$ , there is a temptation to assign a value to it that lies in the centre of this interval, i.e., the value zero. One argument in support of this choice is that in the absence of further information it is optimal in terms of its maximum possible deviation (unity) from the unknown value. Making this choice, however, is of some concern because the electrical engineer would wish to understand the influence of the lack of knowledge of  $\rho(x, y)$  on the uncertainty associated with the power meter calibration. Therefore, it is appropriate to examine the functional dependence of the measurement result and its associated uncertainty on  $\rho(x, y)$ .

The correlation is just one of the several quantities of concern to the electrical engineer, who generally wishes to understand the dependence of the uncertainty associated with an estimate of the value of a quantity as a function of a number  $n$  of parameters or variables. Consider the provision of an  $n$ -dimensional mesh of values of the quantities on which the uncertainty depends. Such a mesh would form the basis for various types of visualization. The mesh values would typically be provided by evaluating a model that often comprises as its inputs the values of the influence quantities and the associated uncertainties. The example below falls into this category.

#### 4.1.2 Frequency dependence

For this study, the ‘independent variables’ for a visualization would be  $u(x)$ ,  $u(y)$ ,  $\rho(x, y)$  and  $f$ , and the ‘dependent variable’  $u(m)$ . The first three such variables could be taken as spatial variables and  $f$  as a ‘time-evolution’ variable. Thus, a display would consist of the time evolution of the ‘shape’ of  $u(m)$  as a function of  $u(x)$ ,  $u(y)$  and  $\rho(x, y)$ .

In order to mimic plausible behaviour of  $x$  and  $y$ , consider a spiral formed using

$$\begin{bmatrix} x \\ y \end{bmatrix} = Cf \begin{bmatrix} \cos Kf \\ \sin Kf \end{bmatrix},$$

for suitable constants  $C$  and  $K$  and a range for the frequency  $f$ . Realistic values for these constants are  $C = 0.01 \text{ GHz}^{-1}$  and  $K = 20 \text{ GHz}^{-1}$ , with a range of frequencies  $f$  from 0 to 18 GHz. The resulting spiral starts at the origin and rotates clockwise as the frequency sweeps through its range, terminating at (0.18, 0). Figure 6 shows points on the spiral at frequencies 0, 1,  $\dots$ , 18 and the straight-line segments joining successive points.

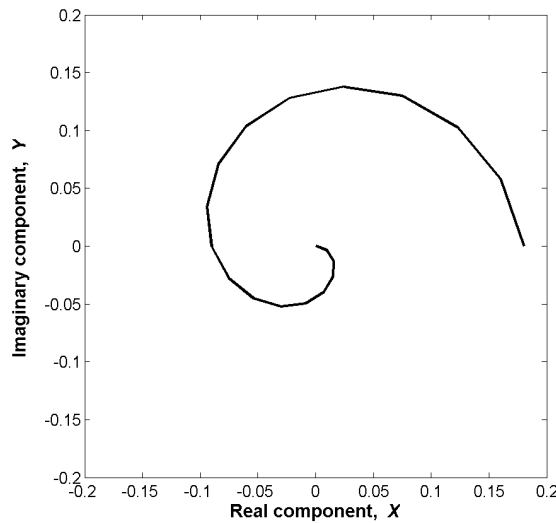


Figure 6: Straight-line segments joining points on the spiral  $[x, y] = Cf[\cos Kf, \sin Kf]$ , for  $C = 0.01 \text{ GHz}^{-1}$  and  $K = 20 \text{ GHz}^{-1}$ , at frequencies  $f = 0, 1, \dots, 18 \text{ GHz}$ .

#### 4.2 Calculation phase

The standard uncertainty  $u(m)$  associated with an estimate  $m$  of the value of  $M$  depends on  $x, y, u(x), u(y)$  and  $\rho(x, y)$ . Consider here the dependence on  $u(x), u(y)$

and  $\rho(x, y)$ , for particular choices of  $x$  and  $y$ .

The purpose of this section is to

- Specify the LPU and MCS evaluations of the standard uncertainty  $u(m)$  associated with an estimate  $m$  of  $M$  for given values of  $x$ ,  $y$ ,  $u(x)$ ,  $u(y)$  and  $\rho(x, y)$
- Specify, for given values of  $x$  and  $y$ , the calculation of the surface composed of those points

$$(u(x), u(y), \rho(x, y))^T$$

that correspond to a given (target) value of  $u(m)$ .

Details of how this information is used to provide the visualizations is given in section 4.3.2.

#### 4.2.1 The law of propagation of uncertainty

Applying the law of propagation of uncertainty,

$$u^2(m) = \left(\frac{\partial M}{\partial X}\right)^2 u^2(x) + \left(\frac{\partial M}{\partial Y}\right)^2 u^2(y) + 2 \left(\frac{\partial M}{\partial X} \frac{\partial M}{\partial Y}\right) u(x)u(y)\rho(x, y), \quad (8)$$

where all partial derivatives in the above expression are evaluated for  $X = x$  and  $Y = y$  [5, Clause 5.2.2]. It follows that

$$u^2(m) = 4x^2u^2(x) + 4y^2u^2(y) + 8xyu(x)u(y)\rho(x, y). \quad (9)$$

This expression permits  $u(m)$ , the standard uncertainty associated with the estimate  $m = 1 - x^2 - y^2$  of  $M$ , to be evaluated in terms of  $x$ ,  $y$ ,  $u(x)$ ,  $u(y)$  and  $\rho(x, y)$ .

A re-arrangement of expression (9) gives

$$\rho(x, y) = \frac{u^2(m) - 4x^2u^2(x) - 4y^2u^2(y)}{8xyu(x)u(y)}. \quad (10)$$

This expression permits points  $(x, y, u(x), u(y), \rho(x, y))^T$  defining the *iso-surface*  $u(m) = \gamma$  for specified  $\gamma > 0$  to be determined. Specifically, for a given  $u(m) = \gamma$ , form a  $N_x \times N_y \times N_{u(x)} \times N_{u(y)}$  hyper-rectangular mesh, and evaluate  $\rho(x, y)$  for each point on the mesh using expression (10).<sup>20</sup>

<sup>20</sup>Here, the suggestive notation  $N_x$  is used to denote the number of  $x$ -values, etc.

The following considerations arise in an implementation of the scheme described above for calculating points on an iso-surface relating to constant  $u(m)$ .

Firstly, given  $x$ ,  $y$ ,  $u(x)$ ,  $u(y)$  and  $u(m)$ , the computed value of  $\rho(x, y)$  must satisfy

$$-1 \leq \rho(x, y) \leq +1$$

for  $(x, y, u(x), u(y), \rho(x, y))^T$  to be a (valid) point on the iso-surface.

Secondly, for the cases  $x = 0$  or  $y = 0$  or  $u(x) = 0$  or  $u(y) = 0$ , either

- no value of  $\rho(x, y)$  satisfying expression (9) exists, e.g., if  $x = y = 0$  and  $u(m) \neq 0$ , or
- infinitely-many values satisfying expression (9) exist, e.g., if  $x = y = 0$  and  $u(m) = 0$ .

Finally, let  $\alpha = 2xu(x)$  and  $\beta = 2yu(y)$ . Then, expressions (9) and (10) become, respectively,

$$u^2(m) = \alpha^2 + \beta^2 + 2\alpha\beta\rho(x, y),$$

and

$$\rho(x, y) = \frac{u^2(m) - \alpha^2 - \beta^2}{2\alpha\beta}.$$

An iso-surface of *reduced* dimensionality, composed of points  $(\alpha, \beta, \rho(x, y))^T$ , can be formed using the variables in this expression. For any point on the surface,  $\alpha$  corresponds to any  $(x, u(x))$ -pair such that  $2xu(x) = \alpha$ , and similarly for  $\beta$ . In general, it can be worthwhile to inspect a model to see whether its dimensionality can be reduced.

#### 4.2.2 Monte Carlo simulation

A key task in the application of MCS to the problem formulated in section 4.1 is to be able to draw random samples  $(x_k, y_k)^T$ ,  $k = 1, \dots, N$ , where  $N$  is the number of Monte Carlo trials, from a bivariate Gaussian distribution with expectation  $(x, y)^T$  and uncertainty  $V_{x,y}$  given by expression (7). A way in which this task can be carried out is given in appendix C.

For each random sample  $(x_k, y_k)^T$  so obtained, the model (6) is used to determine corresponding values  $m_k$  of the output quantity, viz.,

$$m_k = 1 - x_k^2 - y_k^2, \quad k = 1, \dots, N.$$

The sample mean of these values of the output quantity, viz.,

$$\hat{m} = \frac{1}{N} \sum_{k=1}^N m_k$$

is taken as the estimate  $m$  of the value of the output quantity, and their sample standard deviation  $s$  obtained from

$$s^2 = \frac{1}{N-1} \sum_{k=1}^N (m_k - \hat{m})^2,$$

as the standard uncertainty  $u(\hat{m})$  associated with the estimate.

The above evaluation of  $\hat{m}$  and the associated uncertainty  $u(\hat{m})$  is repeated for each combination of values for  $x$ ,  $y$ ,  $u(x)$ ,  $u(y)$  and  $\rho(x, y)$ . Unlike the LPU calculation (section 4.2.1) there is no direct way to calculate, for given values of  $x$  and  $y$ , those points  $(u(x), u(y), \rho(x, y))^T$  that correspond to a given (target) value of  $u(\hat{m})$ . Instead, an ‘interpolation’ scheme is required to extract this information from the set of points  $(u(x), u(y), \rho(x, y), u(\hat{m}))^T$  corresponding to the given  $x$  and  $y$ .

### 4.3 Interactive visualization

A web-based interactive visualization of the ‘uncertainty surfaces’ obtained using LPU and MCS is available.<sup>21</sup> Information concerning its use is given below.

Figure 7 illustrates an example of a ‘surface’ of constant  $u(m)$  generated by this interactive visualization for a typical range of variation in  $u(x)$  and  $u(y)$ , the standard uncertainties associated with the real and imaginary parts of  $\Gamma_M$ . Since, as stated, establishing (even a coarse approximation to) the correlation coefficient  $\rho(x, y)$  associated with  $x$  and  $y$  is (in practice) very difficult, the vertical axis in the visualization is used to represent the full range  $[-1, 1]$  for this quantity.<sup>22</sup>

#### 4.3.1 Operating the visualization

There are two sets of controls available for operating the visualization. The first set, displayed on the left-hand side of the screen (figure 7), enables the user to move the visualization on the computer screen. These controls are labelled *Plan*, *Pan*, *Turn* and *Roll*, in accordance with the type of movement required by the user. Each control is activated by selecting (i.e., ‘clicking’) the appropriate on-screen icon. The visualization is then moved, using the selected control, by the user clicking and dragging across the active area of the visualization.

The second set of controls, displayed on the right hand side of the screen (see figure 8 for a magnified image), enables the user to alter the parameters used

<sup>21</sup>Henceforth, the surface obtained using LPU will be referred to as the ‘LPU surface’ and that obtained using MCS as the ‘MCS surface’.

<sup>22</sup>The label ‘ $r(x, y)$ ’ is used on the vertical axis (in place of ‘ $\rho(x, y)$ ’) in the visualization tool.

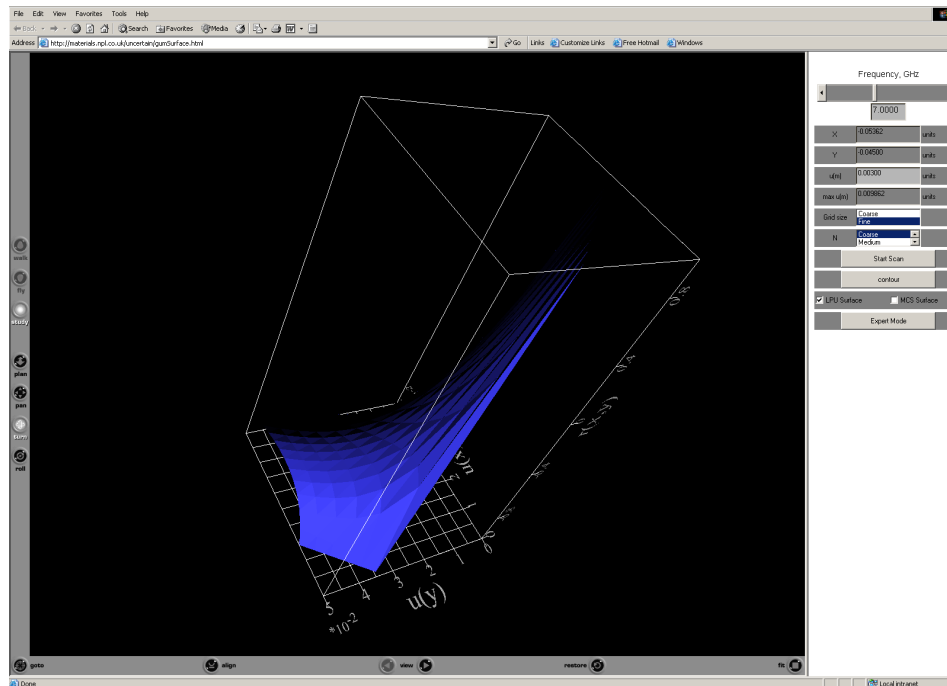


Figure 7: Illustrative surface and controls for a surface of constant standard uncertainty  $u(m)$  associated with comparison loss.

to generate the visualization. These controls are labelled *Frequency*, *X*, *Y*, *u(m)*, *max u(m)*, *Grid size* and *N*. In addition, there are ‘buttons’ labelled *Start Scan*, *contour*, *LPU surface*, *MCS surface* and *Expert mode*. Each of these controls and buttons is explained below.

## Controls

**Frequency.** A slider allowing frequencies to be accessed at integer GHz values ranging from 0 to 18. Alternatively, any frequency value can be entered manually into the box immediately below the slider.

**X and Y.** Values determined automatically, based on the selected frequency and the ‘spiral’ model (section 4.1.2). They are used to simulate the behaviour of a typical power sensor. The use of simulated values for *X* and *Y* is adequate for the purposes of this ‘demonstrator model’ of the visualization software—a ‘production version’ would be modified to import values of *X* and *Y* direct from measurements made using laboratory instruments such as Vector Network Analyzers.

**$u(m)$ .** Required value of  $u(m)$ . The uncertainty surface will only appear on the

Frequency, GHz

7.0000

|                                                 |                                      |       |
|-------------------------------------------------|--------------------------------------|-------|
| X                                               | -0.05362                             | units |
| Y                                               | -0.04500                             | units |
| u(m)                                            | 0.00300                              | units |
| max u(m)                                        | 0.009862                             | units |
| Grid size                                       | Coarse<br>Fine                       |       |
| N                                               | Coarse<br>Medium                     |       |
| Start Scan                                      |                                      |       |
| contour                                         |                                      |       |
| <input checked="" type="checkbox"/> LPU Surface | <input type="checkbox"/> MCS Surface |       |
| Expert Mode                                     |                                      |       |

Figure 8: Magnification of the controls in figure 7.

computer screen if  $u(m) < \max u(m)$ , otherwise a warning message is displayed.

**$\max u(m)$ .** Maximum calculated value for  $u(m)$  occurring within the scale ranges set for the visualization, i.e., the displayed ranges for  $u(x)$  and  $u(y)$ . It is determined automatically.

**Grid size.** *Coarse* or *Medium*—*Coarse* being the default setting. It determines the number of points on a grid within the visualization ‘space’ where uncertainty evaluations are performed. *Medium* will generally produce smoother surfaces, but will increase the time taken to compute the surfaces.

**$N$ .** *Coarse*, *Medium* or *Fine*, corresponding, respectively, to  $N = 1\,000$ ,  $10\,000$  and  $100\,000$ . It determines the number  $N$  of Monte Carlo trials used to perform the MCS calculation. *Fine* should be used to obtain the most accurate results, although the time taken to compute the MCS surface will be greater. *Coarse* or *Medium* settings are recommended when exploring general features in the computed surfaces.

## Switches

**Start Scan.** Allows the frequency to be ‘swept’ automatically, in real time, in integer GHz values, from 1 to 18. Only the ‘LPU surface’ is displayed, since the computation of the MCS surface can take considerable time. The scan can be stopped at any time by pressing the *Cancel* button, which replaces the *Start Scan* button during the scanning process.

**Contour.** Presents a series of ‘slices’ through the uncertainty surfaces at values of correlation coefficient,  $\rho(x, y)$ , corresponding to  $-1.0$ ,  $-0.5$ ,  $0.0$ ,  $+0.5$  and  $+1.0$ . Each slice shows a two-dimensional grid, with axes  $u(x)$  and  $u(y)$ , with contour lines for different values of  $u(m)$ . The numbers on these contour lines correspond to the scale of values for  $u(m)$ , from zero to  $\max u(m)$ , given at the bottom of the screen. An additional contour line, shown in green, is the contour line corresponding to the value for  $u(m)$  selected by the user and displayed as the surface in the main visualization window. Slices through both LPU and MCS surfaces can be displayed using the *Contour* option. However, to display slices through the MCS surface, the MCS surface button must first be pressed (below).

**LPU surface.** A switch allowing the LPU surface to be turned on or off, i.e., displayed or not displayed in the visualization.

**MCS surface.** A switch allowing the MCS surface to be turned on or off. Note that the MCS surface must be re-calculated and re-displayed each time there is a change in the values in the parameter list, e.g., *frequency*, *Grid size* or  $N$ ,

but not  $u(m)$ .<sup>23</sup> This aspect is most important, since any MCS surface that is already shown, but has not been re-calculated and re-displayed, is likely to be based on previous parameter value settings and will therefore, in general, not be the correct surface for the modified display.

**Expert mode.** Provides access to a larger set of controls and buttons. Under normal circumstances, the user should not need to access these extra features, since they are intended for diagnostic and training purposes.

#### 4.3.2 How does the visualization work?

To calculate the LPU surface, formula (10) of section 4.2.1 is evaluated over a two-dimensional grid of values of  $u(x)$  and  $u(y)$  for given values of  $x$ ,  $y$  and  $u(m)$ . Where the surface intersects the  $\rho(x, y) = \pm 1$  planes, interpolation is used to determine the position of the free edge of the surface. The surface is then displayed using flat shading.

To calculate the MCS surface, the MCS procedure described in section 4.2.2 is applied over a three-dimensional grid of values of  $u(x)$ ,  $u(y)$  and  $\rho(x, y)$  for given values of  $x$  and  $y$ . A marching-cubes algorithm [23] is used to find the iso-surface corresponding to the specified value of  $u(m)$ . This surface is then displayed in a similar manner to the GUM surface using flat shading.

#### 4.4 An ‘engineering’ interpretation

When verifying the performance of a power sensor for use at RF and microwave frequencies (e.g., by testing the sensor with respect to a specification limit) it is necessary to determine the ‘mismatch’ comparison loss for the sensor. In general, this measurement will be a function of several different quantities (namely, the reflection coefficients of the measurement source, a reference power sensor and the sensor under test). However, under certain circumstances, only the reflection coefficient of the sensor under test need be considered. The ‘mismatch’ comparison loss  $M$  of the power sensor can then be determined from expression (6), where  $\Gamma_M$  is the complex voltage reflection coefficient of the sensor under test.<sup>24</sup>

Therefore, in order to determine whether a given sensor has met a specification value for its comparison loss, it is necessary to obtain a measurement of  $\Gamma_M$ .

<sup>23</sup>To indicate this requirement, a dialogue box, containing the message ‘Update MCS surface—you need to recalculate the MCS data’, appears automatically whenever there has been a change in the parameter list settings. A re-calculation is initiated by clicking the ‘continue’ button in this dialogue box.

<sup>24</sup>This ‘special case’, although not fully representative of all the intricacies of a sensor’s comparison loss determination, is useful for illustrating the consequences of measurement effects having possible mutual interactions during the measurement process.

Since  $\Gamma_M$  is a complex-valued quantity, this is equivalent to determining two ‘quantities’ simultaneously (i.e., the real and imaginary parts of  $\Gamma_M$ ), along with the associated uncertainty matrix of order two required to represent the uncertainty associated with the measurement.<sup>25</sup>

The uncertainty associated with  $\Gamma_M$  needs to be taken into account when assessing whether the measured comparison loss of the power sensor meets the target specification. Therefore, the operator testing the power sensors (or the designer of the equipment used to perform the test) needs to know, for a given measurement of  $\Gamma_M$ , over what range of values the uncertainty components associated with  $\Gamma_M$  can vary for the sensor’s measured ‘mismatch’ comparison loss to be within a given specification limit. Therefore, for a given measurement  $\Gamma_M$ , the following steps are undertaken:

1. Determine an estimate  $m$  of the value of the sensor’s comparison loss  $M$  (from the measurement of  $\Gamma_M$ ).
2. Check whether  $m$  lies ‘within’ (i.e., is greater than) the comparison loss specification limit  $M_{\text{spec}}$ , i.e., whether  $m > M_{\text{spec}}$ .
3. If the answer is affirmative, determine the amount by which  $m$  exceeds  $M_{\text{spec}}$  to establish an upper limit for the *expanded* uncertainty  $U(m)$  that can be tolerated<sup>26</sup> in the assessment of  $m$  against the specification,<sup>27</sup> i.e.,

$$U(m) \leq m - M_{\text{spec}}. \quad (11)$$

4. If the answer is negative, regard the sensor as unsatisfactory, since its performance is inconsistent with the specification limit.

The designer is therefore interested in those combinations of components of the uncertainty associated with  $\Gamma_M$  that can be accommodated in keeping with inequality (11).

<sup>25</sup>This uncertainty matrix will contain all the necessary information to obtain the uncertainties associated with the real and the imaginary parts, and the correlation coefficient characterizing the degree of mutual dependence between them.

<sup>26</sup>This situation occurs, for example, when a designer of a product’s test bench needs to establish the level of uncertainty that can be tolerated by a given test in order that a certain type of product can be tested in an efficient manner. This decision can affect both the choice of test type and test equipment used to ensure adequate quality control (i.e., including both economic and scientific factors in the decision concerning the fitness for purpose of the test).

<sup>27</sup>The symbol  $U$  represents an expanded uncertainty corresponding to a suitable coverage probability  $p$ . For most cases of compliance assessment against a specification limit (in this area of testing),  $p$  is often taken as 95 %. (This form of compliance assessment is often called ‘inset limits’.)

#### 4.4.1 Example 1—determining compliance to specification

The specification limit for a sensor's ‘mismatch’ comparison loss, at 12.247 GHz, is given as 97.5 %, i.e.,  $M_{\text{spec}} = 0.975$ . This is the smallest value of comparison loss for the sensor to be within its specification.<sup>28</sup>

During the test measurements on the sensor, the real and imaginary parts of  $\Gamma_M$  were found to be  $(-0.052, 0.111)$ , and hence  $|\Gamma_M|^2 = 0.015$ . The mismatch comparison loss is therefore measured as

$$m = 1 - |\Gamma_M|^2 = 0.985.$$

The expanded uncertainty  $U(m)$  associated with the ‘mismatch’ comparison loss measurement must conform to

$$U(m) \leq m - M_{\text{spec}} = 0.985 - 0.975 = 0.010$$

to ensure that this sensor falls within specification. The visualization (figure 9) is used to assist in identifying those combinations of  $u(x)$ ,  $u(y)$  and  $\rho(x, y)$  that satisfy the condition  $u(m) = 0.005$ .<sup>29</sup> These combinations can be seen by inspecting the contour ‘slices’ through the visualization surface, as can general trends indicated by the surface as a whole.<sup>30</sup> If the choices are limited to instances where  $u(x) = u(y)$ , it is appropriate to see where the *straight line*  $u(x) = u(y)$  intersects the contour  $u(m) = 0.005$ .<sup>31</sup>

Now, if, for example,  $u(x) = u(y) = 0.02$  can easily be achieved, but no indication of the value of  $\rho(x, y)$  is available, the following situations can be seen from the contour slices:

| $\rho(x, y)$ | $u(m)$          | The product                              |
|--------------|-----------------|------------------------------------------|
| −1           | $> 0.005$       | Probably rejected as non-compliant       |
| −0.5         | $> 0.005$       | Probably rejected as non-compliant       |
| 0            | $\approx 0.005$ | Compliance cannot be clearly established |
| 0.5          | $< 0.005$       | Can be accepted as compliant             |
| 1            | $< 0.005$       | Can be accepted as compliant             |

<sup>28</sup>During this example, for simplicity, only the ‘LPU surface’ is considered.

<sup>29</sup>Assuming a Gaussian distribution is assigned to the value of  $M$ , and  $p$ , the coverage probability, is 95 %, it follows that  $U(m) = k_{0.95}u(m)$ , where  $k_{0.95} \approx 2.0$  [5]. For the purposes of this ‘demonstrator model’ of the visualization software, the standard uncertainty  $u(m)$ , rather than the expanded uncertainty  $U(m)$ , is visualized. A production version of the software would provide a visualization of  $U(m)$ , which is the more useful quantity for verifying the performance of a power sensor.

<sup>30</sup>It is important to examine the entire surface for the presence of any unusual behaviour that may be present at values of  $\rho(x, y)$  between the contour ‘slices’. Such behaviour includes cusps, singularities, inflections and any other rapid variations in the shape of the surface as a function of  $\rho(x, y)$ .

<sup>31</sup>This is a realistic limitation in the uncertainty structure. It is used currently in PIMMS [28], NPL’s Primary Impedance Microwave Measurement System.

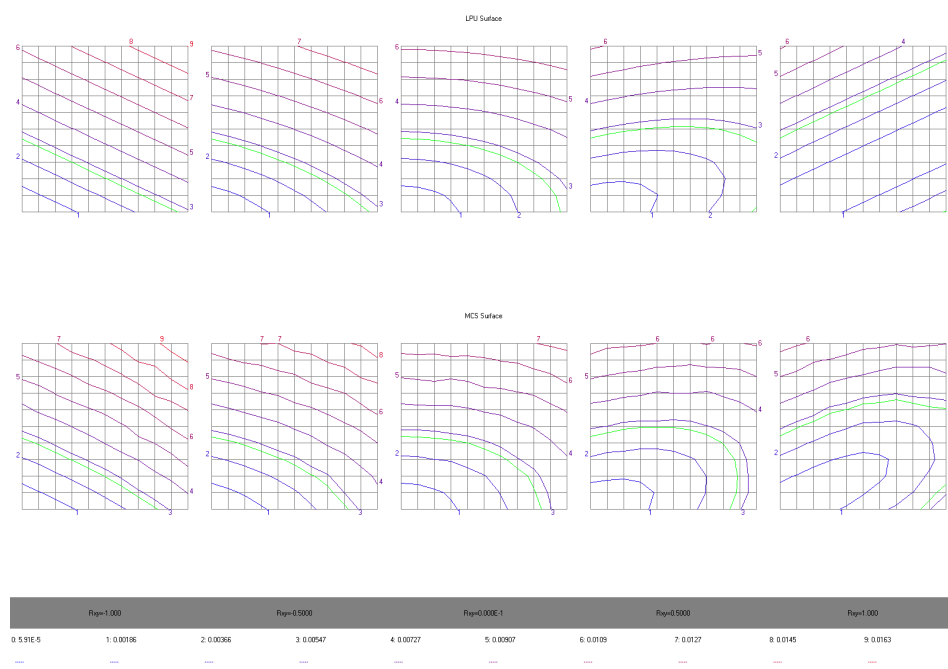
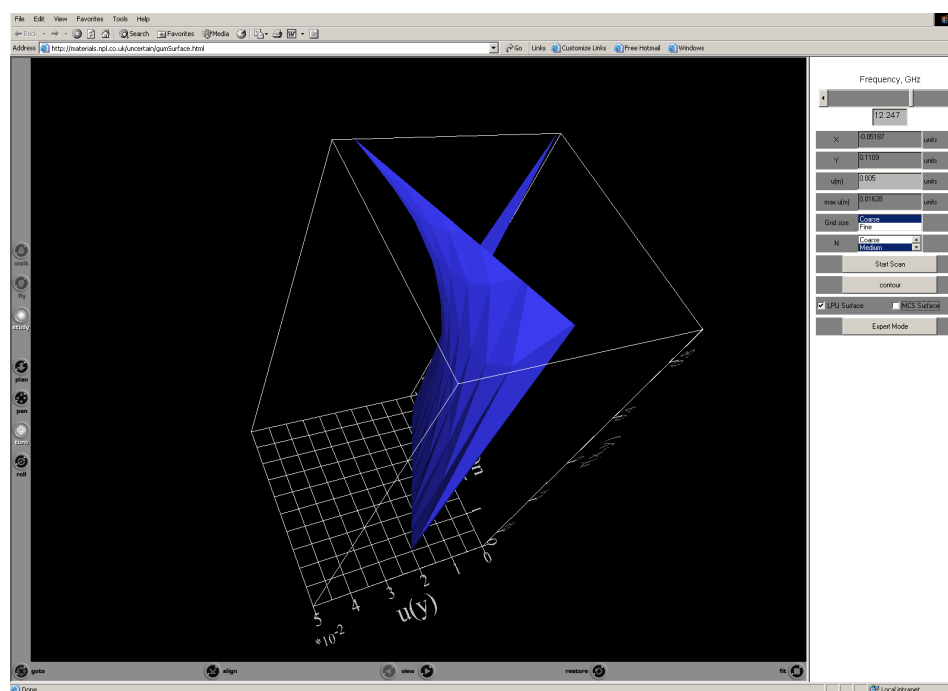


Figure 9: The LPU surface corresponding to a frequency of 12.247 GHz and  $u(m) = 0.005$ , and (bottom) the contours defining the LPU surface and the corresponding MCS surface. The MCS surface is obtained using the 'medium' setting of  $N = 10\,000$  trials.

In order to demonstrate satisfactory compliance with the specification, regardless of the value of  $\rho(x, y)$ , the uncertainty associated with  $\Gamma_M$  must be reduced so that  $u(x) = u(y) < 0.015$ . Such a reduction could be achieved, for example, by using better test equipment to perform the measurements, or by carrying out investigative work to reduce key components in the equipment's uncertainty budget.

#### 4.4.2 Example 2—validating the LPU calculation

Having established the criteria for compliance to the specification in the above example, it is important to verify the calculation used to generate the  $u(m)$  surface. Such a verification can be made by comparison with a surface generated by MCS.

To implement MCS, it is advisable to set the number  $N$  of Monte Carlo trials to a suitable value. If  $N$  is too small, e.g.,  $N = 100$ , the calculation will be subject to considerable sampling error and result in unreliable results. If  $N$  is too large, e.g.,  $N = 10^6$ , the calculation can take too long to complete. The visualization allows the operator to select from three preset values of  $N$ , labelled *Coarse*, *Medium* and *Fine*.<sup>32</sup>

In practice, the *Coarse* and *Medium* settings can be used to detect whether there are any serious discrepancies between the surfaces generated using the LPU and MCS calculation methods. These settings allow the MCS surface to be computed in a relatively short period of time. However, using these settings, the computed MCS surface may appear to be somewhat crinkled. This effect is particularly likely to occur when using the *Coarse* setting. The crinkling is due to the relatively small sample size used to perform the MCS calculations for these settings. Any crinkles should not be confused with systematic discrepancies between the LPU and MCS surfaces, the primary purpose of the validation process using MCS being the detection of systematic differences between the surfaces. Therefore, to investigate more fully any systematic discrepancies, the *Fine* setting should be used for the MCS calculation. However, the consequence will be that the MCS surface will take much longer to compute, e.g., ten minutes or more.

In Example 1, above, the  $u(m)$  surface generated using MCS is 'sufficiently' similar<sup>33</sup> in appearance to that generated using LPU to provide a satisfactory validation for the latter calculation method on this occasion.<sup>34</sup> The similarity between the computed surfaces is because both calculation methods (based on expression (6))

<sup>32</sup>These settings correspond to  $N = 1\,000$ , for *Coarse*,  $N = 10\,000$ , for *Medium*, and  $N = 100\,000$ , for *Fine*.

<sup>33</sup>Judging similarities between surfaces is a rather subjective exercise and requires a significant degree of interpretation by the operator. Generally, under such circumstances, it may be more desirable to establish objective criteria for assessing similarity between such surfaces.

<sup>34</sup>There is some departure between the surfaces for values of the correlation coefficient close to unity.

produce comparable results when the value of  $|\Gamma_M|$  is significantly greater than zero. However, as  $|\Gamma_M|$  approaches zero, appreciable systematic differences between the results produced using the LPU and MCS methods (and hence the generated surfaces) begin to occur. These differences can be seen, for example, at frequencies of 1 GHz and below, where the value for  $|\Gamma_M|$  becomes less than 0.01.<sup>35</sup>

To illustrate this effect (figure 10), repeat the steps followed in example 1, except at a frequency of 1 GHz, and consider a case in which (a)  $u(m) \leq 0.001$  is now required to determine a compliant product, (b)  $u(x) = u(y) = 0.03$  is achieved for the measurement of  $\Gamma_M$ .

In this example, there are appreciable differences between the surfaces obtained from the two calculation methods. Furthermore, if the surfaces are used as the basis of the product test, the following situations can be seen from the contour slices:

| $\rho(x, y)$ | Uncertainty calculation method |             |         |             |
|--------------|--------------------------------|-------------|---------|-------------|
|              | LPU                            |             | MCS     |             |
|              | $U(M)$                         | Test result | $U(M)$  | Test result |
| -1           | < 0.001                        | Pass        | > 0.001 | Fail        |
| -0.5         | < 0.001                        | Pass        | > 0.001 | Fail        |
| 0            | < 0.001                        | Pass        | > 0.001 | Fail        |
| +0.5         | < 0.001                        | Pass        | > 0.001 | Fail        |
| +1           | < 0.001                        | Pass        | > 0.001 | Fail        |

Thus, on this occasion, the method chosen to perform the calculations (i.e., either LPU or MCS) has a dramatic effect on the outcome of the product test. (This outcome is irrespective of the assumed value for the correlation coefficient  $\rho(x, y)$ .) The reason for the effect is that, under these circumstances, non-linearities in expression (6) become significant and so can no longer be ignored. It therefore becomes inappropriate to use the LPU calculation method (which uses implicit assumptions concerning linearity) to perform the uncertainty calculations for this example, and so the MCS method must be used instead.<sup>36</sup>

It is suggested that the LPU calculation method should be used to explore the general behaviour of the uncertainty surfaces generated by the visualization. This suggestion is made because the calculation method is quick to complete and therefore allows the operator to make observations in a timely manner. However, having made general observations concerning the behaviour of the calculated uncertainty

<sup>35</sup>At these low frequencies, it may become necessary to adjust the value of  $u(m)$ , so that it is less than  $\max u(m)$ , in order for the visualization to display the calculated surfaces.

<sup>36</sup>If the LPU calculation method is used (as this is often the method of choice for such calculations) then this example shows that the product test would cause non-compliant product to be accepted (in other words, defective products would be passed as good products).

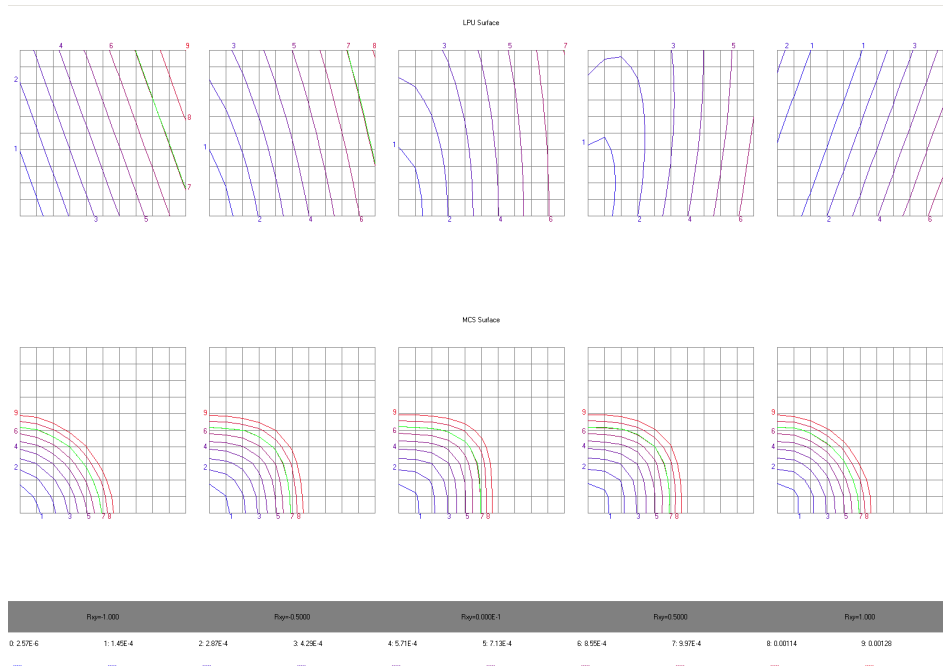
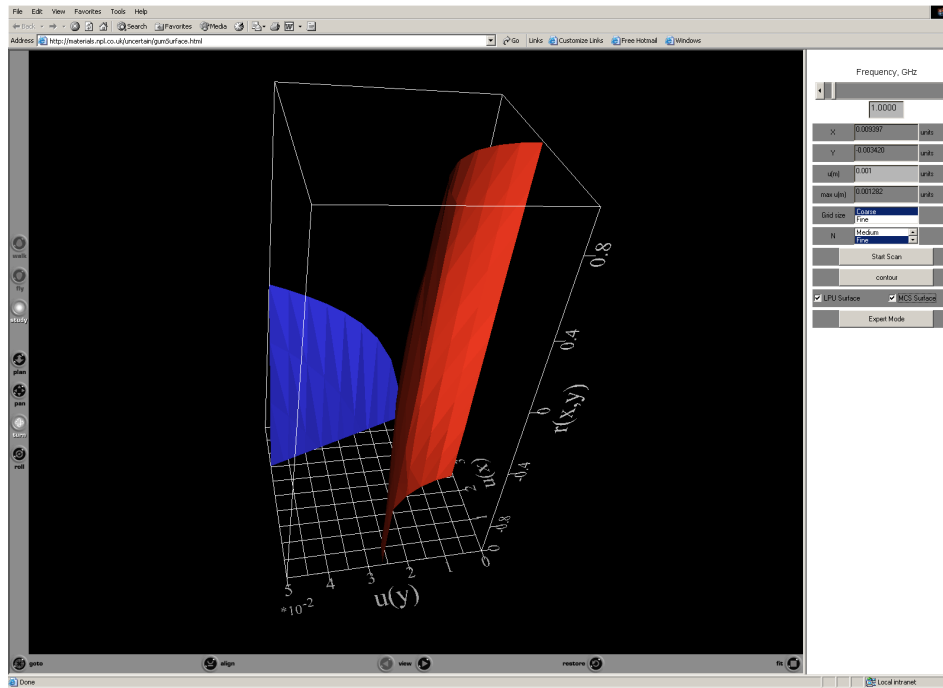


Figure 10: The LPU (blue) and MCS (red) surfaces corresponding to a frequency of 1 GHz and  $u(m) = 0.001$ , and (below) the contours defining the surfaces. The MCS surface is obtained using the ‘fine’ setting of  $N = 100\,000$  trials.

surfaces, it is essential to validate these observations (and any subsequent judgements based on these observations) using the MCS calculation method.

## Disclaimer

In developing the visualizations presented in this document, the authors have performed a range of tests to validate aspects of the visualizations, concentrating mainly on verifying the validity of the mathematical operations underlying the results generated to demonstrate the differences between the LPU and MCS methods of evaluating uncertainties. However, a full validation of every stage of the visualization has not been carried out and the software has not been subjected to NPL's Quality Assurance Procedures. The reader is therefore advised to exercise caution in the interpretation and use of the results and not to take any action based on the results presented here without independent verification.

## 5 Conclusions

This report has considered the visualization of uncertainty regions for vector and multidimensional data, viz., for instances of discrete modelling. It has done so by considering two case studies from the areas of electromagnetic metrology and electrical engineering. The first case study concerns co-ordinate system transformations, as arise in converting measurements from Cartesian (real and imaginary) co-ordinates to polar (magnitude and phase) co-ordinates. The other concerns microwave power meter calibration, particularly the determination of 'comparison loss', as is necessary when testing the performance of a power sensor for use at RF and microwave frequencies with respect to a specification limit.

One aim of the work has been to use visualization to help *educate* a user undertaking such calculations. For example, the visualizations provided as part of the co-ordinate system transformation study show effectively and efficiently the limitations of using LPU to propagate distributions through such transformations. The PDFs that are displayed for the values of magnitude and phase angle are (except in certain circumstances) manifestly different from normal distributions.

A second aim has been to use visualization to assist a user to make *informed* decisions about the result of a measurement. For example, the visualizations provided as part of the comparison loss study permit a user to investigate the uncertainty associated with the measurements (of the components of the reflection coefficient  $\Gamma_M$  of a sensor) that can be tolerated in order for the sensor to pass a product test, and to do so in cases where there is no knowledge about the correlation associated with the measurements.

A number of approaches to undertaking the visualizations have been explored. These include

- (static) two-dimensional plots, e.g., ‘slices’, scatter plots, contour plots, histograms, etc.,
- (static) three-dimensional plots, e.g., elevated surfaces,
- movies in which, e.g., an elevated surface is viewed as an ‘evolution’ of slices,
- three-dimensional plots with controls to allow, e.g., the user to change the viewpoint for the visualization, and
- tools which allow, e.g., the user to modify the ‘data’ that controls the object displayed.

For many problems, as demonstrated by the case studies considered here, it is likely that the use of a combination of these approaches will be required to give most benefit.

Some consideration has been given to the *validation* of visualizations, including the software used for this purpose. Validation is an issue that is important to metrologists, who need to have confidence in the software they use to provide visual representations of objects, functions and relationships, in order that the metrologist is not misled. This is an issue that will require further attention.

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## A The propagation of distributions

The propagation of distributions based on a model of measurement is a viable approach to uncertainty evaluation for three reasons [10]. One, it is consistent with the GUM, falling in the category of the ‘other analytical or numerical methods’ [GUM Clause G.1.5] permitted by it. Two, it provides a more general capability than that given by LPU as described in the GUM [5]. Indeed, the Joint Committee for Guides in Metrology, with its responsibility for the GUM, has prepared a supplemental guide [4] to the GUM on the propagation of distributions. Three, the use of Monte Carlo simulation (MCS) for its broad implementation is feasible because of the power and availability of personal computers.

Consider a model of a measurement in the form of a relationship between a set of mutually independent input quantities and the output quantity.<sup>37</sup> The model can be used to provide the value of the output quantity corresponding to values of the input quantities.

The input quantities are known inexactly. It is required to examine the effect on the value of the output quantity of this imperfect knowledge. This knowledge would be quantified in any one particular situation by assigning probability density functions (PDFs) to the values of the input quantities [5, Clause 4]. The inexactness of the value of the output quantity can also be expressed in terms of a PDF.

The determination of the PDF for the value of the output quantity from the PDFs for the values of the input quantities is known as the propagation of distributions. The expectation of the PDF for the value of the output quantity is taken as the best estimate of the value of the output quantity and the standard deviation of this PDF as the standard uncertainty associated with the estimate. Coverage intervals for the value of the output quantity can also be obtained from the distribution function (DF), viz., the indefinite integral of the PDF.

An estimate of the value of the output quantity is conventionally obtained [5, Clause 4.1.4] by evaluating the output quantity at the estimates (expectations) of the values of the input quantities. However, since a PDF rather than a single number describes the value of each input quantity, an equally legitimate value is given by sampling at random from that PDF. The value of the output quantity so obtained is a valid estimate of the value of the output quantity.

MCS, the most effective general numerical method for the propagation of distributions, involves generating a large number of values of the output quantity. This large number of values is used to approximate the DF for the value of the output quantity, from which the above quantities can be formed. From this approximation to the DF, an approximation to the PDF can be obtained if required.

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<sup>37</sup>Mutually dependent input quantities can also be handled.

The approach extends to problems with more than one output quantity. For each sample taken at random from the PDFs for the value of the input quantities, the corresponding value of the model is determined. The resulting (joint) distribution approximates the distribution for the values of the set of output quantities.

## **B Validating visualizations**

It is possible to produce good, useful scientific visualizations and bad, misleading visualizations [6]. Computer-produced visualizations are also subject to this risk, and errors in visualization software can easily be missed [19]. It is therefore essential that the software that produces visualizations be validated and tested, and that the results of the validation and testing activities be documented and made available to the users of the software.

### **B.1 General issues**

Two types of generic problem exist: the visualization software does not implement the programmer's intention, and the software performs differently from the expectations of the scientist using it [37]. Visualization software projects should thus be approached in the same manner as any other software development project, with the preparation of a user specification and functional specification and the definition of a comprehensive test plan to address these two problems. This specification process needs also to take into account the purpose of the visualization. Is it to give a qualitative understanding of some phenomenon of interest or is the aim to display a definitive representation of an experimental or theoretical result, perhaps including the uncertainties associated with that result? In the context of visualization research, little attention seems to have been paid to the question of visualizing uncertainties [26], at least due partly to the inherent difficulty of defining, characterizing and controlling uncertainty in the visualization process. Not only are there uncertainties associated with the original data, but the process of transforming, interpolating and rendering the data also introduces further sources of uncertainty [26].

The validation of visualization software has to address three questions: the correctness of the original data and of the mathematical manipulations that have been performed on the data, the manner in which the visualization software represents and transforms the data, and the way in which the user of the software understands and interprets the results of the visualization. It is the second and third topics that introduce challenges that go beyond those normally encountered in validating software. The canonical texts within the discipline of visualization tend to concentrate on the third question, which is concerned with communication, i.e., how to assist the user in understanding the information being presented and to avoid misleading the viewer by creating the wrong impression of the data [33, 34, 35]. The validation process itself is not discussed. Nevertheless, it is useful to consider whether validation and testing techniques which have been developed for model validation in other areas of mathematical and software research can be adapted for use in verifying visualizations. The Software Support for Metrology (SSfM) programmes have

produced guides and reports that are of assistance here. The best-practice guide on modelling [1] (incorporating an earlier guide on discrete model validation) defines the validation process as determining whether the results produced are consistent with the input data, theoretical results, reference data, etc. A key question to be considered is whether the model encapsulates all that is known about the system. In addition, does the model demonstrate both internal and external consistency? A model is considered to be internally consistent if its outputs are valid as long as its inputs are valid. External consistency refers to the process of comparing the outputs of the model with other sources of information such as experimental data or other prior information. A model is externally consistent if it is not contradicted by other valid information.

The approach outlined in the previous paragraph has recently been extended to the validation of continuous models [16]. It is recommended that the knowledge and intuition of metrologists should be formally incorporated into the validation process as part of the process of determining internal consistency [16]. The question of whether a result ‘looks right’ or ‘looks wrong’ to an experienced metrologist can be considered to be a valid test. Often, the results of such tests cannot be easily quantified. They are probably most effectively used as a simple ‘pass/fail’ criterion for the model in question, especially when the tests are essentially subjective and two metrologists may not agree, but the tests are nevertheless important. Questions that can be considered in this way concern whether the global properties of the model look right. Are results the right order of magnitude? Do they have the correct sign? Are shapes, sizes and locations of key features correct? Is the behaviour as expected at boundaries, edges and corners? Are there singularities in the model and does the model behave as expected in the region of such singularities? Do zeros and maxima appear in appropriate locations? Is asymptotic behaviour captured correctly? Do different ways of presenting the same data demonstrate consistent results? These questions are directly applicable to visualizations and should be built into visualization test plans.

Clearly, the kinds of test described can be applied most straightforwardly to representations of geometric objects and to experimental and theoretical results that relate to geometrical objects, such as stress fields in an engineering component, or representations of electrical, acoustic, pressure or temperature fields in space. When what is being represented is a purely mathematical object, as is the case in the work reported here, tests based on prior knowledge or intuition may be more difficult to carry out.

The visualization software and the computer screen itself, a two-dimensional surface, produce their own problems. Everyone is familiar with optical illusions which demonstrate that the human eye and brain can be deceived by images, leading to erroneous conclusions about what is being seen. Often such effects arise from tricks of perspective, in which the brain appears to use information it has about the three-dimensional world to re-interpret two-dimensional representations. The question

to be considered during validation, therefore, is whether incorrect results are being masked by the way in which the observer views the image. Alternatively, are the results correct, but is the observer being deceived by the way the brain perceives the image?

A second problem associated with the visualization itself is that of the level of discretization in the image and whether apparent discretization relates to the data being imaged or to the visualization process itself. A simple example here is the use of contour lines or colours to represent a numerical scale. Are sufficient colours or lines being used (indeed are they available) to represent the data adequately? Are specific local behaviours, which might indicate a problem with the visualization, hidden by the visualization itself?

An issue of concern for metrologists is that of ensuring that a visualization of discrete data does not create the impression that the data are continuous, and vice versa [26]. The simplest example is the plotting of a smoothly varying line through discrete data points, which creates the impression that data are continuous. To represent uncertainties in discrete, one-dimensional data, each point can be plotted with its associated uncertainty. Representing data is more difficult in higher dimensions. For example, the impression almost always created by contour lines and isosurfaces is that the original data from which the contours and surfaces have been derived are continuous, even where this is not the case.

An interesting example of how one might be misled by discretization has been observed by one of the authors of this report in commercial finite element software. The image in question was of an engineering component, a part of a spherical shell. If the software was asked to display the location of the nodes defined in the model or to show the shapes of the main areas of the components that made up the model, the smoothly curved nature of the surface was immediately apparent. However, when the software was asked to display the elements that made up the surface, these were represented as flat surfaces, so that the shape in question appeared to be composed of a number of facets. In fact, in the case of finite element modelling, such an observation may be helpful in that it may indicate the need for a finer mesh density for the problem of interest.

Further concerns relate to the working of the visualization software itself. For example, has the correct algorithm been used in the construction of the visualization [22, 38, 39]? Is the visualization software performing additional mathematical operations on the data to be imaged, such as interpolation or co-ordinate system transformation? Can these operations be checked by the use of test data sets?

Useful guidance on developing test data sets for validating visualizations is available [19] and the interested reader is referred to this work for further information.

## **B.2 Validation of the law of propagation of uncertainty**

Central to the validation of an uncertainty evaluation undertaken using LPU is the extent to which the PDFs for the values of the output quantities obtained from LPU and MCS are consistent. The validation of the use of LPU for models having a single output quantity is considered as part the first supplemental guide to the GUM [4]. The matter is also considered in the SSfM best-practice guide to uncertainty evaluation [10]. The situation is relatively straightforward, because the (univariate) PDFs determined using LPU and MCS can be superimposed graphically (on a plane surface). They can also readily be compared numerically, e.g., in terms of the endpoints of the shortest 95 % coverage intervals for the two PDFs [4, 10]. The situation for models having more than one output quantity is more complicated, because the PDFs for the values of the output quantities take the form of (hyper-)surfaces, and comparison (visual and numerical) is more difficult.

## C Multivariate Gaussian distribution

This appendix considers random sampling from the most important multivariate distribution used in practice, the multivariate Gaussian distribution. An  $n \times 1$  vector of expectations  $\boldsymbol{\mu}$  and an uncertainty matrix  $V$  of order  $n$  define the parameters of the  $n$ -dimensional Gaussian distribution.

Any number  $q$  of values can be sampled from this multivariate (or joint) Gaussian distribution [31] using the following procedure:

1. Form the Cholesky factor  $L$  of  $V$ , i.e., the lower-triangular matrix satisfying  $V = LL^T$ . (To generate  $q$  pseudo-random numbers it is necessary to perform this matrix factorization only once.)
2. Form  $q$  samples from the  $n$ -dimensional standard Gaussian distribution  $N(0, 1) \times \dots \times N(0, 1)$ . Doing so simply means generating an  $n \times q$  array  $Z$  of standard Gaussian variates.
3. Provide the required sample (the Cholesky factor acts as a transformation from the uncorrelated standardized space to that required):

$$X = \boldsymbol{\mu}E + LZ,$$

where  $E$  denotes a  $1 \times q$  vector of ones.

The particularization of the above procedure to a two-dimensional Gaussian distribution is given below. In this case, let the distribution be defined by the  $2 \times 1$  vector of means  $(\mu_x, \mu_y)^T$  and uncertainty matrix  $V$ , where

$$V = \begin{pmatrix} \sigma_x^2 & \sigma_x \sigma_y \rho_{x,y} \\ \sigma_x \sigma_y \rho_{x,y} & \sigma_y^2 \end{pmatrix}.$$

Now,  $V$  has the Cholesky factorisation

$$V = LL^T,$$

where

$$L = \begin{pmatrix} \sigma_x & 0 \\ \sigma_y \rho_{x,y} & \sigma_y \sqrt{1 - \rho_{x,y}^2} \end{pmatrix}.$$

It follows that a sample  $(p, q)^T$  from the required distribution is given by

$$\begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix} + L \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} \mu_x + z_1 \sigma_x \\ \mu_y + z_1 \sigma_y \rho_{x,y} + z_2 \sigma_y \sqrt{1 - \rho_{x,y}^2} \end{pmatrix},$$

where  $z_1$  and  $z_2$  are samples drawn independently from  $N(0, 1)$ , a standardized (univariate) Gaussian distribution with zero mean and unit variance.

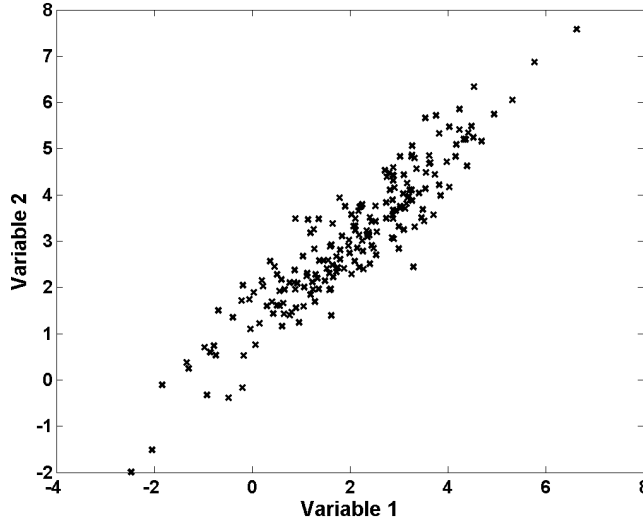


Figure 11: Points sampled from a bivariate Gaussian distribution with positive correlation.

Figure 11 shows 200 points generated from a bivariate Gaussian distribution, using the MULTNORM generator [31], with expectation  $\boldsymbol{\mu} = (2, 3)^T$  and uncertainty matrix

$$V = \begin{bmatrix} 2.0 & 1.9 \\ 1.9 & 2.0 \end{bmatrix}.$$

Similar generators are available elsewhere [13].

In this figure the points “span” an elongated angled ellipse. Were the off-diagonal elements of  $V$  to be replaced by zero, the points would span a circle. Were the diagonal elements made unequal, and the off-diagonal elements kept at zero, the points would span an ellipse whose axes were parallel to the axes of the graph.

## D The probability density function for polar co-ordinates in a special case

Consider the co-ordinate system transformation  $R^2 = X^2 + Y^2$ ,  $\tan \Theta = Y/X$  in Study 1 of section 2.5. Let the joint PDF for the value of  $(X, Y)^T$  be  $g_{X,Y}(X, Y)$  and that for the value of  $(R, \Theta)^T$  be  $g_{R,\Theta}(R, \Theta)$ .<sup>38</sup> Now, the PDFs are related by

$$g_{X,Y}(X, Y)dXdY = g_{R,\Theta}(R, \Theta)dRd\Theta.$$

But

$$dRd\Theta = (\det J) dXdY,$$

where  $J$  is given by expression (3) with  $R$  in place of  $r$  and  $\Theta$  in place of  $\theta$ . It follows that

$$RdRd\Theta = dXdY,$$

and so

$$g_{X,Y}(X, Y)dXdY = g_{R,\Theta}(R, \Theta)RdRd\Theta.$$

Therefore, making the substitution  $X = R \cos \Theta$  and  $Y = R \sin \Theta$ , we obtain

$$g_{R,\Theta}(R, \Theta) = Rg_{X,Y}(R \cos \Theta, R \sin \Theta).$$

Consider the case where

$$g_{X,Y}(X, Y) = g_X(X)g_Y(Y),$$

i.e.,  $X$  and  $Y$  are mutually independent, and

$$g_X(X) \sim N(\mu_x, \sigma^2), \quad g_Y(Y) \sim N(\mu_y, \sigma^2).$$

Then,

$$g_X(X) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{-(X - \mu_x)^2}{2\sigma^2}\right), \quad g_Y(Y) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{-(Y - \mu_y)^2}{2\sigma^2}\right),$$

giving

$$\begin{aligned} g_{R,\Theta}(R, \Theta) &= \frac{R}{2\pi\sigma^2} \exp\left(\frac{-(X - \mu_x)^2 - (Y - \mu_y)^2}{2\sigma^2}\right) \\ &= \frac{R}{2\pi\sigma^2} \exp\left(\frac{-(R \cos \Theta - \mu_x)^2 - (R \sin \Theta - \mu_y)^2}{2\sigma^2}\right). \end{aligned} \quad (12)$$

<sup>38</sup>In this appendix a subscript on 'g' is used to indicate the quantities to which the PDF relates, and to emphasize, e.g., that the PDFs  $g_{X,Y}$  and  $g_{R,\Theta}$  are *different* functions, with the former a function of Cartesian co-ordinates  $X$  and  $Y$  and the latter of polar co-ordinates  $R$  and  $\Theta$ . Elsewhere in this document, this use of subscripts has been omitted and the quantity to which the PDF relates is to be inferred from the argument of  $g$ . A more precise notation for the PDF for quantity  $(X, Y)^T$  is  $g_{X,Y}(\xi, \eta)$ , where  $\xi$  and  $\eta$  are, respectively, values of  $X$  and  $Y$ . However, this notation is regarded as unnecessarily complicated for the purposes of this document.

The PDF corresponding to the marginal distribution for  $R$  is

$$\begin{aligned} g_R(R) &= \int_{-\pi}^{\pi} g_{R,\Theta}(R, \Theta) d\Theta \\ &= \frac{R}{\sigma^2} \exp\left(\frac{-R^2 - \mu^2}{2\sigma^2}\right) I_0\left(\frac{R\mu}{\sigma^2}\right), \quad R \geq 0, \end{aligned} \quad (13)$$

where  $\mu^2 = \mu_x^2 + \mu_y^2$  and  $I_0$  is a Bessel function of imaginary argument. This is the PDF for a Rice distribution with parameters  $\mu$  and  $\sigma^2$ . Similarly, the PDF corresponding to the marginal distribution for  $\Theta$  is

$$\begin{aligned} g_{\Theta}(\Theta) &= \int_0^{\infty} g_{R,\Theta}(R, \Theta) dR \\ &= \frac{1}{2\pi} \exp\left(\frac{-\mu^2}{2\sigma^2}\right) \left(1 + \sqrt{\pi} P e^{P^2} \operatorname{erfc}(-P)\right), \quad -\pi < \Theta \leq \pi, \end{aligned} \quad (14)$$

where

$$P = \frac{\mu_x \cos \Theta + \mu_y \sin \Theta}{\sqrt{2}\sigma}$$

and

$$\operatorname{erfc}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt$$

is the complementary error function.

$g_{R,\Theta}(R, \Theta)$  in expression (12) can be written as the product of a function of  $R$  and a function of  $\Theta$  only when  $\mu_x = \mu_y = 0$ . In this case,  $R$  and  $\Theta$  are mutually independent and the joint PDF for  $R$  and  $\Theta$  can be expressed as

$$g_{R,\Theta}(R, \Theta) = g_R(R)g_{\Theta}(\Theta),$$

where

$$g_R(R) = \frac{R}{\sigma^2} \exp\left(\frac{-R^2}{2\sigma^2}\right), \quad R \geq 0,$$

the PDF for a Rayleigh distribution with parameter  $\sigma^2$ , and

$$g_{\Theta}(\Theta) = \frac{1}{2\pi}, \quad -\pi < \Theta \leq \pi,$$

the PDF for a rectangular distribution with limits  $-\pi$  and  $\pi$ .