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Abstract

METAS VNA Tools is a metrology-grade software suite developed to facilitate measurements using vector network analyzers. Its uncertainty analysis is founded on a comprehensive modeling of the entire measurement process and is implemented through multivariate uncertainty propagation via the *METAS UncLib* library, in accordance with GUM and EURAMET guidelines. Engineered to ensure traceability and compliance with ISO/IEC 17025, *VNA Tools* has been widely adopted by national metrology institutes, as well as calibration and industrial laboratories, owing to its robustness, transparency, and scientific rigor. As it is freely available, the software serves not only as a tool for the dissemination of calibration data but also enables advanced post-processing. Consequently, it provides added value that extends beyond the mere generation of calibration certificates, reinforcing both the seamlessness and integrity of the traceability chain.

Keywords: radio frequency and microwave measurements; scattering parameter; vector network analyzer; digital traceability chain; measurement model; multivariate uncertainty evaluation; automatic differentiation; METAS VNA Tools software; METAS UncLib software

1. Introduction

Vector network analysis [1–4] is fundamental in high-frequency electrical metrology. Measurements with a vector network analyzer (VNA) enable the precise characterization of electrical components and systems. To ensure the reliability and traceability of these measurements to the International System of Units (SI) rigorous modeling of the measurement process is essential [5]. *METAS VNA Tools* [6] is a comprehensive metrology software suite developed by METAS to support the evaluation and uncertainty analysis of VNA measurements. Designed primarily for use in national metrology institutes and (calibration) laboratories, *VNA Tools* integrates measurement models in a modular fashion, facilitating standardized workflows and enabling detailed systematic investigations.

According to [7], metrological traceability requires " ... an unbroken chain of calibrations, each contributing to measurement uncertainty.". As noted in [5] the traceability chain is not necessarily a simple linear structure, it may branch into multiple paths that later converge. *VNA Tools* is built upon the uncertainty engine *METAS UncLib* [8,9], which implements uncertainty propagation in a specific way to support the integrity of traceability chains of diverse architectures. Specifically, it enables the propagation of uncertainty budgets along the traceability chain by maintaining a record of influence quantities and their associated uncertainties. This mechanism preserves the integrity of the traceability chain even in cases where, for example, devices under test (DUTs) calibrated at different times on the same measurement system and/or using the same reference standards are subsequently combined in a later measurement.

The paper is structured as follows: It begins with an introduction to measurements with VNAs and challenges related to it. This is followed by a review of the concept of multivariate linear uncertainty propagation and its implementation using uncertainty objects. Next, *METAS VNA Tools* and *METAS*

UncLib are introduced and the implementation of uncertainty objects is described. Building on these more conceptual foundations, the paper continues by discussing how *METAS VNA Tools* provides added value to the end user in support of the digital traceability chain. Finally, the paper concludes with a brief discussion.

2. VNA Measurements

VNAs measure the reflection and transmission characteristics of a device under test (DUT) in amplitude and phase as a function of frequency, normalized to a reference impedance. VNAs exist in various form factors, ranging from relatively large, highly precise desktop models - typically employed at national metrology institutes (NMI) - to compact hand held devices. Most common configurations feature two or four measurement ports, although models with a larger number of ports are available as well. VNAs are used to perform measurements with different transmission media, including coaxial lines, metallic wave guides, and planar structures.

The quantities measured by VNAs are known as scattering parameters (S-parameters), which characterize components with respect to their reflective and transmissive behavior. S-parameters represent one of various possibilities for describing a linear electrical network, see Figure 1. The S-parameters of individual components can be cascaded to determine the behavior of a larger system, such as a measurement chain. Consequently, they play an important role in radio frequency (RF) and microwave (MW) system design. Moreover, S-parameters are fundamental quantities in RF and MW metrology, as their determination is often a prerequisite for accurately measuring other RF and MW quantities - such as RF power or RF noise - to the need to account for impedance mismatch effects.

S-parameters are two-dimensional quantities and may be presented either in polar (amplitude and phase) or Cartesian (complex numbers) coordinates, as illustrated in Figure 1.
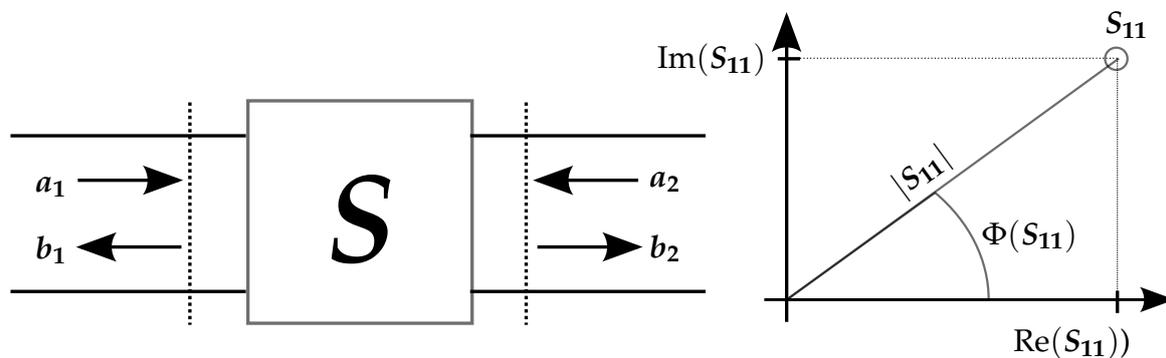
Figure 1. S-parameter describe reflection and transmission of an electromagnetic signal in a linear network. The example shown here is a two port network. The linear relationships are expressed as $b_1 = S_{11}a_1 + S_{12}a_2$ and $b_2 = S_{21}a_1 + S_{22}a_2$. For compactness, this can be written in vector-matrix form: $b = Sa$. All involved quantities are two-dimensional and can be expressed either in polar coordinates (amplitude and phase) or in Cartesian coordinates (real and imaginary components).

S-parameters typically exhibit significant frequency dependence, necessitating repeated measurements at sufficiently small frequency intervals. For broad frequency ranges over tens of GHz, it is common to acquire several hundred measurement points to adequately capture the frequency response of the DUT.

A notable characteristic of VNAs is that the measurements are inherently inaccurate due to unavoidable systematic errors. These errors arise from leakage, loss, mismatch effects, and variations in electrical paths within the measurement setups. These systematic errors need to be determined by measuring a set of known characterized reflection and eventually also transmission standards, a process referred to as VNA calibration. The subsequent measurement with the DUT is then corrected with the error coefficients determined in VNA calibration, a process referred to as VNA error correction.

Various established VNA calibration algorithms are in use [10], with their suitability depending on the specific measurement scenario. Influencing factors include the DUT characteristics, VNA architecture, availability of calibration standards, required accuracy, and practical constraints. VNA calibration and VNA error correction are founded on error models, which are often represented graphically using so-called signal flow graphs. Signal flow graphs are particularly effective depicting linear networks, and established methods exist [11,12] for deriving mathematical equations that relate the measured S-parameters, the unknown S-parameters of the DUT, the characterization data of the calibration standards, and the error coefficients (systematic errors). These equations are used both to determine the error coefficients from the measurements of the calibration standards and to correct the DUT measurement.

The SI traceability of VNA measurements is established through the use of characterized calibration standards. At the top level, national metrology institutes (NMI) perform a primary electrical characterization of suitable calibration standards using a combination of analytical and numerical modeling, as well as dimensional and electrical measurements to establish direct traceability to the SI units [13–15]. These primary standards are used to calibrate a VNA, which then can be employed to characterize a set of secondary calibration standards. In this way, traceability is propagated through the various levels of the metrological pyramid to the end user, via sets of VNA calibration and verification standards. Calibration standards serve as reference standards for disseminating traceability, while verification standards provide an independent assessment of the validity of the measurement model and consequently also the associated uncertainty evaluation.

Central to the integrity of the traceability chain is the reliable determination of the measurement uncertainty associated with S-parameter measurements. According to the Guide to the Expression of Uncertainty in Measurement (GUM) [16], uncertainty evaluation should be based on a measurement model that relates the observed quantity to the true value of the measurand, accounting for all relevant influences. In VNA metrology, the modern form of a measurement model is derived from the error models used for VNA calibration and VNA error correction. The signal flow graphs of the error models are further extended to include additional effects influencing the measurements, such as VNA linearity, drift and noise, cable movement, and connector repeatability [10]. The mathematical equations derived from the signal flow graphs constitute the measurement models.

Due to the two-step measurement sequence (VNA calibration and VNA error correction) these equations become inherently complex. Furthermore, all terms in the model are two-dimensional, necessitating the use of multivariate methods [17–19] to account for correlation effects. Many influencing factors exhibit a significant frequency dependence, meaning that uncertainty calculations must be repeated for each frequency point. Overall, the evaluation of the measurement uncertainty associated with VNA measurements is a demanding task, which requires dedicated software.

3. Measurement Models and Uncertainty Evaluation

A measurement model is a fundamental element in the evaluation of uncertainties associated with the results of the measurements. It has the following basic mathematical form

$$
\begin{aligned}
y_1 &= f_1(x_1, x_2, \ldots, x_N) \\
y_2 &= f_2(x_1, x_2, \ldots, x_N) \\
&\vdots \qquad\qquad \vdots \\
y_M &= f_M(x_1, x_2, \ldots, x_N)
\end{aligned}
$$

In vector notation this can be expressed as

$$
\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) \tag{1}
$$

Each component of the output quantity $\boldsymbol{y}$ is functionally dependent on the input quantities contained in $\boldsymbol{x}$. The uncertainty associated with the input quantities is represented by a covariance (uncertainty)

matrix V_x with squared standard uncertainties as the diagonal elements and covariances as the off-diagonal elements.

$$V_x = \begin{pmatrix} u^2(x_1) & u(x_1, x_2) & \dots & u(x_1, x_N) \\ u(x_2, x_1) & u^2(x_2) & \dots & u(x_2, x_N) \\ \vdots & \vdots & \ddots & \vdots \\ u(x_N, x_1) & u(x_N, x_2) & \dots & u^2(x_N) \end{pmatrix}$$

The correlations between input quantities are captured in the off-diagonal elements, which can be written as $u(x_i, x_j) = r(x_i, x_j)u(x_i)u(x_j)$ with $r(x_i, x_j)$ denoting the correlation coefficient between x_i and x_j. It is well known, see e.g. [17], that the propagation of the uncertainties V_x, associated with x, to uncertainties V_y, associated with y, is governed by the following equation.

$$V_y = J_{y,x} \cdot V_x \cdot J'_{y,x} \tag{2}$$

here, $J_{y,x}$ represents the Jacobian matrix (the $'$ indicating the transpose), which contains the derivatives of the components in y with respect to the components in x.

$$J_{y,x} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \dots & \frac{\partial y_1}{\partial x_N} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \dots & \frac{\partial y_2}{\partial x_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_M}{\partial x_1} & \frac{\partial y_M}{\partial x_2} & \dots & \frac{\partial y_M}{\partial x_N} \end{pmatrix}$$

These equations form the general mathematical framework of linear uncertainty propagation, as described in [16,17]. This approach relies on a linear approximation of the measurement model and is generally sufficient for a reliable evaluation of measurement uncertainties. In cases involving significant non-linearity, the GUM supplements [17,20] promote the use of the Monte Carlo method to propagate distributions representing the state of knowledge.

VNA Tools is to a large extent based on linear uncertainty propagation, largely for performance reasons. Accordingly, the subsequent discussion will focus on the linear approach, although a similar framework can be implemented for Monte Carlo based uncertainty propagation.

For simple cases, such as a single output quantity without correlations, linear uncertainty propagation can be performed manually or using spreadsheet software. However, this approach becomes impractical when multiple output quantities, correlations, or complex equations are involved. In such scenarios, software-based computation is preferred. An intuitive approach involves explicitly programming the derivatives, i.e. the Jacobian matrix of the entire set of equations, and computing V_y using (2).

In the following, we discuss how (2) can be evaluated more efficiently using the technique of automatic or algorithmic differentiation (AD), see e.g. [21–23], and how the explicit storage of large covariance matrices can be avoided while still maintaining correlation tracking. The technique was introduced into metrology already some time ago [24–26], and is based on uncertainty objects.
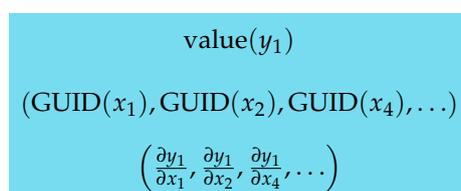
4. Uncertainty Objects

Any measurement model represented by a mathematical equation, as in (1), can be decomposed into a sequence of elementary operations and functions, such as the basic arithmetic operations (addition, multiplication, etc.) and transcendental functions (trigonometric, logarithmic, etc.). This decomposition is illustrated graphically in Figure 2.
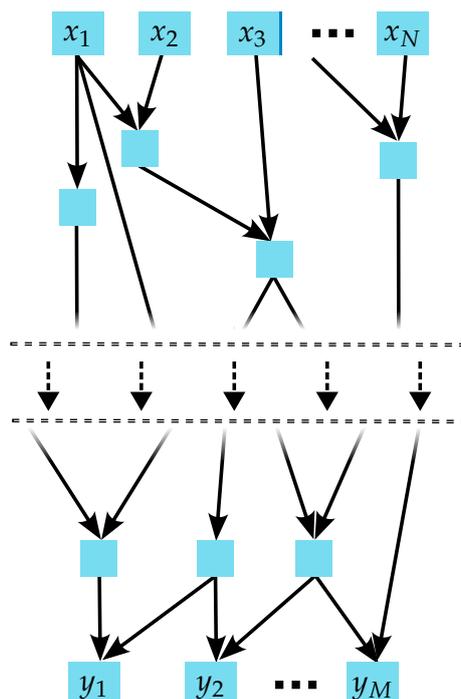
Figure 2. Graphical representation of a measurement model (equation) decomposed into elementary operations and functions. x_1, x_2, ... and y_1, y_2, ... denote the input and output quantities, respectively. Each blue box in-between constitutes an elementary operation, the output of which becomes an input to the next operation. This is indicated by the arrows.

The top layer of blue boxes, labeled as x_i, $i = 1 \ldots N$, represents the input quantities into the measurement model. The bottom layer, labeled y_i, $i = 1 \ldots M$, corresponds to the output quantities. The intermediate blue boxes represent elementary operations with the arrows defining the inputs to these elementary operations. Each intermediate result serves as the input to the next elementary operation, ultimately constructing the full equation. Computers internally decompose arbitrarily complicated equations into such elementary steps<, a process that can be exploited through the implementation of the technique of AD. Each blue box in Figure 2 corresponds to an uncertainty object, which encapsulates the value, a list of dependencies and the sensitivities with respect to those dependencies, as shown in Figure 3.

$$\text{value}(y_1)$$

$$(\text{GUID}(x_1), \text{GUID}(x_2), \text{GUID}(x_4), \ldots)$$

$$\left(\frac{\partial y_1}{\partial x_1}, \frac{\partial y_1}{\partial x_2}, \frac{\partial y_1}{\partial x_4}, \ldots \right)$$

Figure 3. Schematic representation of the contents of an uncertainty object, here illustrated for y_1. It contains the value (best estimate), a list of input quantities on which y_1 depends (dependencies identified by GUIDs, globally unique identifiers) and the sensitivities (partial derivatives) of y_1 with respect to these dependencies.

The value represents the numerical estimate of the quantity. The list of dependencies identifies the relevant x_i, on which the intermediate result depends. The list of sensitivities contains the derivatives of the intermediate result with respect to the relevant x_i. As the equation tree is traversed, these lists are updated at each step. For operations involving a single input, the dependency list remains unchanged. For operations involving two inputs (e.g., binary arithmetic operations), the two dependency lists are concatenated, with duplicate entries removed. To ensure uniqueness and consistency, the x_i are assigned globally unique identifiers upon creation. The list of sensitivities is updated using the chain rule and sum rule of differentiation. This requires the explicit programming of the derivatives for the

entire but also manageable set of elementary mathematical functions. Once implemented, derivatives of arbitrary complicated equations can be computed automatically and with machine precision. For a more detailed introduction and examples, see [24].

The use of AD eliminates the need to manually program derivatives of complex equations, thereby reducing the potential for coding errors. Moreover, by employing object-oriented programming techniques, uncertainty objects can be manipulated as if they were ordinary numerical values, with the propagation of uncertainties handled automatically in the background.

With the information in the uncertainty objects, the covariance matrix for any set of intermediate or final results can be computed on demand using (2). Because dependencies are tracked explicitly, there is no need to store large covariance matrices, which offers significant advantages for both the evaluation and communication of measurement uncertainties. Questions regarding the extent of correlation information to be calculated, stored and transmitted become obsolete. Providing the y_i and x_i objects suffices to compute uncertainties and correlations as needed. Furthermore, correlations of measurements on the same measurement system but e.g. at different points in time will still be recognized, due to the unique identifiers of the shared input quantities.

5. *METAS VNA Tools* and *METAS UncLib*

VNA Tools is a free software suite that operates independently of the VNA firmware. The software controls VNA settings and measurement sequences directly from a PC, processes raw measurement data, and performs all calculations externally. It has a wide range of features, which are not further discussed here. Details can be found in [6,27,28]. In the following the focus remains on the evaluation of measurement uncertainties and the seamless dissemination of digital traceability.

VNA Tools integrates several key components to facilitate comprehensive and reliable uncertainty evaluation in accordance with the EURAMET VNA Guide [10], which advocates rigorous modeling of the entire measurement process. It incorporates relevant measurement models that consider all influence quantities across various calibration and error correction algorithms and different transmission line media. A dedicated database stores the characterization data of these influences, which are essential for determining the associated uncertainties. The software also features a measurement journal that logs all relevant actions during the measurement process with time stamps, such as measurements, re-connections, and cable movements, thereby enabling accurate tracking of uncertainty contributions. Both random and systematic effects are appropriately addressed, with particular attention given to the time-dependent nature of drift and its correlation across measurements. The software also generates comprehensive and detailed uncertainty budgets, which support further investigations by identifying dominant uncertainty sources and guiding improvements in measurement setups and procedures. A verification process is also supported to ensure the appropriateness of the applied measurement models.

Uncertainty propagation is handled by an engine based on the *METAS UncLib* library [8], which performs multivariate uncertainty propagation in accordance with GUM Supplement 2 [17]. The library supports three different modes of uncertainty propagation, linear propagation (according to [16,17]), numerical propagation via Monte Carlo methods (according to [17,20]) and propagation based on higher order Taylor approximations of the measurement model.

METAS VNA Tools centers around the linear uncertainty propagation module *LinProp* of the *UncLib*. The *LinProp* module adheres to the principles outlined in sections 3 and 4, encapsulating value, dependencies and sensitivities in so-called *LinProp* objects. Input quantities for the measurement models are instantiated as *LinProp* objects based on influence data stored in the *VNA Tools* database. Due to the object oriented implementation, any subsequent calculations with these objects automatically update the internal content of the *LinProp* objects in the background.

From a data management perspective, *VNA Tools* introduces a robust storage concept using dedicated and documented XML and binary formats [29], capturing the complete dependency and sensitivity information of the *LinProp* objects. This capability is particularly valuable for communi-

cating measurement results, enabling modular and traceable uncertainty evaluation throughout the traceability chain. Export and import to and from other common data formats is supported as well.

A further valuable and convenient feature of *VNA Tools* is its virtualization capability. NMIs and accredited calibration laboratories are required to declare their measurement scope as part of their quality assurance and for mutual recognition. This scope includes measurement ranges and associated best uncertainties. The uncertainties associated with S-parameter measurements depend not only on frequency, but also on the value of the measurand. *VNA Tools* has built in a virtual VNA that samples possible measurand values in the complex plane and automatically generates tables of best uncertainties as a function of frequency and measurand value.

6. Support of the Digital Traceability Chain

The delivery of a calibration certificate often marks a discontinuity in the traceability chain, as the recipient typically receives only a list of values and associated uncertainties. Efforts related to digital calibration certificates aim to address this issue by providing the data in electronic form and enabling machine-readable certificates. *VNA Tools* offers significant added value to the end user, extending beyond the mere distribution of certificates and calibration data, particularly through its advanced handling of uncertainties.

METAS issues S-parameter calibration certificates in digitally signed electronic format. For illustrative purposes, the certificates include a limited subset of the data in tabular form. The complete dataset is provided electronically and referenced in the certificate via a hash key, ensuring unique assignment and enabling the detection of any deliberate or accidental modifications. The certificates are issued in PDF/A3 format (ISO 19005-3) [30], which supports direct embedding of calibration data within the certificate file. Embedding into a machine-readable digital calibration certificate, as promoted by [31,32], is also supported. The calibration data is stored in one of the documented *VNA Tools* data formats [29], allowing full restoration of the information contained in the *LinProp* objects.

Due to the free availability of *VNA Tools*, recipients of calibration certificates have full flexibility in utilizing the calibration data. By loading the data into the software, users can reconstruct the *LinProp* objects with the exact same state of information as the provider. This enables users to characterize their own working calibration standards based on the received characterized standards. The same mechanism applies when working standards are used to calibrate items at the next level of the traceability chain. In this way, traceability dissemination from one level to the next occurs without disruption or loss of information.

The approach to uncertainty handling, i.e. by keeping track of dependencies and sensitivities and by updating them at each calibration step, offers several advantages over traditional methods that rely solely on propagating uncertainties and covariance matrices. This mechanism ensures that the full uncertainty budget is propagated along the traceability chain and is incrementally supplemented with additional contributions from each measurement step. The end user thus gains access to the accumulated uncertainty budget of the entire traceability chain. This supports current trends in data provenance and scientific transparency and is valuable for systematic investigations of measurement processes. Furthermore, with the information contained in the *LinProp* objects, users can display uncertainties and correlations on demand.

Traceability chains that deviate from a simple linear structure are not uncommon. Typically, multiple calibration and verification standards are used in a VNA measurement. These standards may not have been calibrated during the same campaign, but their characterization may still be traceable to common reference standards. Such correlations are recognized during uncertainty evaluation and verification. Thanks to the unique identifiers of dependencies within the *LinProp* objects, shared influences are properly accounted for, helping to prevent both underestimation and overestimation of measurement uncertainty in complex traceability scenarios.

7. Discussion

Providing uncertainty and correlation information through *LinProp* objects introduces a certain level of abstraction. However, achieving the same level of comprehensiveness and integrity in the traceability chain using direct representations of uncertainties and covariances would be difficult, if not impossible.

End users, however, have different needs and may not be interested in the full detail offered by the mechanisms described thus far. Practical constraints, such as file size limitations, may also apply. Disseminating *LinProp* objects along the traceability chain can result in file sizes reaching tens or even hundreds of megabytes. To accommodate different needs and limitations, *VNA Tools* provides the capability to truncate dependencies and replace them with uncertainties and covariances at any desired level. This reduces file size at the expense of some information loss.

Commercial solutions are also available [33,34] that incorporate the *VNA Tools* suite. These tools offer a more guided and controlled approach to VNA measurements, which may be advantageous for less experienced users compared to the flexibility provided by *VNA Tools*. These commercial solutions maintain a high level of interoperability with *VNA Tools* through its documented data formats [29]. For example, the solution described in [33] allows exporting the entire project, including the measurement journal, for further analysis in *VNA Tools*. This feature is particularly useful when a technician performing routine calibration encounters an unusual result that requires more systematic investigation by a metrology specialist.

These commercial tools interact with *VNA Tools* via the Real Time Interface (RTI), a stable, high-level software interface that provides access to *VNA Tools* functionality. Many measurement laboratories already operate within overarching software environments that support testing, calibration, development, or production processes. The RTI facilitates the integration of *VNA Tools* into such environments, thereby promoting its adoption and usability.

The combination of interoperability, flexibility, and adaptability has made *VNA Tools* suitable for use across all levels of the traceability pyramid—from national metrology institutes to industrial laboratories. As a result, the software, along with its underlying models and data formats, has evolved into a quasi-standard that helps overcome fragmented structures and supports the digital transformation of metrology [35].

Overall, *VNA Tools* contributes to the development towards a truly digital and seamless traceability chain, thereby promoting good metrological practice. Key elements include the use of uncertainty objects, which enable the propagation of uncertainty budgets and the tracking of correlations across diverse traceability chain designs. Equally important is the support provided to users beyond the calibration certificate, with flexibility and customizability tailored to specific needs. There is potential to extend this approach further by embedding the measurement journal and, potentially, the measurement models directly into the certificates, thereby advancing the concept of full data provenance [36] or data lineage in metrology.

Finally, *METAS UncLib* is freely available as a standalone, general-purpose uncertainty engine that incorporates the essential mechanisms discussed. It can be applied in other areas of metrology to implement systems similar to *VNA Tools* for VNA measurements. Solutions in other domains that utilize uncertainty objects carrying complete traceability information - readily shareable with customers - can play a pivotal role in driving the digitalization of the global metrology infrastructure.

Abbreviations

The following abbreviations are used in this manuscript:

AD	Automatic (Algorithmic) Differentiation
DUT	Device Under Test
GUM	Guide to the Expression of Uncertainty in Measurement [16]
MW	Microwave
NMI	National Metrology Institute
RF	Radio Frequency
RTI	Real Time Interface
S-Parameter	Scattering Parameter
SI	International System of Units
VNA	Vector Network Analyzer

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