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The digital transformation and novel calibration approaches

Die digitale Transformation und neuartige Kalibrierungsansätze

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Abstract: In this paper we describe how the digital transformation (i.e., the adoption of digital technology) of society affects National Metrology Institutes like VSL. This digital transformation has many different aspects of social, economic and technical nature. In this paper we will mainly focus on some mathematical and statistical aspects which are important for modelling measurement instruments and analyzing measurement data. We will discuss how modern techniques like artificial intelligence, digital twins, digital calibration certificates and the introduction of the new definition of the SI system of units affect national metrology institutes. Important changes are the usage of complex algorithms and models in measurement instruments, as well as the introduction of novel calibration approaches and the digitalization of the services provided by NMIs.

Keywords: Digital transformation, digitalization, calibration, artificial intelligence, virtual instrument, digital twin, new SI, self-X-solution, metrology network.


1 Introduction

In society a digital transformation is taking place. This transformation also affects National Metrology Institutes like VSL in various ways. This paper addresses some mathematical and statistical aspects of this transformation which are relevant for modeling measurement instruments and analyzing measurement data. Novel algorithms developed by the artificial intelligence (AI) community have found their way into measurement instruments, and the mathematical models used inside instrumentation and for data processing can be very complex [15, 1, 39]. Advanced mathematical models of measurement instruments have led to so-called ‘Virtual Instruments’ and ‘Digital Twins’ [11, 16]. For some measurement instruments these models are essential to get a correct measurement value, for others they enable to calculate a reliable value of the measurement uncertainty.

At the hardware side the number of sensors providing measurement data is rapidly increasing, and modern ICT solutions make it possible to continuously read out large numbers of sensors real time (‘Internet of Things’) and store large amounts of measurement data (‘big data’). This requires an adaption of metrology to the digital age [6]. To be able to keep up with the established concept of metrological traceability of sensors shorter and cheaper traceability chains are required. The redefinition of the SI system of units in terms of natural constants has made ‘one-step’ traceability chains conceptually possible [35]. New technologies based on quantum technologies are being...
developed to implement these new definitions in small, affordable primary standards [28].

Finally, the service of metrology institutes is shifting to a more digital form. A first step was to replace paper certificates by digitally signed ones. The new development is to make the certificates fully machine readable, and to develop a full software chain that produces, reads and uses these digital certificates [33, 14, 13].

VSL [37] is the National Metrology Institute (NMI) of the Netherlands and as such it maintains the national measurement standards. NMIs like VSL make it possible that measurement results can be presented in an 'absolute', traceable way. Traceability means that results are expressed in the SI system of units, can be linked back to primary standards which realize the SI units from their definitions, whereby each measurement result is accompanied by a measurement uncertainty.

In this paper we will present some important aspects of this digitalization of metrology and the novel calibration approaches that accompany it.

2 Virtual instruments and metrological digital twins

Advanced mathematical models of measurement systems are becoming more and more widespread. Some of them have been around already for some time, others are more recent. In the metrological community these models, which should also include explicit modeling of error sources, have usually been called 'Virtual Instruments'. More recently, the concept of 'digital twins' has been introduced. According to [4], a digital twin is defined as “a virtual representation that serves as the real-time digital counterpart of a physical object or process.” This means that the state of the mathematical model should be updated with the state information which should be provided by the instrument. This involves more than only the measurement result itself, but could include, e.g., the position of a moving frame of the measurement instrument or its internal temperature. Some examples of digital twins in industrial contexts can be found in [16].

An example of a virtual instrument is the Virtual Coordinate Measurement Machine (VCMM) [11]. In a VCMM the machine mechanics are carefully modelled including all potential error sources like ruler errors, squareness, flatness, probe shape and temperature induced errors. The magnitudes of these error sources must be determined by means of a traceable calibration. In a next step the uncertainty of the parameter(s) of interest is calculated using a Monte Carlo method, i.e., by simulating different realizations of the individual error sources and evaluating the spread of the calculated value of the measurand. The measurand could be, e.g., the radius of a measured sphere or lens, which is fitted through a measured point cloud of \((x, y, z)\)-coordinates. If this virtual instrument is to be transformed to a digital twin, the actual position of the moving parts of the instrument should be measured and transmitted to the digital model. If the measurement task is supervised and action should be taken based on what is happening, then this digital twin extension can be worthwhile. In the case of a relatively simple pre-programmed measurement task, an extension of the virtual instrument to a digital twin may not be worthwhile. In Figure 1 the qualitative difference between a virtual instrument and a digital twin is schematically illustrated. Whereas the virtual instrument only receives and processes the main measurement data of interest and calculates the measurand value and uncertainty, a digital twin is aware of the complete status of the instrument and can act based on all the sensor data it receives. In the case of a CMM one could imagine that the digital twin proposes or autonomously decides to measure more points in a certain area based on the measurement data, or pause the measurement if it detects temperature gradients, as it is aware of certain temperature induced deformations in the instrument. These decisions are translated into outputs or system control data that are passed to the actuators of the instrument.

Calculating the uncertainty of a measurand with the help of a virtual instrument usually requires many model evaluations, in particular when the Monte Carlo method is used. With the increase of processing speed of modern

![Figure 1: Qualitative difference between a virtual instrument and a digital twin.](image-url)
computers, it is now also possible to use the virtual instrument approach for computationally more intensive problems. E.g., it has been used at VSL to assess the uncertainty of a flow meter (sonic nozzle) using a computational fluid dynamics (CFD) model of the flow and randomly varying the input parameters [21]. A study regarding systematic effects involving various flow patterns was performed by the German national metrology institute PTB in [38] for an ultrasonic and an electromagnetic flow meter. A next step of this study could be to construct virtual instruments for such flow meters that estimate the uncertainty of the measured flow rates as function of the measured data and all flow profiles that are consistent with the measured data (e.g., the measured fluid speed for each of the ultrasonic paths).

In a recently started project [2] a virtual instrument for a scatterometer is being developed, which involves solving Maxwell equations for electromagnetic waves propagation. The measurement principle of this scatterometer is described in [23]. In this particular set-up a camera image of the sample is made from which the geometrical parameters of the periodic sample are being estimated. In Figure 2 examples of geometrical parameters are shown together with simulated and measured images.

Parameter estimation is done by model inversion in the following way. The forward model, which is based on Maxwell equations for electromagnetic waves propagation, has as output the image that is obtained for a given set of geometrical parameters of the sample. By using an optimization method, the geometrical parameters are selected that minimize the difference between simulated and measured image. In an additional loop some parameters modeling uncertainties (e.g., imperfections of the instrument) can be varied, and this will then give the uncertainty of the measurand (which in this case can actually consist of up to five parameters if they are all assumed unknown). As the inner optimization loop is relatively time consuming, it can be very interesting to use a well-trained neural network (or another appropriate mathematical function) as fast surrogate model.

Another application for such a fast surrogate model would be the case in which the scatterometer measurement is used for in process control of a production machine. In this case the measurement result should become available within a few seconds. In Figure 3 the structure of the uncertainty calculation for the different cases is graphically displayed. The main difference is whether there is a computational model for calculating the measurand value $y$ from the data $x$ and some parameters $a$, i.e., $y = f(x,a)$, or if there is a computational model for calculating the (simulated) measurement data based on an assumed value for the measurand, i.e., $x = g(y,a)$.

3 Model based measurements, data driven models and artificial intelligence

3.1 Physical models

In simple metrological measurements the relationship between the actual measurements and the value of the measurand is straightforward and well understood. E.g., one can measure the lengths of the sides of a square and multiply them to get the area of the square. There also exist less straightforward measurement models. In VSL’s scatterometer monochromatic light is focused on a periodic sample (e.g., a grating) and the refracted light is measured by a camera. Based on the recorded light intensities geometrical and/or optical parameters (e.g., refractive indices) of the sample are determined using a computational model of the measurement set-up based on Maxwell equations.
the best fit parameters are determined by an optimization procedure, i.e., the parameter values that result in the best correspondence of the simulated image with the measured image. The problem is thus an inverse problem and due to the repetitive solution of the Maxwell equations it is computationally expensive and therefore relatively time consuming. As the complex mathematical model is an essential part of the measurement, we call this a model-based measurement.

### 3.2 Data driven models using artificial intelligence

For a physically inspired model to be an accurate representation of the reality, it is not only necessary to understand the underlying physical principles, but it is equally important to be very careful in the bookkeeping of the numerical values, signs, orientations of coordinate frames, etc. It can thus be time consuming to assure that the predictions of the physics-based model are correct. A final, empirical correction may still be needed. Furthermore, an accurate physics-based model can be computationally expensive and therefore slow, which is a problem when it needs to be evaluated many times, e.g., in an optimization routine, or when results are needed in real-time, e.g., in a feedback control loop of a machine. In these cases, more simple surrogate models can be used. Besides using more classical numerical methods, these substitute models can now also be based on techniques from the area of artificial intelligence (AI), be completely or partly data driven and they can be much faster (once the model has been constructed) than complex physical models. A popular choice are neural networks which are especially reputed for good accuracy in image processing. In some cases, data driven models are more precise in comparison to physical models, which are often only an approximation to the real process.

In a joint research project [31] the possibility of constructing a fast neural network to complement the much slower physics-based model for a scatterometer is being explored. The prior training of the neural network is a slow process and will be based on a large number of simulations using the physics-based model. Potentially the architecture of the neural network can be optimized by using information about the physical process, i.e., creating a ‘physics informed neural network’ (PINN), [29]. There is an active research community dealing with this type of networks [24]. One approach to make the neural network aware of the physical equations governing the process is to explicitly take them into account in the loss function that is minimized when calculating the optimal internal parameters of the network. In this way the parameters are not only tuned to the specific data at hand, but also the structure of the underlying equations (e.g., partial differential equations) is taken into account. This can make the network more ro-
bust and the predictions for fresh data outside the domain covered by the training data can be more reliable. See [18] for an example involving the seismic wave equation. When the physical equations are not known beforehand, one can also use a neural network to discover these equations from the data. See [3] for an example how this can be done.

This approach can also help to make the results produced by the neural network more explainable. There is much current research in the “XAI-community” (eXplainable Artificial Intelligence) to methods for making the output of AI algorithms better interpretable. So instead of treating an AI algorithm as a black box for which it is unclear why the algorithm arrived at a certain output, the solution should be explainable to humans. We will not cover this research field in more detail here. In reference [32] more details can be found.

### 3.3 Other applications involving artificial intelligence

The last section dealt with replacing computationally expensive physical models by much faster neural networks and possibly other AI methods. Another application of AI methods is to improve the performance of low-grade instruments. Such instruments may be sensitive to a lot more than only the physical quantity of interest. By measuring these influence quantities and fitting a complex AI based mathematical model, the performance of the instrument can be considerably improved. A good example for this approach is the case of low-cost air quality sensors. By means of some additional sensors, and fitting a neural network to the training (calibration) data, the uncertainty of the amount-of-substance fraction of the target gas can be reduced considerably [36].

In the health sector AI algorithms are becoming more widespread and this also includes the measurement instruments used, especially the ones in the field of medical imaging. There are even methods to replace complete measurement systems by other systems combined with AI. This is the underlying idea for synthetic CT scans that are produced based on MRI images [5]. For the medical diagnosis a CT scan is desired, involving an exposure to potentially harmful radiation for the patient. However, the patient is measured using MRI, which is much less harmful. Based on a large set of training data, the AI algorithms are now able to construct a synthetic CT image, which gives the medical doctor already valuable information, and a real CT scan may not always be needed anymore. It is well possible that in industrial settings virtual or synthetic measurements can be performed whereby certain measurement instruments become obsolete as they can be replaced by other measurement instruments in combination with AI.

Yet another application involving AI that metrology institutions are looking into are the measurements made by autonomous vehicles (AVs) [12]. By means of complex AI algorithms camera images are processed and fused with lidar, radar and inertial measurement unit data resulting in a measured distance to an object, which is expressed in the SI unit meter [22]. The question is what the measurement uncertainty of the reported distance is. Classical sensitivity analysis and propagation of uncertainties through the model is not fully feasible and satisfactory, as it is not always clear how to perturb the input quantities in a real-

**Figure 4:** (Taken from [29]) Graphical representation of one type of Physically-Inspired Neural Network (PINN): the loss function that is used for optimizing the model parameters, is extended with a loss part related to the fulfillment of the governing physical equations (in this example the Navier-Stokes equations for fluid flow).
istic and metrological sound way (e.g., how to perturb the camera image). It’s also not clear what the boundaries of the tested input domain exactly are. Are specific measurement conditions interpolation or extrapolation [25] and is the outcome of the algorithm trustworthy or not at all?

Some more examples of metrological applications involving AI are the usage of a deep neural network for computational optical form measurements [15], invertible neural networks in relation with uncertainty calculations for grazing incidence X-ray fluorescence [1] and a deep neural network used for calibrating misalignments in the interferometric measurement of freeform surfaces [39].

3.4 Implications for traceability and calibration

There is a considerable implication of the usage of advanced mathematical models and black box AI-algorithms to the traceability and the calibration of instruments. In the most classical setting, the measurement instrument measures the one-dimensional quantity of interest in a direct way (e.g., length measurement with a caliper) and the calibration consists of simply comparing two numbers. The calibration points are taken at regular steps in an interval of interest, and the calibration is assumed to be valid for the full interval based on mathematical interpolation of the calibration results at the measurement points. This establishes the core of the traceability of the instrument.

In a CMM the diameter of a sphere is not directly measured, but derived from the measured \((x, y, z)\)-coordinates of a number of measurement points. The function to calculate the best-fit sphere from a point cloud is well understood. By means of a VCMM, or even analytically in the case of a least squares fit, the uncertainty of the sphere radius can be assessed. The values of parameters for the uncertainty calculation by means of the VCMM can be determined by means of a calibration of the individual sources of uncertainty of the CMM in a part of or in the entire machine volume. It is also clear what interpolation means: using the CMM in the calibrated and characterized measurement volume. As long as the VCMM model is validated, the calculated uncertainties are reliable, and the extend of the traceability is clear.

The measurement of geometrical parameters by means of a scatterometer is more involved. The inversion of the model \(x_{\text{meas}} = g(y, a)\) can be ill defined and multiple, quite different, solutions may exist for the vector-valued measurand \(y\). Prior knowledge on the approximate range of \(y\) is usually needed. If this prior knowledge is available, the uncertainties \(U(a)\) of the influence parameters \(a\) are relatively small and the physics based mathematical model based on the Maxwell equations is used, the calculated uncertainty may still be deemed appropriate as long as one has assured that all sources of uncertainty are covered by the model. So, a traceable calibration using a scatterometer is theoretically possible. (Note that assuring that the uncertainty budget for a scatterometer is complete and accurate is a challenging task and part of the work in [2].)

In the case of using black box AI-algorithms for calculating the measurand, it may not be clear if the algorithm behaves as expected for new input and if it follows sound physical principles. For the scatterometer case it is not directly clear if an algorithm trained with simulated images will work in the same way with slightly different measured images. And if it works with a specific set of camera images, will it still work if some camera settings like the contrast level are changed? This type of questions becomes even more important in the case of autonomous vehicles which may identify objects and determine the distance to them based on camera vision only [34]. If the AI model works for images taken under specific circumstances, in which circumstances is it still expected to work, and when possibly not? If a measurement device using black box AI algorithms is calibrated, to what extent is it traceable, and what means interpolation? Can unusual input be detected [25]? Which sources of uncertainty need to be accounted for [20, 10]? It is clear that a substantial research effort is needed to fully answer these and similar questions. In the document [19] the strategy of PTB regarding AI is presented.

4 Quality control of measurement instruments and self-X-solutions

In the last section we presented some examples of how AI methods can assist in the calculation of the measurement results. In this section we look at aspects related to quality control and self-X-solutions.

4.1 Quality control of measurement instruments

AI-algorithms can be used for quality control of measurement systems by means of a meta-analysis of the available measurement data. If a substantial amount of well-structured measurement and/or calibration data is available, unsupervised AI algorithms can be used to find patterns and clusters in the data. This can give new insights
related to relationships between measurement results and measurement conditions, conditions in which measurements are likely to fail, and insights in the health of the measurement instrument itself. E.g., a need for recalibration of the instrument could be discovered before its deadline based on a fixed time schedule. A necessary step needed for fully releasing the potential of AI algorithms for quality control is a using consistently a well-structured uniform data format for saving all data and storing them in a systematic way.

### 4.2 Self-X-solutions

Another way of improving the quality control of measurement instruments is by using so-called self-X-solutions. In general, ‘self-X’ can indicate a great variety of capabilities: self-configuring, self-healing, self-correcting, self-optimizing, self-provisioning, self-managing, self-healing, self-protection, self-calibrating, etc. [17]. Clearly, not all self-X features are relevant for measurement instruments, and the underlying ideas covered by the self-X terminology are not all entirely new. Self-correcting of a sensor in a network can be realized when redundant information is present, at least part of the time [30]. The sensor can compare its measured value with the mean of a large set of neighbouring measurement values or with the result of one particular reference sensor and correct its results. An example is the self-correction of air quality sensors. If it is assumed that pollution levels are homogeneous around 3 a.m. due to the absence of people and/or traffic, the correction factors (e.g., the background offset) of the low-cost air quality sensors can be adjusted by comparing the measurement results with the results of a high-grade reference station. A variety of self-diagnosis and self-calibration strategies for low-cost air quality sensor networks can be found in [27].

The term self-calibration may refer to the possibility of calibrating an instrument by itself in the field. E.g., an A/D-converter of a temperature measurement instrument can be calibrated by measuring a set of built-in, stable resistances at regular time intervals. This can be useful, as the A/D converter may be most prone to drift. However, the resistors themselves will have to be calibrated at some (longer) time intervals as well, so this doesn't completely replace calibration at a reference laboratory. (In this example the measurement element of the device (e.g., the 100 Ohm resistance of a Pt100 sensor) will need recalibration as well at some point in time.)

Complete self-calibrating (traceable) systems require that primary measurement standards that realize the SI units are integrated into the measurement device. This is impossible for the traditional way of realizing these units, as this is done using large and expensive measurement set-ups in national metrology institutes. However, some NMIs like NIST in the ‘NIST on a chip’ program [28], are exploring the possibility of making much smaller and cheaper primary measurement standards that operate according to the principles of quantum physics. The result would be that primary realizations of the SI units can be available ‘anywhere and anytime’, be it probably with a larger uncertainty than what is possible in an NMI. Using such small primary standards, an instrument can be truly ‘self-calibrating’. This leads to the concept of ‘one-step-traceability’: instead of having a (potentially) long chain of comparison measurements between the references and working standards at an NMI, standards at intermediate calibration laboratories and the instrument of interest itself, the instrument is directly (in ‘one-step’) compared to a primary standard.

Note that the redefinition of the SI system of units in terms of fundamental natural constants in 2019 [35] has made this one-step-traceability idea conceptually possible. E.g., before 2019 the reference for the kilogram was a physical weight stored at the BIPM laboratories in Paris, which made ‘one-step-traceability’ by definition impossible outside the BIPM, at least for quantities involving the SI unit kilogram. Traditional traceability chains can be long and labor intensive to realize. In the current situation in which large numbers of sensors with a somewhat higher measurement uncertainty are being installed in industry, smart cities and at home, future ‘SI on a chip’ solutions may offer a reasonable solution for realizing SI traceability at an affordable cost.

### 5 Digitalization of NMI services and European cooperation

In this section we present how NMI services are being digitalized by developing digital calibration certificates, and how the digital transformation of metrology institutes is helped by European cooperation initiatives.

#### 5.1 Digital calibration certificates

In the realm of the digital transformation of metrology institutes the services provided by NMIs become more digitalized. Digital client portals where a customer has an overview of his order and certificates are being created.
The paper calibration certificate has remarkably long survived in our modern world, but finally it seems to get replaced by a digital counterpart. At this moment most digital certificates are digitally signed pdf-files, which cannot be interpreted by a machine in a standardized way. A European effort has been made in the SmartCom project [33] to design a structured and machine-readable format by using xml-files. Using this scheme and some supplementary domain specific conventions NMIs will be able to produce digital certificates that are automatically interpretable by a computer and exchangeable (i.e., it doesn’t matter which NMI has provided the certificate, the data format remains the same). To take really advantage of these digital certificates, the customer must implement some software at the receiving side so that the data from the calibration certificate can be automatically read, processed, and stored. This latter development still seems to be largely ‘work in progress’.

5.2 European Metrology Network for mathematics and statistics

There is a large need for research in the area of digitalization, novel technologies and AI regarding how these developments can be integrated in the metrological landscape. In order to come to a common European approach, prioritize the research needs, share the workload and prevent duplication of work in metrological research, the umbrella organization of European NMIs Euramet [9] has created several ‘European Metrology Networks’ (EMNs). The topics of advanced mathematical modeling, uncertainty calculations and artificial intelligence are being addressed by the EMN for Mathematics and Statistics in Metrology (MATHMET) [8]. The EMN MATHMET is actively engaging with industry, academia and research institutes in a stakeholder consultation process which will be used to create a strategic research agenda. This will yield a roadmap for prioritizing the research topics. The EMN members are also actively discussing a quality management system that can be used to assess software and data in order to come to a joint understanding and definition of software and data quality. Joint research proposals of NMIs, academia, research institutes and industry are submitted in the European Partnership for Metrology program [26] in order to get the necessary funding to make the roadmap indeed happen and produce the necessary bits of knowledge still missing for a fruitful digital transformation of the metrological landscape.

As noted earlier, the digital transformation of metrology encompasses more than incorporating novel mathematical and statistical methods in the measurement process. Other EMNs are addressing other aspects. To name one, EMN Advanced Manufacturing [7] addresses the required new and enhanced metrology methods needed in advanced manufacturing to assure the quality of manufacturing processes and the resulting products in the context of advanced manufacturing. As digital methods and automated measurements are of high-interest to advanced manufacturing, this EMN is also very relevant for the digital transformation of industry, be it more focusing on the hardware side of measurements.

6 Conclusion

In this paper we gave a short overview of how the digital transformation of society is present in metrology institutes and in measurement solutions. We discussed the metrological counterpart of digital twins, the advance of AI in measurement models and quality control and the emergence of self-X-solutions. Arguably the most relevant self-X-solution from a metrological point of view is self-calibration. This is conceptually possible with the redefinition of the SI in terms of fundamental natural constants which are available anywhere and anytime. Society is now waiting for technological solutions which indeed implement primary metrological reference standards in a small format (e.g., on a chip) at affordable cost. This would enable one-step-traceability solutions without the need of sending the equipment to an NMI or secondary laboratory for calibration. However, we don’t expect that these ‘SI on a chip’ solutions will be available for all relevant quantities in the near future, and they will probably have a higher measurement uncertainty than the reference standards at metrology institutes. The need for NMIs will thus also remain in future.

Solutions based on AI can make new measurements possible or existing measurements faster. However, we expect that at NMIs, at the top of the traceability chain, primary instruments realizing the SI units will continue to be based on well-understood fundamental physical laws and associated well-understood equations. For primary standards AI can help with quality control, but we don’t expect it to be an essential part of the primary instrument itself in the near future. A large research topic for NMIs is how to validate (secondary) measurement instruments and processes that heavily rely on AI.

European collaboration between NMIs is essential in order to prioritize the research topics in the digitalization domain, share the workload and prevent duplication of
work. For mathematical, statistical and AI related topics the EMN MATHMET is coordinating this, whereas other EMNs address other topics.

Only the future will really tell us which new and unforeseen opportunities the digital transformation of metrology will offer to the metrological community and its stakeholders.

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