PTB Competence Center
"Metrology for Virtual Measuring Instruments" (VirtMet)

In the course of digitalization, the importance of simulations and *in silico* experiments is increasing rapidly. In many areas, so-called "virtual measurements" as simulations based on physical-mathematical modelling and statistical methods are now in everyday use. For example, simulations serve to gain a better understanding of the real experiment, to plan new experiments or to evaluate existing ones. In the meantime, simulations are increasingly being used as an essential part of measurement, usually as part of an inverse problem.
In this development, the task of metrology is to secure confidence in simulation results if they are to be used in the same way as real measurements. Concrete existing examples at PTB include the Tilted-Wave Interferometer or the Virtual Coordinate Measuring Machine. In a national workshop "Metrology for Virtual Measuring Instruments" organized by PTB in March 2018, the following overarching questions and cross-sectional tasks were identified for these and other application examples:

1) How do you ensure trust in simulation results?
2) How can virtual and real measurements be compared?
3) What standards are required for interfaces, metadata and data formats?
4) How can virtual experiments for complex measurement systems with large amounts of data be handled using machine learning methods?

PTB's treatment of these issues requires continuous and intensive interdisciplinary cooperation. For this reason, the PTB Competence Center "Metrology for Virtual Measuring Instruments" was established, in which the existing expertise is bundled, and the interdisciplinary exchange is continuously promoted. The centre is coordinated and supported by the AG PSt1 "Koordination Digitalisierung" (Coordination of Digitisation) in order to realise a possible linkage of the developments in VirtMet with other PTB projects in the field of digitisation. In addition, the competence center will further strengthen the exchange and cooperation with external partners in this area with regular workshops.

Based on concrete working points, the higher-level questions will be dealt with in cross-departmental projects. By embedding the projects in the competence centre, there will be an intensive and regular exchange between all participants in order to exploit synergy effects and pursue a joint strategy.

Areas involved in the PTB

OU	name	skills
1.0	Mechanics and acoustics	Digital twins in the range of mechanical sizes
1.5	Liquids	Calibration of flowmeters
4.2	Image and wave optics	Calibration of optical measuring instruments
5.3	Coordinate metrology	Virtual coordinate measuring machine
6.2	Medical Imaging	Metrology for imaging techniques
6.4	Neutron radiation	Metrology for imaging techniques
7.5	Heat and vacuum	Calibration of flowmeters
8.4	Mathematical modelling and data analysis	Simulation Methods, Measurement Uncertainty and Machine Learning

Simulations for medical imaging methods using X-rays

Background

Due to the non-linear behavior of current imaging techniques using X-rays (CT, mammography), new measures are required for the evaluation of image quality. The development of such measurements and their reliable determination is crucial for an optimal balance between necessary radiation exposure and required image quality for reliable diagnostics. The development of so-called "model observer" and the characterization of their uncertainty is a current research direction. Virtual experiments can significantly support this development.

Current status

In 2016, the PTB started the development of methods for the assessment of image quality in CT and mammography in a cooperation of the departments 6 (ionizing radiation) and 8 (medical physics and information technology). In addition to the development of new estimation methods [1-3], virtual experiments for CT and mammography are currently being developed. The aim is to achieve a simulation that is as realistic as possible. The virtual experiments shall be used for the development and validation of methods for the evaluation of image quality.

In this field, PTB cooperates with 3 national reference centres for mammography (Münster, Oldenburg, Marburg), the EUREF centre in Nijmegen (NL), the University of Leiden (NL), the CEA (F), NPL (UK), as well as Charité and TU Berlin.

Goals and outlook

The PTB is currently financing a postdoctoral position and a PhD position to strengthen the area. Half of both positions are located in departments 6 and 8. In addition, the PTB will apply for a European project (EMPIR) in 2018 and aims at coordination. The PTB is actively involved in committees (e.g. AK CT) with the aim of implementing the procedures developed at the PTB in practice. Cooperation with industry is being sought.

Interdepartmental character and embedding in VirtMet

The project is already very well organised across departments. Through the embedding in VirtMet, the approaches and solutions developed in the project become accessible to other areas as well, and a continuous, active exchange takes place.

Transfer of the VCMM concept to other areas and for use in Metrological Digital Twins

Motivation

The VCMM (Virtual Coordinate Measuring Machine) developed at PTB has been used very successfully for many years in the field of coordinate measuring technology for process-accompanying measurement uncertainty determination and measurement process optimization in science and industry. The established PTB process, which was awarded the Braunschweig IHK Technology Transfer Prize in 2005, meets the requirements of international guidelines and standards. Due to the complex structure and the time-consuming programming of necessary software modules, a transfer to other metrological areas has hardly taken place so far. A dissemination of the established VCMM concept to other metrological areas within PTB and industry through the development of a universal modular system for virtual measurement processes (VMP) is therefore promising and will result in numerous third-party funding (in funding programs or direct industrial cooperations).

Current status

The VCMM was developed at PTB about 20 years ago and has since been extended by additional measuring tasks and systems in coordinate metrology. Larger manufacturers such as Zeiss and Hexagon have implemented the VCMM in their coordinate measuring machines and, for example, presented it as a key topic at the Control 2018 trade fair. Five accreditations also prove the interest of the industry. The use of the VCMM concept in so-called digital twins, for example, was successfully tested at PTB's digital weighing unit as an integral part of the Planck balance currently under construction and will be integrated into the planned digital processes in the competence centre "Wind" (CCW), in particular in the area of the torque standard measuring equipment (DM-NME).

Goals and outlook

The extension of the VCMM concept to other areas of PTB serves the strategic goal of actively supporting industry and economy in the change of digitization through the development of "virtual measurement systems" and "digital twins". The following concrete steps are to be taken to this end:

1. Cross-departmental structure of a VMP modular system:
    - Revision/extension of the VCMM module concept and the interface definitions as a basis for use in the VMP modular system
    - Documentation and provision of the VMP construction kit in a central repository at PTB for the fast representation of virtual measurement processes for industry (for quality assurance reasons initially as PTB service)
    - Provision of a selection of API wrappers
    - Connection to the TraCIM service (especially for implementation in external software)
    - Creation of a formalized validation concept with catalogue of requirements
2. Validation and optimization of the VMP modular system through sample applications
    - VMP for Planck Scale (Dissertation Dept. 1, ongoing) and DM-NME
    - VMP for gearing (validation and transfer) and optical distance sensors
3. Preparation of basic documents for the transfer to the calibration service

Interdepartmental character and embedding in VirtMet

The transferability of the VCMM concept to other metrology areas makes this proven and well-controlled procedure usable for all PTB departments. The VMP modular system with all modules and documentation should be administered by a central office at PTB, which also advises other interested parties and minimises duplication of work and the risk of undesirable developments. The specific applications must be developed and maintained in the departments or departments. Newly created modules must be entered into the VMP construction kit in consultation with the central coordination office and the documentation database updated jointly. Once the universal VMP kit has been developed, it is directly applied to pilot applications in Divisions 1 and 5 and optimized for general use. By embedding the project in VirtMet, the later expandability to other areas and departments will be considered from the beginning and the methodical approaches to digital twins and simulation-based evaluations of the VMP construction kit will be compared with those of the other projects.
The VCMM has extensive experience in gaining *confidence in the simulation results* through verification comparison measurements on selected standards and under very different measurement conditions. In this way, the *comparability of the virtual and the real measurements is* also ensured, as the resulting dispersion of the simulation results and the resulting measurement uncertainty leads to conformity under consideration of the calibration uncertainty. Last but not least, the high acceptance of this established concept is clearly demonstrated by the accreditations carried out by the DAkkS for many years. The creation of *interface definitions* for the communication of the individual modules of the VMP library based on the previous knowledge from the VCMM is a focal point of the research project intended here. The VCMM today and the future applications of the VMP modular system offer an excellent basis for the development of intelligent measurement processes through *machine learning*. Decisions such as test process suitability. In the future, the optimum test process can be performed by the measuring process or device itself.

Tilted-Wave Interferometer (TWI) as Example for Hand-in-Hand Calibration of Real and Virtual Experiments

Background

The optical industry uses aspheres and free-form surfaces in modern optical systems, which, however, place very high demands on metrology. Optical measurement techniques have a prominent role to play here, as they do not damage the measurement objects. The industry urgently needs a return in optical asphere/free form metrology, which is not yet available.

Current status

The non-contact Tilted-Wave Interferometer (TWI) is used at PTB. With its measuring principle, the optical effect of the measuring system and the object being measured on wave fronts is recorded by a camera from a large number of directions of incidence [4]. The resulting interference fringe pattern is very complex, and only by simulating the measurement process and solving several inverse problems can the surface shape of the object be deduced. The virtual experiment is part of the modelling of the measurement process. The central objective of PTB is the determination of uncertainty, which is to be determined by combining the virtual experiment with the real measurement setup [5,6].

At PTB, the topic is dealt with equally by FB 4.2 and FB 8.4. PTB also cooperates with the University of Stuttgart, where the basic measuring principle was invented, and Mahr GmbH, which markets a commercial version of TWI. Internationally, there is cooperation with many NMIs, universities and companies within EMRP/EMPIR projects as well as with the Nanotechnology Competence Center Ultra Precise Surface Treatment. (CC UPOB), which has established itself as an expert forum for aspheres and free-form metrology and manufacturing.

Goals and outlook

The further development of the TWI concept is integrated in PTB's work and research programme in topic area 5: Length, dimensional metrology. The project has a particular impact on the promotion of the German and European optical industry and the associated manufacturers of measuring instruments. Aspheres and free-form surfaces are an outstanding future-oriented development in optical systems and have an impact on high-end camera systems, industrial camera systems and also camera applications in the automotive and consumer sectors. The goal is to develop a key role for PTB in optical aspheric and free-form surface metrology by realizing a high-precision traceability by combining real and virtual experiments. The transfer of this return to industry will enable much more precise production there and will in particular have a very positive effect on German and European competitiveness.

Interdepartmental character and embedding in VirtMet

The TWI is a striking example of a mathematics-based optical measuring instrument. This is also reflected in the treatment of the topic at PTB, which takes place in equal parts in the fields of image and wave optics and mathematical modelling and data analysis. Regular joint working meetings in Braunschweig and Berlin are an integral part of the work on the topic. A central part of the project is the uncertainty determination of the TWI, which can be determined from the sensitivities obtained from the simulations. In addition, within certain limits (i.e. typically above 50 nm uncertainty) a comparison can also be made with high-precision coordinate measuring machines.

The question of the comparability of virtual and real measurements does not arise with the TWI principle, since the virtual experiment is part of the real measurement. However, the questions of reliable characterization of the virtual part of the measurement to be dealt with by the TWI will also play an elementary role in other projects in VirtMet. The TWI is also a very complex measuring system in which machine learning processes can be very helpful, especially in the calibration strategy of the optical system and the optimal positioning of the test specimen.

Development of a virtual flow meter

Background

The aim of this project is to establish numerical flow simulations as a reliable and practicable tool for the calibration and uncertainty determination of flowmeters (DFM). The FB 7.5 has been working with various manufacturers of flowmeters (e.g. FLEXIM or KROHNE) for a long time. Important work contents are CFD simulations to simulate different flow configurations and to analyze their effects on the measuring instruments. In recent years, FB 8.4 has been involved in a number of EMRP and EMPIR projects, which involved flow simulations (EMRP ENG58, EMPIR 16ENG07) and the determination of uncertainties (EMRP NEW04). The possibility of virtually assessing flowmeters with significantly higher accuracy using simulations would not only strengthen current research cooperations, but would also enable further project partnerships (e.g. through a joint EMPIR project in Energy or Industry Call). With the development described above, it would be much more advantageous for manufacturers to develop new measuring instruments and further improve existing ones.

The planned work will be complemented by the development of a virtual flow meter for water meters in FB 1.5 as part of an ongoing EMPIR project, which is to enable the estimation of the influence of water quality on the measurement quality of water meters. In a second step, the framework set up in the project will be transferred to the calibration of flowmeters in order to determine the influence of dynamic measurement conditions on the measurement deviation in the future and thus be able to make a statement on the calibration quality.

Current status

Preliminary work within the framework of cooperation in past third-party-funded projects of the departments 7.5 and 8.4 has already led to four joint journal papers in this field and thus created a sound basis [7-10]. The EMPIR project METROWAMET, started in 2018, will be coordinated by the department 1.5 and will aim at the development of a virtual flow meter with focus on water meters.

Goals and outlook

Flow simulations are becoming increasingly important in the industrial environment, as they represent a cost-effective alternative to expensive prototype production and complex measurements. By developing methods that lead to a virtual measuring device, flowmeters can be optimized on the computer and correction factors can be adapted to the respective flow conditions. This means that a large number of costly and time-consuming measurements can be saved when developing and evaluating new measuring instruments. Therefore, it is necessary for PTB to provide suitable data of uncertainty considerations and calibrated test cases for the approval of heat meters for the simulation of pipe flows in order to achieve a higher accuracy of the calculations and their improved uncertainty quantification and to enable an increased reliability of the prediction of the measured value.

Interdepartmental character and embedding in VirtMet

The measurement of the flow of liquids plays an important role in many areas, for example in industrial applications, pharmaceuticals and medical technology or in the measurement of water consumption in one's own household. Accordingly, the measuring instruments, measuring conditions and the requirements to be fulfilled by the instruments are manifold. The virtual flowmeters under development or planned at PTB will cover DFM for an essential range of the applications mentioned.

Due to the possibility of high-precision measurements in Department 7.5, parameters of the turbulence models can be newly determined. The expertise available in Department 8.4 is to be used to identify the most important parameters and constants of the turbulence models and to implement the new parameters/equations in a software package. A surrogate model is to be developed based on measurement data and selective simulations. For this purpose, a suitable measurement database and suitable methods for surrogate modelling must be identified and created. By solving the inverse problem, the measuring error resulting from the flow characteristic and the measuring principle can be corrected. In addition to the uncertainty of the measurement, the uncertainty contribution based on the model parameters must also be determined by a suitable mathematical procedure. For this purpose, polynomial chaos [11] can be used, for example, in which statistical distributions are assigned to the parameters and their effects on the calculated measurement uncertainty are quantified.

Thus, this project combines detailed expertise from several departments and enables new insights. Divisions 7.5 and 8.4 can build on already well-established cooperation from which both sides benefit. Thus, experimental considerations can be supported by CFD simulations and simulation results can be validated by experimental results.

By embedding the project in VirtMet, other areas can also benefit from the resulting expertise. CFD simulations already play an important role in the research and development of flow sensors. Although PTB can partially validate the simulations by means of highly accurate (here: laser-optical) measurements, it has turned out that the deviations between simulation and measurement are sometimes very high. Therefore, questions of trust in simulation results, comparability of virtual and real measurements as well as suitable interfaces, metadata and data formats are of central importance for this project. Since very large amounts of data have to be generated and processed during both the simulation and the measurement of flows, it may also be helpful in the future to resort to methods of machine learning.

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