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Validation and reliability of the 3D calibration evaluation algorithm for SPM

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Abstract

Novel marker-based 3D standards, in the form of cascading step-slope pyramids, enable the calibration of three scaling factors and three coupling factors of scanning probe microscopes using only a single sample and a single measurement. They offer better convenience than conventional methods and are therefore increasingly applied. From a quality management perspective, it is of high importance to validate the evaluation algorithm of the 3D calibration strategy and analyze its error contribution. This paper proposes and develops a new software validation method based on both synthetic data and measurement data. Finally, results of our study are discussed, and the impact of the computational error on the measurement uncertainty is examined.

Keywords: software validation, 3D calibration, calibration standard, calibration uncertainty

1. Introduction

Contemporary metrology increasingly relies on complex computations executed by evaluation software. The software processes the measurement data and delivers final measurement results. However, computational errors can often wield substantial influence on measurement uncertainty or even dominate it. Therefore, it is imperative to explicitly recognize the role of the software and validate its correctness.

Software validation has been the subject of extensive research and application across various branches of metrology. For example, Todhunter *et al* [1] presented a method for the performance validation of surface texture parameter

calculation software, with a specific focus on functional surface texture parameters. Chiboub *et al* [2] generated reference softgauges to test minimum zone fitting algorithms. Some metrology institutes already offer validation services for specific algorithms. The Physikalisch-Technische Bundesanstalt (PTB), for instance, offers the TraCIM (Traceability of Computationally-Intensive Metrology) service for validating Least-squares fitting algorithms and Chebyshev minimization algorithms [3]. Bui and Vorbürger [4] at the National Institute of Standards and Technology have developed a web-based system for testing surface metrology algorithms. This paper aims to demonstrate our efforts in validating a complex evaluation algorithm of a novel 3D calibration method, and in analyzing its error contribution on measurement uncertainty.

Scanning probe microscopy (SPM) [5–7] stands as an essential tool for research and industrial inspection at the nanometer scale. However, instrument distortion can compromise image quality and introduce uncertainty in quantitative evaluations. Therefore, the necessity of calibration arises, serving to rectify distortions and ensuring the traceability of measurements.

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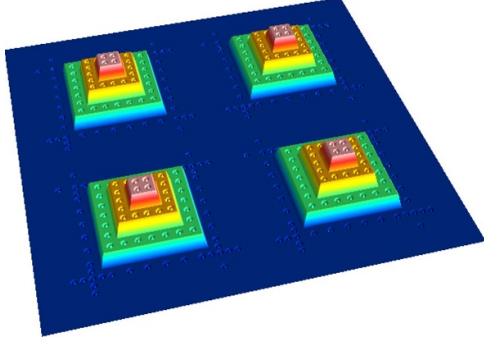


Figure 1. 3D calibration standard with ring-shaped nanomarkers on the substrate and the terraces of the pyramids.

Garnaes *et al* [8] proposed a 3×3 calibration matrix for calibrating and correcting linear systematic distortions in closed-loop SPMs. This calibration matrix is represented as:

$$M = \begin{bmatrix} C_x & C_{xy} & C_{xz} \\ 0 & C_y & C_{yz} \\ 0 & 0 & C_z \end{bmatrix}. \quad (1)$$

In this context, the x and y axes collectively define the horizontal plane, and the z -axis corresponds to the vertical dimension. The variables C_x , C_y and C_z signify the linear scale coefficients, while C_{xy} , C_{xz} and C_{yz} indicate the coupling between the corresponding axes. For an ideal SPM, these linear scale coefficients should be 1, and the coupling coefficients should be 0. However, in real SPMs, these values can deviate. The deviations may range from some tenths up to several tens of percent [9].

The conventional calibration process for SPMs comprises separate lateral and vertical calibration steps involving more than one calibration standards. In the horizontal plane, lateral linear scale coefficients C_x and C_y and the coupling coefficient C_{xy} are calibrated using a 2D grating with homogeneous pitch structures. For the vertical dimension, the linear scale coefficient C_z is calibrated using a step height standard. To determine the coupling coefficients in the vertical planes (C_{xz} and C_{yz}), an additional calibration procedure is required, often involving the use of a line standard with triangular line profiles [8].

Three-dimensional pyramidal standards developed by Ritter *et al* [10, 11] provide a novel approach to calibration within the measurement volume of SPMs. Ring-shaped markers, called nanomarkers, are located across the reference field at multiple height levels. The centers of the nanomarkers serve as precise 3D reference points, as illustrated in figure 1.

The calibration process compares the 3D coordinates of nanomarkers measured by a user's tool to their known reference 3D coordinates, obtained through traceable measurements using e.g. a metrological atomic force microscope (AFM) at National Metrology Institutes (NMIs) [12]. Following a least-squares affine 3D fitting of the measured coordinates to the reference coordinates of nanomarkers, this approach enables the calibration of three scaling factors as

well as three coupling factors of the user's tool. This calibration can be achieved with just one standard and one single measurement, offering the distinct advantage of simplicity and ease of use when compared to conventional nanoscale standards.

The company point electronic offers a dedicated software tool for computing 3D coordinates of nanomarkers from measured images. The software tool is delivered to customers along with a 3D pyramidal standard and its calibrated reference coordinates. As the software tool plays an essential role in the calibration chain, it is pivotal to validate the software to ensure the reliability of the calibration process.

In this paper, the evaluation algorithm of 3D calibration software is presented in section 2 as the basis of the research. Then, section 3 introduces a new software validation method. Section 4 presents the results of the validation, with a particular focus on assessing the impact of computational errors on calibration uncertainty.

2. Evaluation algorithm of 3D calibration

In addition to being accurate and robust, the 3D calibration algorithm is designed to prioritize speed and flexibility. The algorithm's flexibility is demonstrated by its ability to handle measurement data from various devices and its independent of sample orientation. To accelerate evaluation while ensuring high reliability, the algorithm uses prior knowledge of the geometry of the calibration samples. These so-called layout data facilitate the definition of marker size and shape, allowing for the minimization of search areas. This prior knowledge aids in setting up the most suitable model for the specific device during parameter estimation, eliminating redundancies and achieving accurate and reliable results.

Computation involved consists of two essential tasks. One is the detection of nanomarkers from microscopic images. It includes the calculation of 3D coordinates of nanomarkers from images measured by both the metrological AFM and the tool under calibration. The other is the least-squares affine 3D fitting of measured coordinates to the reference coordinates, allowing the calculation of three scaling factors as well as three coupling factors of the tool.

2.1. Marker detection

The 3D calibration samples are designed in such a way that circular markers are positioned on the substrate and terraces of pyramid-shaped structures. Distinct types and sizes of the markers are designated for different measurement instruments. Circular features are chosen because they provide rotation invariance and high accuracy in measurement and feature detection through image processing operators.

The marker detection process follows a multi-step approach. Initially, topographic data are transformed into height maps, enabling the application of various image processing methods. A modified Hough circle transformation [13] is employed for marker detection, capable of working

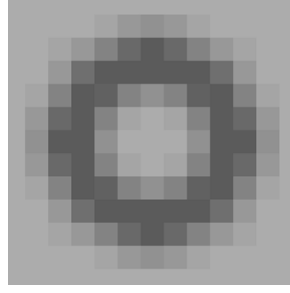


Figure 2. Automatically generated marker template, blurred with Gaussian noise.

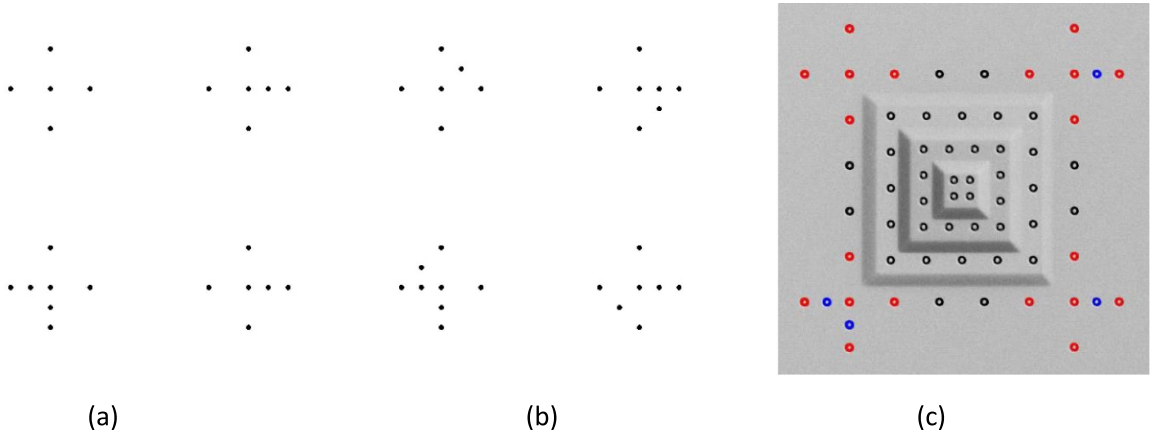


Figure 3. Finder structures are formed by markers with non-symmetric distribution, shown as (a) 4-bit coded finder structure; (b) 8-bit coded finder structure; (c) 4-bit coded finder structures on the calibration sample providing sample orientation information.

with different types of markers and being invariant to reverse contrasts, accommodating ring-shaped or circle-like markers, as well as deepened or protruding structures. The results yield candidates for the marker lateral positions and associated feature diameters.

The next step involves verifying the results obtained in the preceding step. Using the known geometry of the markers, feature matching methods are adapted. A synthetic image of the marker is generated from the known design data and blurred with Gaussian noise, as shown in figure 2. The template scale is applied from the original measurement data or optionally from the resulting Hough diameters. The lateral marker positions are then detected using a cross-correlation algorithm. By applying a threshold value for cross-correlation results of markers, the marker candidate list can be refined, containing only reliable marker positions, and rejecting any incorrect detections in the previous step. These positions are then compared with layout data to determine sample orientation and define search areas for the subsequent marker position detection.

Various methods, including image correlation, least-squares-matching, or the preferred image matching with paraboloid adjustment [14], are applied to achieve sub-pixel accuracy in the lateral center detection of the markers. The results provide the final lateral positions of the markers, each with a unique identifier.

The orientation of the measured data compared to the reference sample orientation, is determined by analyzing the non-symmetric distribution of the markers on the sample. Each pyramid on the calibration sample contains four special finder structures arranged into a corresponding code, as shown in figure 3. These codes, defined uniformly for all samples, are stored in a dedicated description readable by the image processing software. Currently, two different code systems are supported: 4 bit which enables 16 different tags, and 8 bit which enables 256 different tags.

Finally, the height value of the marker center is determined using standard interpolation methods, such as bilinear or optionally bicubic height interpolation in the original measurement data. The measured 3D coordinates of the markers are then ready for the estimation of the calibration parameters, as illustrated in figure 4.

2.2. Evaluation of calibration coefficients

Once the 3D coordinates of the marker centers are determined, the transformation of the measured coordinates is evaluated by comparing the marker positions to their known reference coordinates, obtained through traceable metrological instruments at NMIs.

As already mentioned in equation (1), a 3×3 matrix M which comprises six linear calibration coefficients (i.e. three

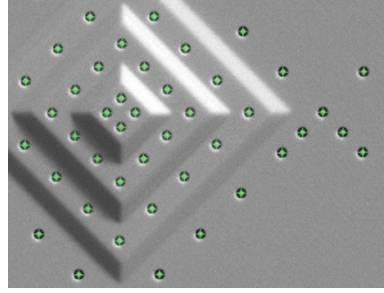


Figure 4. The 3D coordinates of the markers are determined.

Table 1. Pre-configured parameter setups in the estimation model.

Transformation	Parameters	Number of parameters	Remarks
3D shift	t	3	Only shift (e.g., for drift analysis)
3D rigid	t, R	6	Rigid adjustment (e.g., for device comparison)
3D similarity	t, R, c	7	Simple calibration with similar scales
3D non-isotropic	t, R, C_x, C_y, C_z	9	Calibration with individual scales
3D affine with lateral shear	$t, R, C_x, C_y, C_z, C_{xy}$	10	Complete linear scan system calibration (e.g., for scanning electron microscopy (SEM) application)
3D affine with spatial shear	$t, R, C_x, C_y, C_z, C_{xy}, C_{xz}, C_{yz}$	12	Complete linear calibration (e.g., for SPM application)

scale and three coupling coefficients) is to be determined for calibrating the geometrical properties of the user's tool. Additionally, to account for the rotational and translational misalignment of the standard when it was measured in the metrological instrument and in the user's tool, a 3×3 rotational matrix R and a spatial translation vector t are employed to depict the 6 degrees-of-freedom movement between the measured and reference coordinates. Thus, the transformation model encompasses up to 12 parameters.

Given the measured coordinates $S = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$, reference coordinates $S' = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix}$, and translation vector $t = \begin{bmatrix} t_x \\ t_y \\ t_z \end{bmatrix}$, the transformation model is defined as [10]:

$$S' = R \cdot M \cdot S + t. \quad (2)$$

The calibration coefficients estimation is over-determined due to the surplus of measured markers compared to the number of fittings parameters. Consequently, a least-squares parameter estimation (LSE) is applied to solve this over-determined equation system. The mean point error serves as a criterion for the quality of the 3D transformation evaluation. Calculated from the square root of the weighted residues, this

mean point error represents the remaining distances in all directions of the marker coordinates after the 3D transformation. A small mean point error indicates a highly linear measurement system primarily affected by small random errors, while a large mean point error suggests additional error sources like gross errors or systematic non-linearities. Gross errors are optionally detected as outliers and eliminated using statistical tests within the applied data snooping process [15].

In addition to the resulting scale and coupling coefficients, various statistical results from LSE facilitate further analysis of the transformation and, consequently, the calibrated user's tool. For example, the residuals after the application of the optimal parameter model describe the remaining errors vector in space. This enables the analysis and accuracy estimation of lateral distortions, non-linear height distribution, or other systematic errors in general.

In cases where no reference coordinates are available, two sets of coordinates obtained from two non-calibrated devices or successive measurements on the same device can be compared. In such a case, although being not traceable, the results offer useful information about the relative orientation, scale, and coupling of the two coordinate systems, thus for comparing different 3D measurement instruments or for analyzing the stability of a tool (i.e. drift analysis).

The implemented software offers an option to apply different transformations with different pre-configured parameter setups, as listed in table 1. Users can choose the most suitable

models for their applications. If no prior knowledge about the device is available, different models can be evaluated based on the resulting statistical values.

3. Methodology of software validation

It is crucial to identify, and if possible, rectify errors associated to the evaluation algorithm before its application in 3D calibration. In addition, it is essential to analyze how these errors may affect the uncertainty of the 3D calibration. Therefore, a validation scheme on 3D SPM calibration evaluation algorithm is implemented, as illustrated in figure 5.

The concept of the validation is as following. Assume a (virtual) tool has a given geometrical properties (M). In its simulated measurement, the tool will distort an ideal artifact and result in a simulated data set D . By feeding D to the software, its output M^* can be obtained. The difference between M and M^* indicates the contribution of the computation error on the calibration process. In realizing the validation scheme mentioned above, a key step lies in the generation of reference pairs (D, M) .

3.1. Generation of the reference matrix M

To generate the reference matrix M , the Monte-Carlo method is employed. The boundary conditions, i.e. the upper-limit and lower-limit of parameters, are set based on our experience of SPM calibration as follows:

For the three linear scale coefficients C_x , C_y and C_z : [0.99, 1.01].

For C_{xy} : [-0.01, 0.01].

For C_{xz} and C_{yz} : [-0.05, 0.05].

In conventional calibration procedures, the calibration of coupling factors in vertical planes, C_{xz} and C_{yz} , are more complicated and therefore less frequently executed. Considering the potential inaccuracy associated with C_{xz} and C_{yz} , it is reasonable to assume a maximum deviation of 5% for these two parameters. The other four parameters are considered more accurate, and therefore a maximum deviation of 1% is specified.

Within the specified boundary conditions, the six coefficients are randomly generated using uniform distributions. This method ensured that the reference matrix M is generated reflecting the practical conditions and potential uncertainties in SPM calibration.

3.2. Generation of the reference data D

As shown in equation (2), a pixel S' on the artifact surface in the ideal coordinate system is transformed into position S within the instrument coordinate system when a surface topography measurement is performed.

The equation (2) can be expressed as:

$$S = M^{-1} \cdot R^{-1} \cdot (S' - t). \quad (3)$$

The generation procedure of reference data $D = \{S_{ij}\}$ simulates the above measurement process. A result is demonstrated in figure 6. It maps the artifact surface in the instrument coordinate system and acquires a pixelized image through sampling.

To summarize, the generation of the reference data D encompasses three key steps:

- Generating an ideal artifact surface.
- Performing coordinate transformation.
The vector t and matrix R demonstrates the misalignment of the artifact. In the validation, elements in the vector t and the matrix R are uniformly distributed random values. The translations along the three axes are within the range of $\pm 1 \mu\text{m}$, while the pitch, yaw and roll are within the range of $\pm 2^\circ$.
- Sampling in the instrument coordinates.

In our study, two methods are employed for obtaining the ideal artifact surface S' :

- Synthetic SPM images: These images are generated from the given feature geometries (i.e., ground truth values) of 3D standards using the software tool, referred to as VirtualSPM, developed at the PTB [16]. Since the positions of nanomarkers are known in synthetic images, this method allows not only the assessment of the computation accuracy of the calibration matrix M but also evaluating the precision of nanomarker centers localization. This approach helps in determining the primary source of the computational errors, whether they come from the nanomarker center position determination or from the least-squares affine 3D fitting. Thus, the reliability of the 3D calibration software can be studied thoroughly.

Various measurement influencing factors can be simulated on the synthetic images for investigating their impacts. As an example, uniformly distributed noise within a range of $\pm 2 \text{ nm}$ is introduced to three measurement axes to investigate the impact of measurement noise.

- Real AFM images: These images are obtained from a metrological AFM and are considered the ideal artifact surface. Unlike the synthetic images, real measurements are subjected to e.g. noise and other measurement artifacts e.g. AFM tip and contaminations. The advantage of using real images lies in their ability to reveal and quantify the impact of these influences on the computation, thus allowing the examination of the robustness of the evaluation algorithm. The disadvantage is, however, the ground truth about the positions of nanomarkers is not available. Consequently, it only allows the assessment of the computation accuracy of the calibration matrix M . In this study,

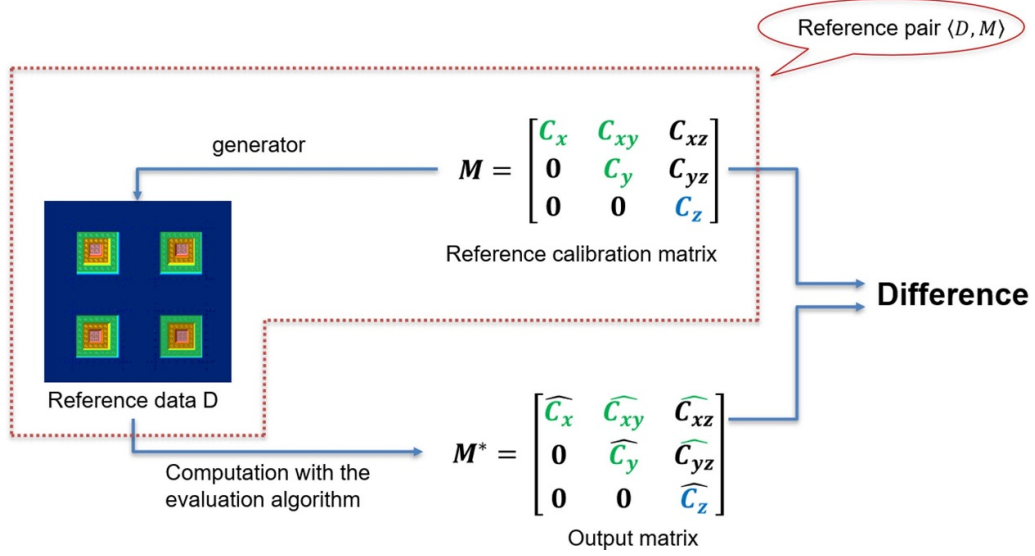


Figure 5. Proposed validation scheme for the 3D calibration evaluation algorithm.

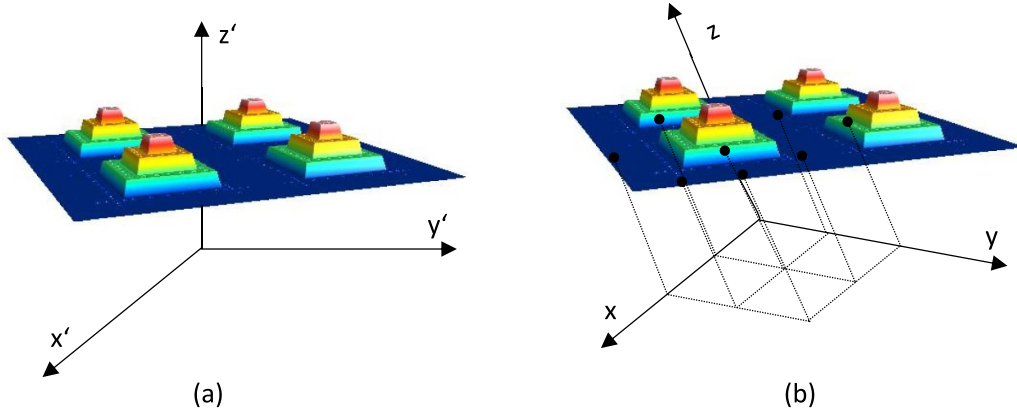


Figure 6. Schematic diagram of generating the reference data **D**, shown as (a) the artifact surface in the ideal coordinate system; (b) the artifact surface in the instrument coordinate system and image is acquired after sampling.

the validation utilizes images acquired from Metrological Large-range SPM (Met. LR-SPM) [17, 18].

Two 3D calibration standards, named MMC40 and MMC80, are studied in the validation. The numbers in the names of these standards, namely 40 and 80, indicate the sizes of their respective reference fields, which are 40 μm and 80 μm . The standards have a feature height of 1.8 μm and 3.9 μm , respectively. The layout of both standards is a pyramid array composed of four 4-step pyramids, as shown in figure 7. The standard MMC40 features a total of 352 nanomarkers, while the standard MMC80 contains 272 nanomarkers.

4. Results

Validation results, depicted in figure 8, present a comparison between outcomes obtained from synthetic images and a measurement image, based on the standard MMC40 with 1024×1024 pixels. The horizontal axes represent the input

reference coefficients. The vertical axes display the computational errors, with the result shown in red for the synthetic images without noise, blue for the synthetic images with noise, and black for measurement images.

As shown in figure 8, the distributions of the evaluated coefficient C_z are similar for the synthetic image with noise (shown in blue) and the measurement image (shown in black). These distributions span a much larger range compared to the synthetic image without noise (shown in red), unlike the situation observed for other coefficients. This observation suggests that the evaluation of C_z is more susceptible to noise in the evaluation algorithm compared to other coefficients. This sensitivity can be attributed to the fact that the lateral coordinates of nanomarkers are determined by the cross-correlation algorithm, which exhibits better potential in rejecting the influence of noise than the height interpolation algorithm used for calculating of the z -coordinates. Consequently, this result indicates that the vertical position evaluation algorithm for nanomarkers needs further improvement in terms of noise resistance.

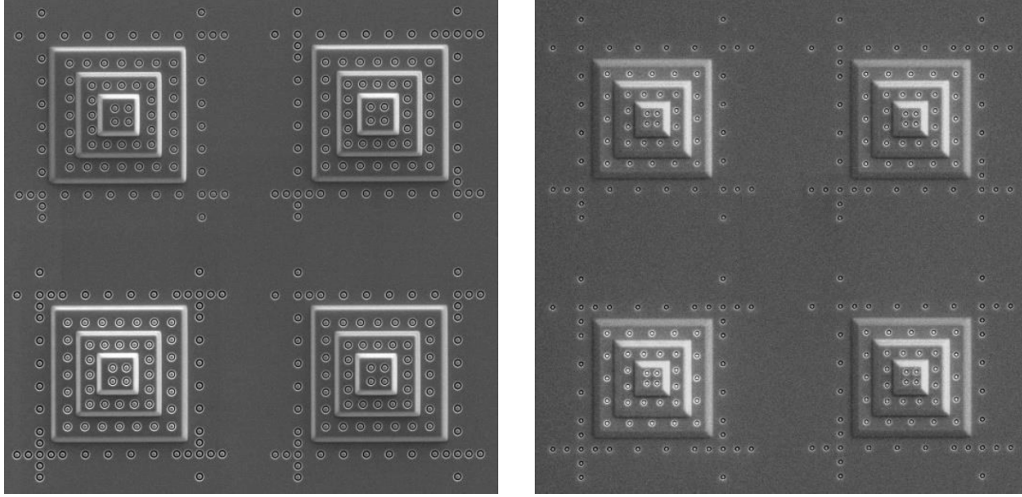


Figure 7. SEM images of the 3D standards MMC40 (left) and MMC80 (right).

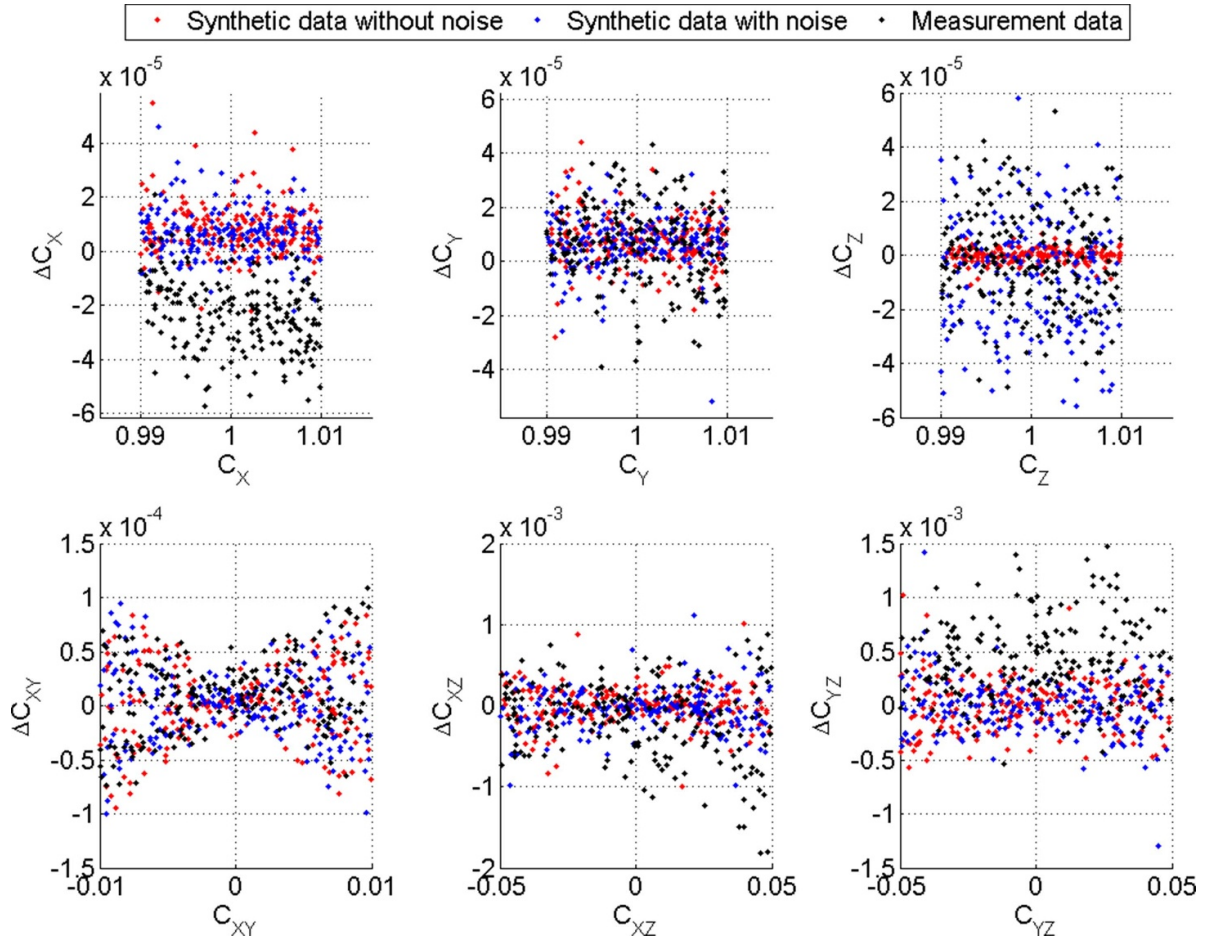


Figure 8. Computational errors assessed using synthetic images (red and blue) and a measurement image (black), based on the standard MMC40 with 1024×1024 pixels.

It is also worth noting that the computational errors for the three coupling coefficients tend to increase as the input coefficients deviate more from their ideal values. Conversely, the

computational errors for the three scale coefficients remain relatively constant and are not significantly impacted by variation in their corresponding coefficients.

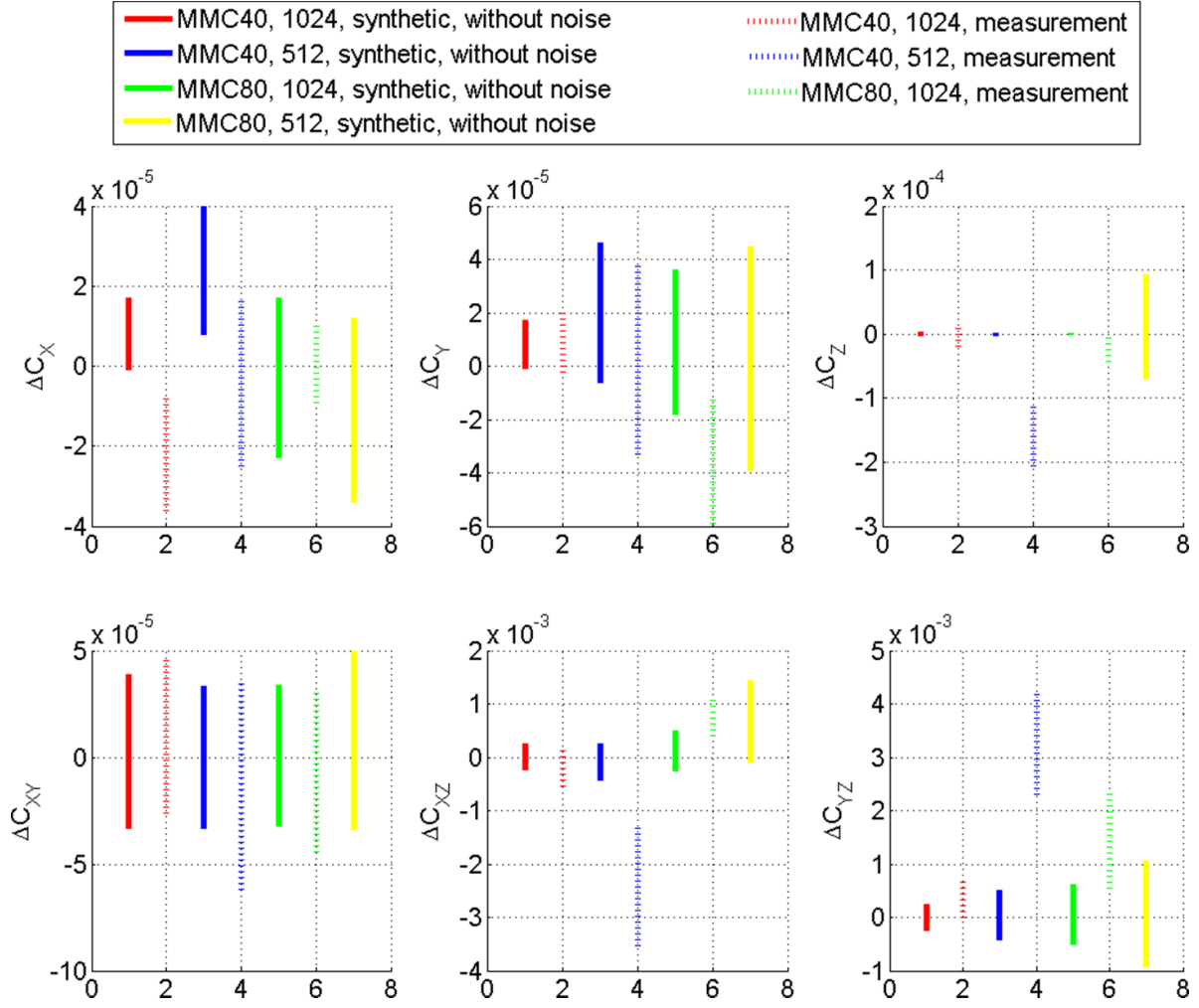


Figure 9. Computational errors assessed on standards MMC40 and MMC80 measured by 1024×1024 pixels and 512×512 pixels.

Figure 9 displays the validation results for both standards MMC40 and MMC80, with images of 512×512 pixels and 1024×1024 pixels. The result for the standard MMC80, based on 512×512 pixels measurement image, is not presented because the software fails to evaluate due to insufficient pixel density in practice. The inner marker plateau has only 5 pixels if the image is measured with 512×512 pixels, and consequently noise will have a big influence on the results. For this reason, 1024×1024 pixels are recommended in practice. Nevertheless, this study tries to understand the impact of different pixel numbers on the computation.

In the graph, the midpoints of the line segments represent the mean values of the computational errors, while the segment lengths correspond to 2 times the standard deviations (2σ). In general, the computational errors using the standards MMC40 are marginally smaller than those observed with MMC80, and errors tend to be slightly reduced when working with 1024×1024 pixel images compared to 512×512 pixel images.

The computational errors for the coefficients C_x , C_y and C_{xy} are below 10^{-4} . Most computational errors for the coefficient C_z also fall below this threshold, except for the result based on

the MMC40 512×512 pixels measurement image. The computational errors of the coefficients C_{xz} and C_{yz} exhibit about one order of magnitude larger than others. This can be attributed to three possible factors:

- In the boundary condition setting, the variations of C_{xz} and C_{yz} are more pronounced compared to other coefficients.
- C_{xz} and C_{yz} are influenced by evaluations both in the horizontal plane and in the vertical direction.
- The geometric setup of the calibration sample or, in mathematical terms, due to the inadequate distribution of the model concerning the vertical shearing. Because of the small height of the sample, minor position errors lead to significant vertical angle deviations. When using the complete calibration area, the height-to-length ratio is about 1:20, which is comparable to the relationship between ΔC_{xy} and ΔC_{xz} (or ΔC_{yz}) (see figure 8).

To understand the contribution of the computational errors to the overall calibration uncertainty, the computational errors (2σ) from both the synthetic and measurement images are compared with the overall expanded calibration uncertainty

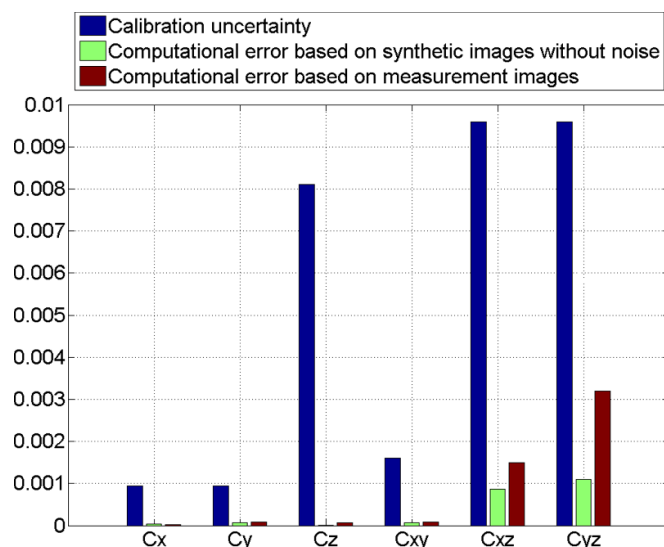


Figure 10. Computational errors (2σ) from both synthetic and measurement images are compared to overall calibration uncertainty, indicating that the developed 3D calibration evaluation algorithm and software are reliable in context of the state-of-the-art calibration uncertainty.

($k = 2$) of 3D calibration of the Met. LR-SPM, as presented in figure 10. The computational errors for C_{xz} and C_{yz} , are approximately 1/5–1/3 of the overall uncertainty, indicating their significant impact. In contrast, the computational errors for the other four coefficients are smaller than 1/10, so their influence on the evaluation process is negligible.

It is worth noting that in the aforementioned example, computational errors contribute a relative significant contribution on overall calibration uncertainty, as the Met. LR-SPM is proved to be one of the most accurate calibration tools for 3D objects of comparable size. For measurements with user instruments, computational errors will be even less significant. Thus, the results indicate the developed 3D calibration evaluation algorithm and software are reliable in context of the state-of-the-art calibration uncertainty.

5. Summary

Complex 3D calibration algorithm and software is designed to automatically detect the 3D positions of markers on the calibration artifact with sub-pixel accuracy, robustness, high speed, and flexibility. Validation of the algorithm and software is an essential task from the perspective of quality management. This paper presents a methodology for such validation. To verify the computational error of the 3D calibration algorithm, reference calibration matrices are generated using Monte-Carlo method under specified boundary conditions. The reference data are applied using synthetic SPM images and real measurement images.

As the result, the computational errors of the coupling coefficients C_{xz} and C_{yz} can reach up to 1/3 of the overall calibration uncertainty budget of a metrological SPM for these coefficients, highlighting their unignorable impact. For other

coefficients, namely C_x , C_y , C_z and C_{xy} , computational errors remain relatively small, with a limited impact on the calibration process. The study validated that the developed 3D calibration evaluation algorithm and software are reliable in context of the state-of-the-art calibration uncertainty.

Although the focus of this study is on the 3D calibration of SPMs, it should be mentioned that the pyramidal 3D standard is applicable for calibrating a diverse range of 2D and 3D microscopes, such as conventional 2D SEM, and 3D SEMs [19], which are typically realized using a multi-segment back-scattered electron detector or based on the stereophotogrammetry principle. In addition, new iterations of 3D calibration standards, featuring larger sizes and alternative marker designs tailored for optical metrology (confocal laser scanning microscopes etc) [20], are currently under development. These advancements underscore the growing potential of 3D calibration standards in research and various industries. However, the methodology and results of this study can be readily extended to the calibration of other kinds of microscopes.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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