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A simulation method to estimate task-specific uncertainty in 3D Microscopy

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Abstract:

Traceability in micro-metrology requires an infrastructure of accredited metrology institutes, effective performance verification procedures, and task specific uncertainty estimation. Focusing on the latter, this paper proposes an approach for the task specific uncertainty estimation based on simulation for a generic 3D microscope. The proposed simulation approach is based on the identification and successive parameter estimation of an empirical model of the measured points. The model simulates the probing error based on a Gaussian process model, thus including the correlation among close points. Parameters for the error simulation are estimated by a deep analysis of error sources of the 3D microscope. Validations of the proposed simulation approach are carried out in the case of focus variation microscopy (FVM), considering several case studies. The procedure proposed in the ISO/TS 15530-4 standard are applied for validation.

Keywords: Uncertainty, 3D microscopy, geometrical metrology, micro-metrology, ISO/TS 15530-4, focus-variation.

1. Introduction

Micro-engineered components are important since they can integrate functions and intelligence into products [1]. These products need micro-geometrical metrology to verify their compliance to tolerances. Coordinate measuring systems (CMSs), being suitable for micro-geometrical metrology are in most cases non-contact (optical) instruments, due to their flexibility in accessing the surface of parts, elimination of the risk of damaging small and delicate micro features and fast data acquisition rate [2]. Among the others, 3D microscopy (3DM) seems very promising and already counts a lot of industrial applications, particularly in the field of surface analysis. 3DM gathers technique like coherence scanning interferometry, phase shifting interferometry, confocal scanning microscopy, confocal chromatic microscopy, digital holography, and focus variation microscopy. Most 3DM techniques are based on the sequential acquisition of images of the sample, while changing the distance between the sample and the objective lens.

1.1 Measurement traceability and uncertainty

Regardless of the considered measuring instruments, traceability of measurements is very important for a reliable measurement result in the case of micro-geometrical metrology as well. Traceability requires not only periodical instrument performance verification to check if measuring instruments behave as stated by the manufacturer or according to some predefined performance index, but also measurement uncertainty

49 must be stated to guarantee measurement comparability [3]. The subject of performance
50 verification has been addressed by the authors in previous papers [4, 5]: this paper
51 addresses the problem of the uncertainty estimation.

52 The main reference for measurement uncertainty estimation is the “Guide to the
53 expression of uncertainty in measurement” (GUM) [6]. According to the GUM, when
54 a final measurement result comes from several distinct measurement data processes,
55 the uncertainty is derived based on the propagation of the uncertainty from each
56 uncertainty contributor along the data processing chain, thus GUM requires a closed
57 form mathematical model of the measurement. In addition, for coordinate metrology,
58 measurement uncertainty is “task-specific” [7], i.e. a single measuring instrument can
59 perform several different measurement tasks with different measuring strategies, which
60 are characterized by a different uncertainty [8]; hence the GUM method is difficult to
61 apply.

62 The ISO 15530-3 [9] and ISO/TS 15530-4 [10] standards propose alternative methods
63 to effectively estimate the measurement uncertainty for coordinate metrology. The ISO
64 15530-3 method needs expensive calibrated artifacts; hence it is not suitable when a
65 product has many variants, as it would require many different calibrated artifacts, or
66 when small production volume cannot justify the cost of a calibrated artifact. The
67 ISO/TS 15530-4 simulation method seems more promising in the case of high product
68 or high demand variability. The main drawback of the simulation method is its
69 computational intensity [11], but the continuous reduction of computational costs
70 should reduce this issue.

71

72 *1.2 Simulation approaches*

73 A simulation-based approach seems to be the most promising solution to estimate a
74 task-specific measurement uncertainty, especially for optical-distance sensor
75 instruments, as suggested by Evans [11] in the case of interferometry. Baldwin et al.
76 [9] used a simulation approach to estimate the uncertainty in tactile-CMM
77 measurement. They simulated CMM geometric errors and incorporated them in the
78 kinematic model of the CMM, so that the nominal position of points could be modified.
79 Kruth et al. [12] proposed a similar approach, with addition of part form deviation as
80 an uncertainty source. Cheung et al. [13] also used a similar approach to estimate the
81 uncertainty in the case of free-form surface measurements. All these simulation
82 approaches neglect the presence of spatial correlations among the sampled points.

83 In general, a simulation approach relies on a point perturbation process (an error
84 simulator) generating a perturbation of a reference cloud of points, as shown in Figure
85 1. Detailed explanation of the framework applied to CMMs was described by Trapet
86 and Waldele [14]. The scheme consists of two paths, the first one (Figure 1: black
87 arrow) estimates a measurement result Y , while the second one (Figure 1: red arrow)
88 estimates the measurement uncertainty U . The first path is explained as follows: a point
89 cloud is obtained by the selected measuring system using a defined measuring strategy.
90 This point cloud is then processed to calculate the measurement result Y . The second
91 path starts from the same sampled point cloud. A point perturbation process by
92 measurement error simulation is applied to the original point cloud. The perturbed point
93 cloud is processed by the same numerical algorithm that gathered to the measurement
94 result and the results are stored. The simulation of the error is repeated for an adequate
95 number of times (usually a few thousand) and the simulated measurement results are
96 stored. The estimated uncertainty u_{sim} ($U = 2 u_{sim}$) of a measurement is the sample
97 standard deviation of the stored results from the simulation runs.

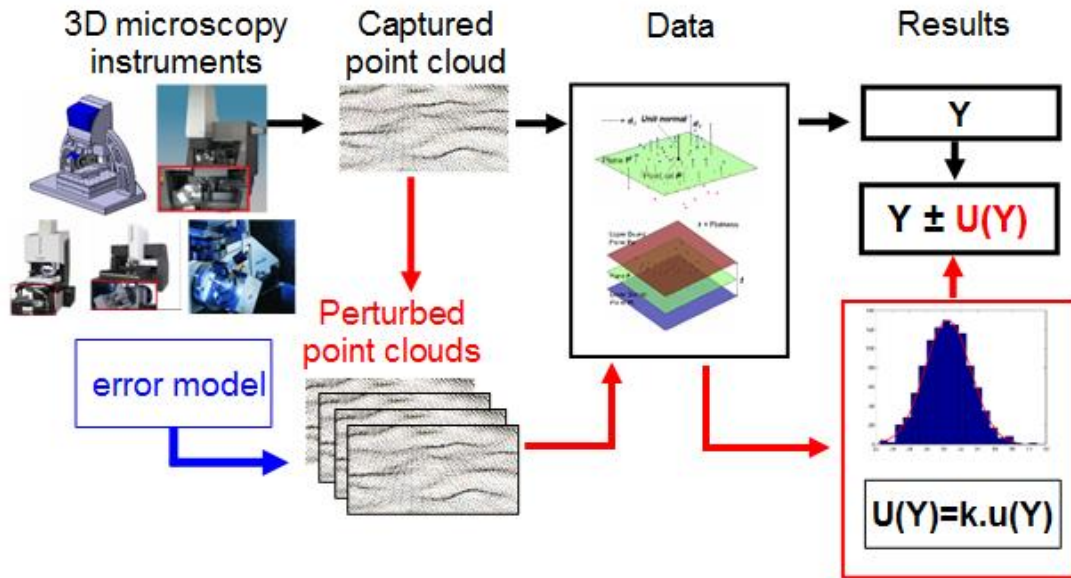


Figure 1: Framework a simulation method for the uncertainty estimate.

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99

100

101 1.3 Research aim

102 In this paper, a simulation-based approach considering spatial correlation among
 103 points is proposed. The proposed model does not directly take into consideration
 104 physical phenomena related to interactions between materials and light; rather the
 105 model includes the effect of the physical interaction between the materials and the light
 106 inside several uncertainty sources, e.g. material types, and parameters of the simulation.

107 There are several technical reasons behind this consideration. First, even if well-
 108 established physical models exist for the interaction between electromagnetic waves
 109 and matter, their application is numerically impractical to apply and to the degree of
 110 accuracy required for 3DM measurement simulation. In general, the intensity value on
 111 each single pixel is not completely independent of the others. Hence, a single ray
 112 coming to the complementary metal-oxide semiconductor (CMOS) sensor has some
 113 degree of correlation with its neighbor ray of light [15]. And finally, some techniques
 114 add an additional contribution to the correlation among points, as the optimization
 115 function allowing the identification of the coordinates of the single point is calculated
 116 considering the neighboring pixels, selected by a windowing process [15].

117 Hence, to empirically model this phenomenon, the basis of the methodology is a
 118 Gaussian process [16], in which data are randomly distributed according to a
 119 multivariate Gaussian distribution, whose covariance structure depends on the spatial
 120 distribution of points. The multivariate Gaussian process can capture and simulate the
 121 correlation among points.

122 This paper is structured as follows. Section 2 describes the mathematical model
 123 allowing the simulation of the correlated points. Section 3 introduces Focus Variation
 124 Microscopy (FVM) as technology considered for the validation of the approach, and
 125 then focuses on the estimation of the parameters required to run the simulation. Finally,
 126 section 4 validates both the model and the estimation of the parameters according to the
 127 ISO/TS 15530-4 standard.

128 2. Task-specific uncertainty estimation by simulation in 3DM

129 The proposed approach relies on a point perturbation process (an error simulator)
 130 adopting a Gaussian process model taking into account the correlation among points,

131 as shown in Figure 1. A correlation means that the error behavior of a point depends on
 132 other points within a certain distance from it. The simulation approach (figure 1, blue
 133 box) uses a Gaussian process model completely defined by a variogram function, we
 134 call it “variogram error model”. The need of this kind of model arises from the how a
 135 3DM measurement is taken. As explained in section 1.3, it is expected that the
 136 measurement errors of the single sampling points are not independent but correlated.
 137 An independent simulation of them could then lead to a simulation far from the reality.
 138 The use of a Gaussian process described by a variogram error model allows the
 139 simulation of non-independent measurement errors, coherently with the measurement
 140 method.

141

142 2.1 Mathematical model for the simulation of a perturbed cloud of points

143 The core of the uncertainty estimation by simulation is the model for the perturbation
 144 of the point cloud. In general, the perturbation of the cloud of points is given
 145 ε_{θ_x} , ε_{θ_y} , ε_{θ_z} , which are rotation errors with respect to x , y and z axes, and ε_x , ε_y , ε_z i.e.
 146 linear errors along x , y and z directions, respectively. Once these perturbations have
 147 been generated for each point, \mathbf{p}_i' , the coordinates of a single perturbed point, can be
 148 generated from the original measured points \mathbf{p}_i , (both are expressed in homogeneous
 149 coordinates) by multiplying the measured points \mathbf{p}_i time an error matrix, \mathbf{T}_{err} , that is:

150

$$151 \quad \mathbf{p}_i' = \mathbf{T}_{err} \mathbf{p}_i = \begin{bmatrix} 1 & -\varepsilon_{\theta_z} & \varepsilon_{\theta_y} & \varepsilon_x \\ \varepsilon_{\theta_z} & 1 & -\varepsilon_{\theta_x} & \varepsilon_y \\ -\varepsilon_{\theta_y} & \varepsilon_{\theta_x} & 1 & \varepsilon_z \\ 0 & 0 & 0 & 1 \end{bmatrix} \mathbf{p}_i \quad (1)$$

152

153 In 3DM most of the error terms can be neglected. In fact, the x and y coordinates are
 154 not directly measured, but considered at their nominal value, as defined by the objective
 155 lens magnification and the sensor size of the 3DM. Moreover, during the scan the x and
 156 y do not move, and the translation along z is very small, so rotation errors are negligible.
 157 As such, the model can be simplified considering only the ε_z term.
 158 A correlated error for the i -th point, ε_{z_i} , is generated by sampling from a multi-variate
 159 Gaussian distribution. The multivariate normal distribution density function is
 160 formulated as:

161

$$162 \quad f(\mathbf{p}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{|\boldsymbol{\Sigma}|} (2\pi)^m} e^{-\frac{1}{2}(\mathbf{p}-\boldsymbol{\mu})\boldsymbol{\Sigma}^{-1}(\mathbf{p}-\boldsymbol{\mu})} \quad (2)$$

163 where m is the dimension of the multivariate, i.e. the number of points, \mathbf{p} represents the
 164 random vector with mean $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ is a $m \times m$ variance-covariance matrix which
 165 represents correlation. As the cloud of points is being randomly perturbed, the $\boldsymbol{\mu}$ term
 166 is set equal to 0. There are several ways of modelling $\boldsymbol{\Sigma}$. Among the others, we have
 167 selected the use of the variogram $2\gamma(\bullet)$ [16]. The variogram is well known and widely
 168 applied in spatial statistics, as its estimation is more robust compared to competitor
 169 method. The variogram function, together with the mean vector $\boldsymbol{\mu}$, fully characterizes
 170 the Gaussian process. Here we will address only isotropic homogeneous variogram
 171 function, as they are the simplest type of variograms, to simplify the discussion.
 172 Moreover, they have been found to be adequate for our case study. Details on non-
 173 isotropic homogeneous variograms can be found in the proposed literature. An isotropic
 174 homogeneous variogram function is defined as:

175

176 $2\gamma(\mathbf{x}_1, \mathbf{x}_2) = 2\gamma(h) = E[(Z(\mathbf{x}_1) - Z(\mathbf{x}_2))^2]$ (3)

177

178 where $2\gamma(\bullet)$ is the variogram function, h is the lag (distance) between the generic
 179 locations \mathbf{x}_1 and \mathbf{x}_2 , and $Z(\mathbf{x})$ is a response function at \mathbf{x} (in 3DM the z -coordinate of a

180 point). Please note that the assumption $2\gamma(\mathbf{x}_1, \mathbf{x}_2) = 2\gamma(h)$ implies the variogram is isotropic.

181 The typical shape of a $\gamma(\bullet)$ function is illustrated in Figure 2. Example functions suitable

182 to model isotropic homogeneous variogram models, but many more exist in literature,

183 are:

184

$$\gamma(h) = \begin{cases} 0 & h = 0 \\ n + s \left(1 - \exp\left(-3\frac{h^2}{r^2}\right) \right) & h \neq 0 \end{cases} \text{ Gaussian model}$$

185

$$\gamma(h) = \begin{cases} 0 & h = 0 \\ n + s \left(1 - \exp\left(-3\frac{h}{r}\right) \right) & h \neq 0 \end{cases} \text{ Exponential model} \quad (4)$$

$$\gamma(h) = \begin{cases} 0 & h = 0 \\ n + s \left(1 - \exp\left(-3\frac{h}{r}\right) \right) & 0 < h \leq r \\ n + s & h \geq r \end{cases} \text{ Spherical model}$$

186

187 where s , n , r are a sill, nugget, and range, respectively. These three parameters

188 characterize all variogram models (Figure 2). Nugget (n) is a non-zero limit

189 representing a discontinuity in a variogram origin. The nugget represents the pure white

190 noise included in the random error. Sill (s) quantifies the error dispersion at infinite

191 distance, i.e. global correlated and uncorrelated measurement noise. Range (r) is a

192 measure of the distance up to which the measurement noise is significantly correlated.

193 Supposing the variogram error model and its parameters are known, having defined

194 a set of locations \mathbf{x} , the Σ matrix can be built as

195

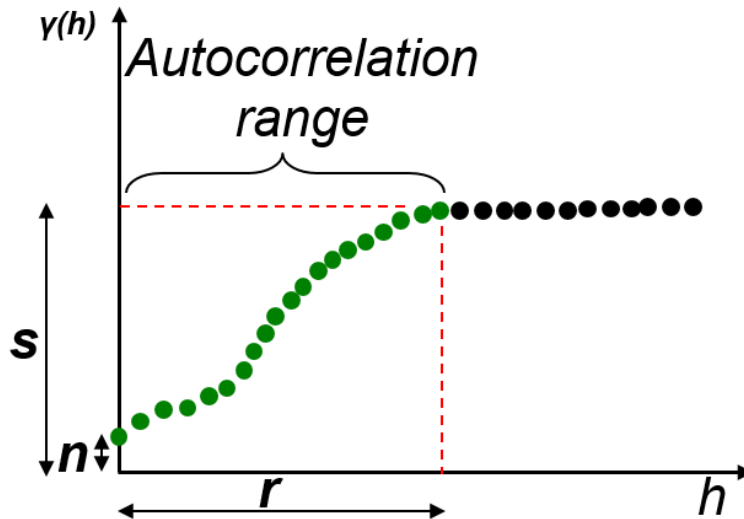
196 $\Sigma_{ij} = s - \gamma(\mathbf{x}_i, \mathbf{x}_j)$ (5)

197

198 Once the Σ matrix is known any multi-normal random number generator can be applied

199 to generate the ε_{zi} term at the \mathbf{x}_i location.

200



201

202

203

Figure 2: Illustration of variogram function and its s , r , n parameters.

204 2.2 Estimation of the variogram parameters for the simulation

205 The variogram model and its parameters need experimental identifications and
206 evaluations. From experimental data, a least-square method is usually adopted to fit the
207 empirical model of the variogram. Given a set of observations $Z(\mathbf{x}_i)$ (e.g. a single scan
208 of a surface by 3DM), the value of the variogram at distance h can be estimated as
209

$$210 \hat{\gamma}(h) = \frac{1}{2|N(h)|} \sum_{N(h)} \left(Z(\mathbf{x}_i) - Z(\mathbf{x}_j) \right)^2 \quad (6)$$

$$211 N(h) = \{ (\mathbf{x}_i, \mathbf{x}_j) \mid \|\mathbf{x}_i - \mathbf{x}_j\| = h \} \quad (7)$$

212

213 In the specific case of 3DM, as the points are locate on an evenly spaced grid, the
214 possible values of h are well defined, so there are a series of well-defined values of
215 $\hat{\gamma}(h)$. The $\hat{\gamma}(h)$ are then fitted, considering different variogram models. Based on R^2
216 of the least-square fitting, the best-fitted variogram model is selected, and then, the n ,
217 s , and r parameters are estimated.

218 The least square estimation of the s , n , and r parameters is in general applicable to a
219 single sampled surface. It is then evident that the resulting parameters will be specific
220 for the particular condition at which the scan has been conducted, e.g. material type. To
221 have parameters that can be applied in a larger variety of conditions, we must modify
222 them in order to take into account other uncertainty contributors. While the estimate of
223 the nugget and the range can be properly estimated on a single scan, the sill, being
224 representative of the overall variability of the measurement noise (correlated and
225 uncorrelated), should include all the uncertainty contributors, and not only those from
226 the condition at which it has been characterized so far. Hence, the parameter s resulting
227 from the least square fitting shall be combined with other error sources before the
228 simulation, according to the formula:

229

$$230 s_{sim} = \sqrt{s^2 + \sum s_i^2} \quad (8)$$

231

232 where s is the sill originally obtained from the fitted model of the variogram and s_i
233 is the contribution related with the i^{th} source of error. The estimate of the s_i terms
234 require a deep analysis of the specific uncertainty sources affecting a particular 3D
235 microscope, and an extensive experimental investigation of them. Anyway, once the
236 contributors are known, their value can be extended to any future measurement.
237

238 3. Case study: the uncertainty estimation for a Focus Variation Microscope

239

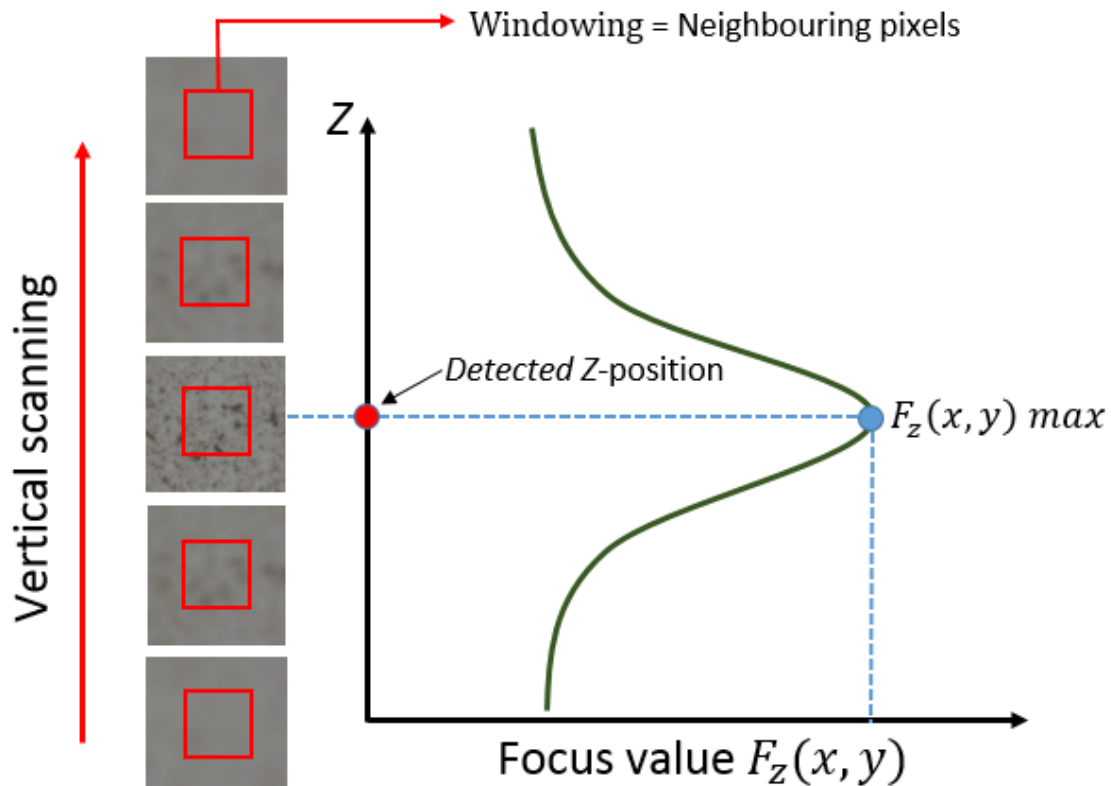
240 Focus variation microscopy (FVM) is considered in this study as an example of 3DM.
241 The FVM instrument used to demonstrate the proposed simulation approach is a 4th
242 generation FVM instrument by Alicona Imaging GmbH.

243 A FVM works based on the local focus condition of a stack of images taken at
244 different distances from the measured surface to the FVM objective lens. The FVM
245 working principle is as follows (see Figure 3): first, a stack of images is taken over a
246 specified range of z -level (the distance from the measured surface to the scanning
247 objective lens); the stack image acquisition is usually obtained by mechanically moving
248 the objective lens of the FVM. For each z -level and for each pixel of the related stacked
249 images, a focus value $F_z(x, y)$, which is a contrast of a pixel with respect to its
250 neighboring pixels, is calculated. In most cases, the more the image is in focus, the

251 higher the focus value is. For each pixel a mathematical fitting procedure is applied to
252 the calculated focus values at each level, and the detected z -coordinate of a point is
253 determined corresponding to the z -level with the highest $F_z(x, y)$ [15].

254 One fundamental advantage of a FVM instrument compared to other optical
255 microscopy is its large working volume and its long working distance of the objective
256 lens. This fundamental advantage provides the possibility of measuring the geometrical
257 properties of a part.

258 The FV values calculated for each (i, j) pixel locations are obtained by comparing its
259 contrast with respect to the intensity of its neighbor pixels.
260



261
262 Figure 3: FVM working principle by calculating a focus value inside a windowing
263 area.
264

265 3.1. Estimation of the variogram parameters

266 Different materials can be characterized by different variograms. In this study, we
267 consider calibrated plates in aluminum (Al), stainless steel (SS), and titanium (Ti) for
268 the variogram characterizations. It is worth to note that the variogram characterization
269 data need to be obtained from a real surface in order to take into account the physical
270 properties of the real measured surface, e.g. a roughness effect, local slope effect,
271 reflectance effect, measurement angle effect and speckle noise effect of the surface to
272 be included into the simulation process. Hence the variogram model takes into account
273 the material type as uncertainty source. The variogram data from the actual surface
274 measurements from the mentioned three materials will be used for uncertainty
275 estimation with industrial case studies (section 4).

276 The variogram characterization, required to estimate the degree of a spatial
277 correlation among points, is a fast procedure. The procedure only takes one single
278 measurement with a single image field of a surface to be measured. It is worth noting
279 that from a single image, a total of \sim one million points are obtained. A single image is

280 sufficient to characterize the variogram because in an empirical variogram estimate
 281 every couple of points counts as a variance estimate replica.

282 The flatness of the three materials was calibrated by means of a traceable CMM with
 283 $E_{0,MPE}=2+L/300 \mu\text{m}$. Methods selected for the calibration are multi-position and multi-
 284 measurement strategies. A total of four different positions for the part were considered
 285 during the calibration of the plates. For each position, five measurements were repeated.
 286 By this method, an uncertainty contribution of the volumetric error of the CMM is also
 287 taken into account in the total calibration uncertainty. The results of the calibration and
 288 their uncertainty are (notation is based on GUM [4]): aluminum = 25.1(8) μm , stainless
 289 steel = 4.8(1) μm , and titanium = 4.1(2) μm .

290 To yield the data on which to define the variogram models, the plates were measured
 291 having the optical axis of the FVM approximately perpendicular to the plate itself, using
 292 the scan parameters in Table 1. The empirical variogram was then evaluated on these
 293 scanned surfaces. The variogram models in Eq. 4 are least-square fitted and the
 294 parameters s , n , and r are calculated. The model is selected based on the highest R^2
 295 value of the data fitting. Table 2 presents the selected variogram models and their R^2
 296 value for the considered three materials (Al, SS, Ti). Detailed variogram
 297 characterizations can be found in [17]. The nugget effect has been indicated equal to 0
 298 because its value did not differ significantly from 0. This indicates a very strong
 299 statistical correlation among measurement errors at short distances, which is due to the
 300 FVM measurement principle based on a focus value calculated over a small patch of
 301 pixels.

302 Regarding the vertical and lateral resolution, they are set following the default values
 303 proposed by the instrument manufacturer with a 5 \times objective lens. It is worth noting
 304 that the selected lateral resolution is larger than the pixel size of the instrument. For the
 305 5 \times objective lens, the pixel size is 1.76 μm . But, the actual resolution (the smallest
 306 distance between two features that can be resolved) will be larger than the pixel size
 307 due to the working principle of the instrument. As the measuring principle of the
 308 instrument needs the consideration of a patch of pixels around the considered point to
 309 calculate the focus measure that defines the z -level of the point, the effective resolution
 310 is reduced by the averaging effect of the focus measure estimated on the patch (see
 311 figure 3).

312 **Table 1** Measurement parameter for Al, SS, and Ti materials.

| Material | Exposure time [μs] | Contrast | Vertical Resolution [μm] | Lateral Resolution [μm] |
|-----------------|---------------------------------|----------|---------------------------------------|--------------------------------------|
| Aluminum | 114.4 | 1.33 | 0.4 | 7.82 |
| Stainless steel | 116.4 | 1 | 0.4 | 7.82 |
| Titanium | 224 | 1 | 0.4 | 7.82 |

313

314 **Table 2** Selected variogram model for Al, SS and Ti.

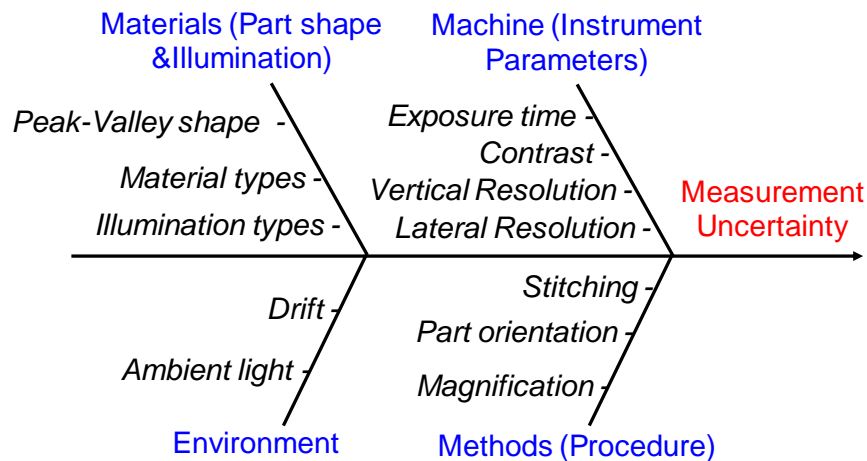
| Material | Variogram model | R^2 | s [μm] | n [μm] | r [μm] |
|----------------------|-----------------|-------|-----------------------|-----------------------|-----------------------|
| Aluminum (Al) | Exponential | 0.56 | 31 | 0 | 114 |
| Stainless steel (SS) | Exponential | 0.78 | 2.8 | 0 | 56 |
| Titanium (Ti) | Gaussian | 0.71 | 3.9 | 0 | 18 |

315

316 3.2. Estimation of the contributors to the sill value for the simulation

317 An extensive experimental campaign was carried out to estimate the various s_i terms
 318 involved in FVM measurements. Therefore, the physical aspects of a FVM
 319 measurement, considered as uncertainty sources, are included into the simulation.

320 A FVM uses a sensor to take a series of images at different distances from a surface.
 321 A focus value is then calculated and a height is associate to each pixel. In case, stitching
 322 can be applied to increase the size of the scan. This process is prone to a lot of
 323 uncertainty sources that cannot be considered by the experiment proposed in section
 324 3.1. Therefore, more uncertainty sources are estimated. Figure 4 schematically depicts
 325 the main uncertainty contributors in FVM measurements.
 326



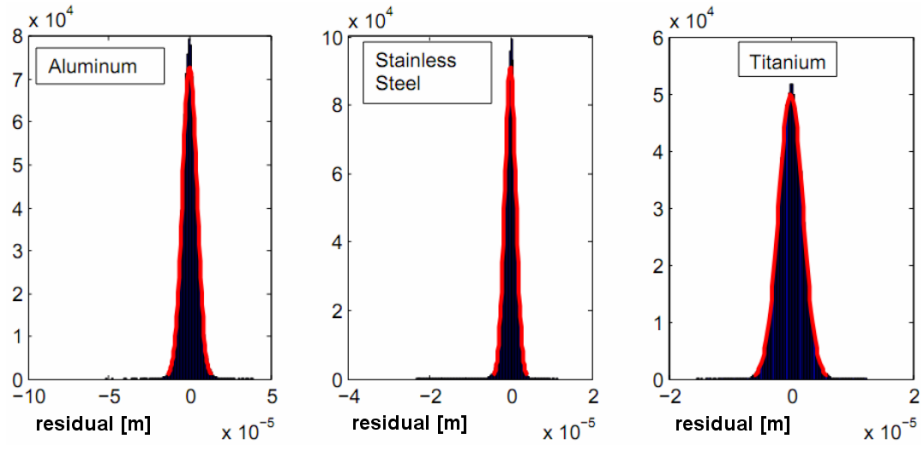
327
 328 Figure 4: Diagram of the uncertainty contributors in FVM measurements [17].
 329

330 An extensive experimental campaign has been conducted to study and quantify the
 331 effect of the mentioned factors and to include them into the simulation parameters. The
 332 three materials already mentioned were considered: aluminum (Al, specular surface),
 333 stainless steel (SS, lambertian surface), and titanium (Ti, lambertian surface). The
 334 numbers of points produced by a FVM measurement ranges from ~1 to ~4 million 3D
 335 spatial points. The analysis of variance (ANOVA) has been used to determine the
 336 significance of the factors.

337 Outliers were removed from the obtained datasets before measurement results could
 338 be extracted. This procedure is important since a large data point set is obtained from a
 339 single measurement cycle and outlying points among these (points presenting a very
 340 large algebraic deviation compared to other points in the scan) could reduce the
 341 accuracy of the measurement result. A simple outliers removal procedure has been
 342 applied, i.e. points having a deviation greater than 3σ from the fitting plane or cylinder
 343 of data points (depending on measured form) were removed, where σ is the sample
 344 standard deviation of all point deviations, that are distances from points to the fitted
 345 geometry.

346 A Shapiro-Wilk test, applied to the residuals (errors) of measured points, proved
 347 normality of the deviations with p -value around 0.8 for all the datasets. Figure 5 shows
 348 the histogram of the deviations (residuals) of points to the fitted plane for the three
 349 materials. The red line is the fitted Gaussian density function. The standard deviation
 350 (σ) of the residuals is presented in Table 3.

351 In this uncertainty characterization studies, the standard deviation σ of measurement
 352 residuals due to different parameters and measurement conditions is considered as
 353 parameter characterizing the impact or effect on the measurement uncertainty. The
 354 measurement residuals are σ of point deviations (a point distance error) to a fitted
 355 geometry, e.g. a plane, sphere and cylinder.
 356



357
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Figure 5: Histogram of residual from a fitted plane for the Aluminum, Stainless steel and Titanium materials.

Table 3 Standard deviation of residuals for the three materials.

| Material | σ [μm] |
|----------------------|----------------------------|
| Aluminum (Al) | 4.49 |
| Stainless steel (SS) | 1.37 |
| Titanium (Ti) | 2.00 |

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3.2.1 Influence of ambient light and different magnification lenses

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A randomly structured surface of a polymeric injection-molded part was used to evaluate this contribution. The polymeric surface is considered because it has a high surface diffusivity and low roughness < 200 nm. Therefore, the surface is smooth and good to estimate the measurement repeatability in the study and to understand the effect of ambient light in a FVM measurement.

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Measurements were carried out at $5\times$ and $10\times$ magnifications, both with the ambient light switched on or off. Numbers of 20 repetitions were carried out with around ~ 1 million points in each measurement repetition. Figure 6a plots the sigma of the residuals obtained by measuring with different lens types and ambient illuminations. In this figure, there are two sections. The left section presents results obtained using the $5\times$ lens in an illuminated or dark room, while the right section presents the result obtained using the $10\times$ lens. The main effect and interaction plot between the objective lenses and ambient light are shown in figure 6b and 6c, respectively.

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From the obtained results, it seems that no influence of the ambient light is present. The different magnification is significant instead. The σ of the residuals at $10\times$ reduces to $2.8 \mu\text{m}$ from the $3.7 \mu\text{m}$ obtained at $5\times$. The interaction between magnifications and ambient light is found to be not statistically significant. The range of σ for the lighted and dark room is around $0.01 \mu\text{m}$. Meanwhile for difference lenses (magnification factor), the range is around $1.3 \mu\text{m}$.

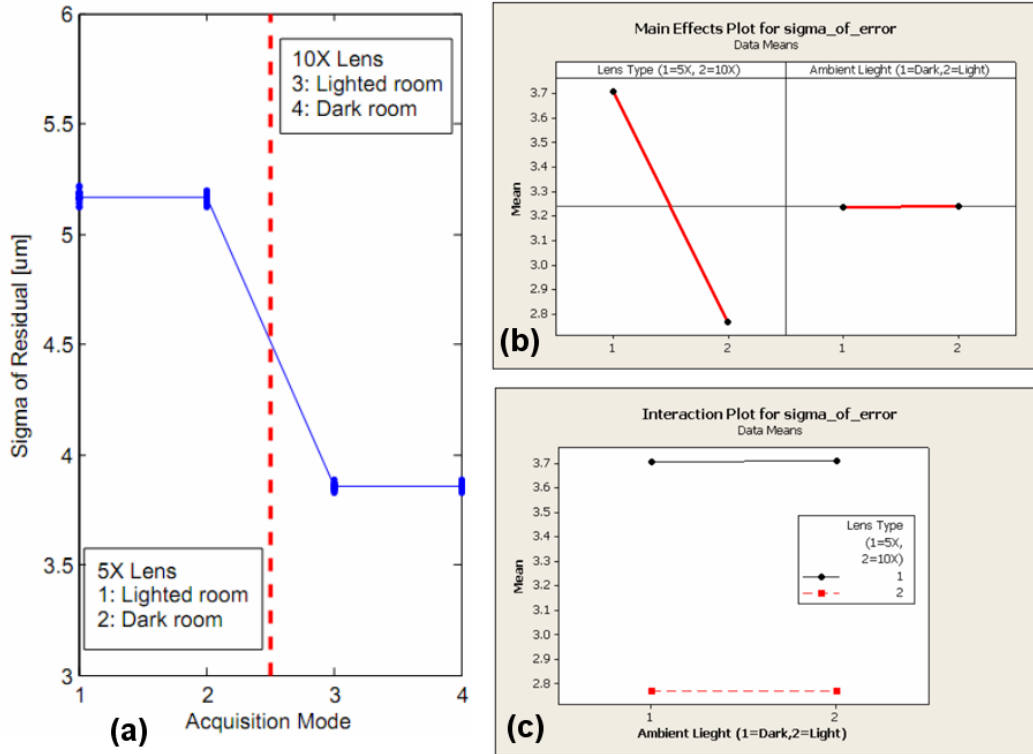


Figure 6: (a) Plot of sigma of residual obtained by different lenses and ambient light, (b) Main effect and (c) Interaction plot between the two factors.

3.2.2 Influence of different types of illumination

In this study, two materials were used, aluminum (specular) and random-structured polymer (lambertian) [18]. A 5× magnification was used. For each sample, 20 measurements were carried out (~1 million points each). The FVM instrument is equipped with three illuminators: axial-light, ring-light and polarized-light. From the analysis, different illuminations significantly affect σ .

From figure 7, for the aluminum surface (specular) the difference of σ from ring-light to polarized light reduces by about 0.6 μm, while for the polymer one, it increases by about 0.45 μm. Furthermore, the σ has inverse behavior when moving from specular to lambertian surface. Note that the plot of σ for the lambertian surface is only for ring light and polarized light since the surface cannot be captured with the axial light. The range of σ the different types of illumination with lambert surface is around 0.5 μm and with specular surface is around 1 μm.

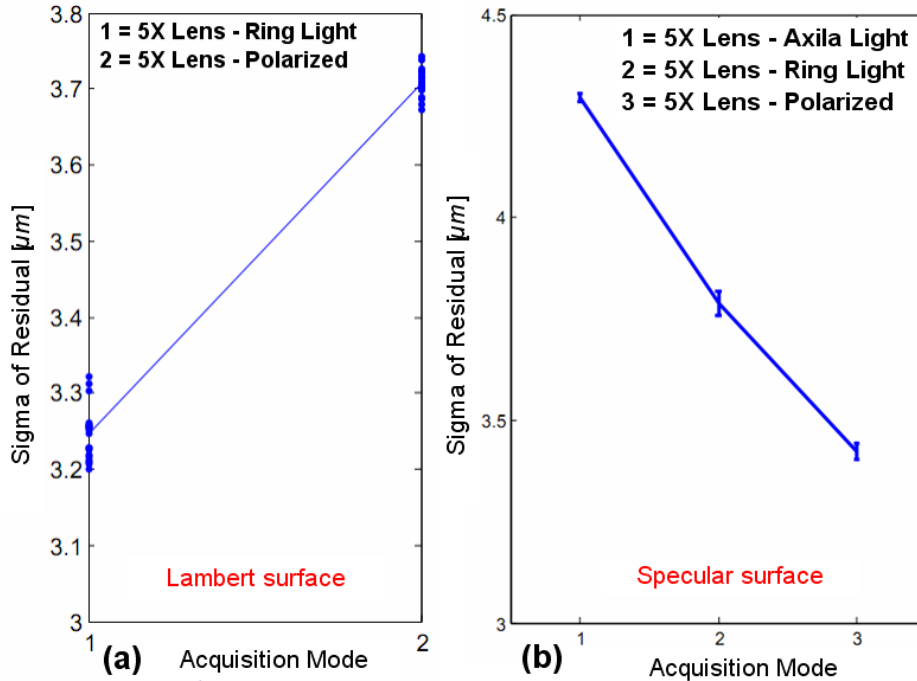


Figure 7: Effect of different illuminations for (a) Lambert surface and (b) Specular surface.

3.2.3 Influence of part orientations (surface slopes)

The three flat samples made respectively of aluminum, stainless steel, and titanium with the addition of coated steel (lambertian) and steel (specular) were used. The measurements were carried out for four different positions and steepness/slope orientations (0° , 5° , 10° , 15°). There are four position types which are combinations of two types of sample placement directions (along x -axis/horizontal or along y -axis/vertical) and two types of rotation directions (clockwise or anti-clockwise). Five measurement repetitions were carried out using the $5\times$ objective lens, so in total 80 measurements were carried out for each material.

From the analysis, it is found that these factors significantly affect the σ . The range of σ for different types of measurement for aluminum, stainless steel and titanium varies around $2.5\ \mu\text{m}$, $2\ \mu\text{m}$ and $1\ \mu\text{m}$, respectively. Figure 8 shows the plot of σ for each experiment as well as the measurement process (position and tilt/orientation direction). Figure 8 shows the plot of σ for different positions and different degrees of steepness (orientation). Note that for steel there are no data when the steepness is higher than 5° due to the specular reflectivity of the steel material, which causes the measurement to fail. The range of σ for the part orientation is around $3\ \mu\text{m}$ considering the highest range value observed is for aluminum-ring light (figure 8 right: blue line).

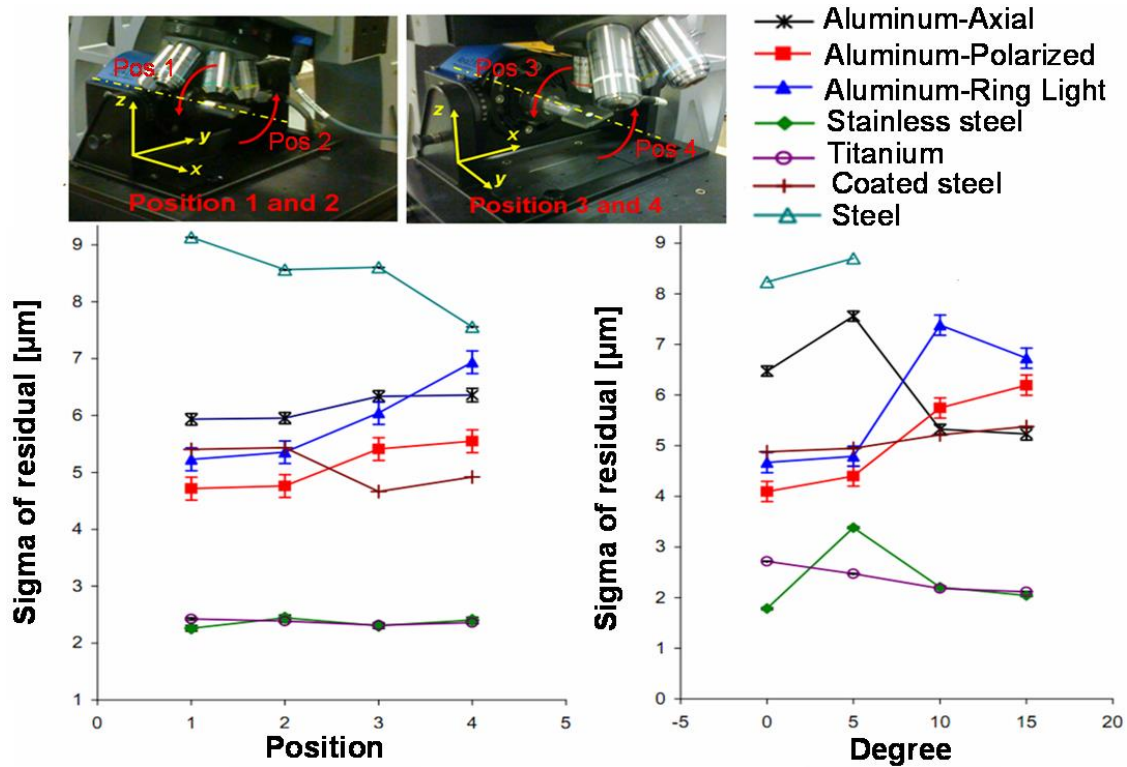
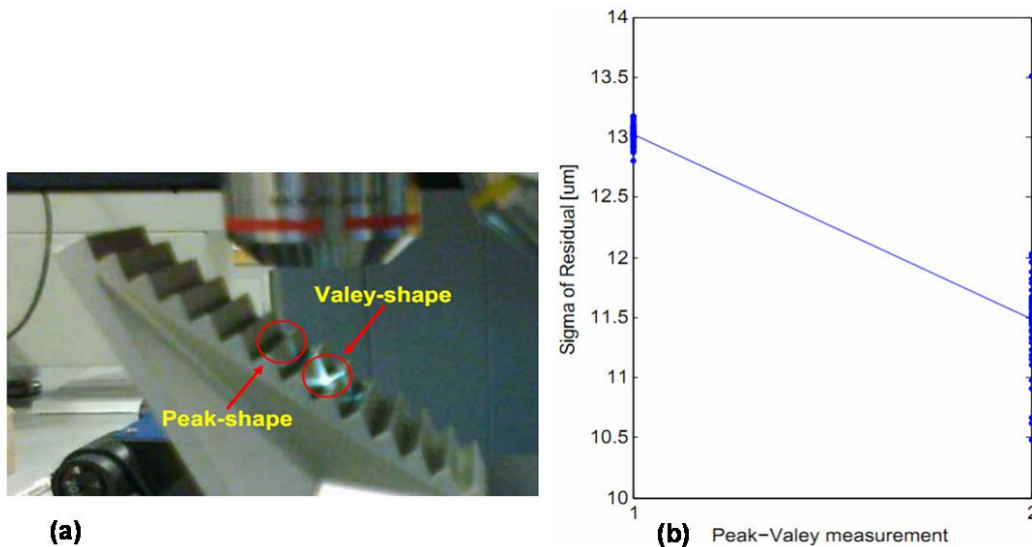


Figure 8: Results of σ for part orientation experiments.

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3.2.4 Influence of peak-valley shape measurements

A machined part having peak and valley features (saw-tooth), made of glazed aluminum with grey color (lambertian), has been used. The edge of the machined part (either peak or valley) was measured 50 times. Each measurement generated about 45000 points. The σ in this case is the standard deviation of the distance of a point to a fitted 3D line representing an edge feature. The results show a statistically significant difference of σ between the two different shapes. The σ of peak measurement is lower by about 1.5 μm with respect to the valley one. The peak-valley measurement and the obtained σ are shown in figure 9. The range of σ for the peak-valley shape contributor is around 2.2 μm (by neglecting some outliers points in figure 9).



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Figure 9: (a) Peak-valley measurement and (b) Obtained σ of residual.

444 3.2.5 *Stitching/no-stitching measurements*

445

446 Two types of sphere measurement were carried out: a single image (no-stitching) and
447 four multiple images measurements. The measured part is an ISO 3290-1 steel sphere
448 [19]. Numbers of 50 measurement repetitions were carried out generating ~750000
449 points per scan for a single image measurements and ~ 3250000 points for multiple
450 ones. Table 4 provides details of the results of a point repeatability. The point is derived
451 from the center of a fitted sphere to the obtained points.

452 The results show that the σ , in x -, y - and z -direction, of measurements by stitching are
453 two times lower than the one without stitching. Hence, by stitching procedure, there is
454 an averaging effect to the calculated position of the obtained points which suppresses
455 part of the random error. Form errors in table 4 are the minimum distance between two
456 concentric spheres covering all the obtained points. The range of σ for the stitching of
457 multiple image measurements is around $0.9 \mu\text{m}$.

458

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Table 4: Repeatability of a single point.

| Measurement type | Form Error / μm | |
|------------------|----------------------------|--------------------|
| | Mean | Sigma (σ) |
| Single image | 13.27 | 2.39 |
| Multiple images | 13.5 | 1.45 |

460

461 3.2.6 *Influence of measurement parameters*

462

463 There are four main parameters of an FVM measurement: exposure time, contrast,
464 vertical and lateral resolutions. These factors can be controlled by the user before the
465 measurement is carried out. A flat sample made of titanium was used for the study.
466 There are four considered levels for lateral and vertical resolution factors and three
467 levels for exposure time and contrast factors. The range of the lateral and vertical
468 resolutions is based on the resolution limit of a $5\times$ objective lens used for the
469 experiments. Conversely, the selected range for exposure time and contrast were based
470 on the range in which a good scan of the surface can be obtained. Table 5 and Table 6
471 present details of the lateral-vertical study and brightness-exposure time study,
472 respectively.

473 From the analysis of experiment for the lateral and vertical resolution factors, it is
474 found that only the lateral resolution is significant. As it can be seen in figure 10, the
475 lower the lateral resolution is, the smaller the σ is. Decimation of points for bigger
476 lateral resolution could be the reason for the reduction of noise since there is an
477 averaging effect in data processing algorithms. There is no interaction effect between
478 lateral and vertical resolutions as it can be observed in figure 11.

479 These results can be applied in practice for geometric measurement, in particular form
480 measurement. As stated by Evans [11] optical instruments have considerably larger
481 noise compared to contact ones. As form measurement is very sensitive to noise a larger
482 lateral resolution is preferable to suppress measurement noise. The range of σ for the
483 lateral and vertical resolution are around $3 \mu\text{m}$ and $0.01 \mu\text{m}$.

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Table 5: Detail of lateral and vertical resolutions influence study.

| Type | Level | Resolution | Lateral point distance [μm] | Number of obtained points | Replication |
|----------|-------|------------------|------------------------------------------|---------------------------|-------------|
| Lateral | 1 | Highest | 1.75 | ~2000000 | 25 |
| Lateral | 2 | Medium (default) | 2.62 | ~1000000 | 25 |
| Lateral | 3 | Medium to low | 4.66 | ~300000 | 25 |
| Lateral | 4 | Lowest | 7.82 | ~100000 | 25 |
| Vertical | 1 | Highest | 2.62 | ~1000000 | 25 |
| Vertical | 2 | Medium (default) | 2.62 | ~1000000 | 25 |
| Vertical | 3 | Medium to low | 2.62 | ~1000000 | 25 |
| Vertical | 4 | Lowest | 2.62 | ~1000000 | 25 |

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Table 6: Detail of brightness and contrast resolution influence study.

| Type | Level | Classification | Value set | Lateral point distance [μm] | Number of obtained points | Replication |
|---------------|-------|------------------|-------------------|------------------------------------------|---------------------------|-------------|
| Exposure time | 1 | Highest | 339 μs | 1.75 | ~1000000 | 25 |
| Exposure time | 2 | Medium (default) | 240 μs | 2.62 | ~1000000 | 25 |
| Exposure time | 4 | Lowest | 110 μs | 7.82 | ~1000000 | 25 |
| Contrast | 1 | Highest | 1.5 | 2.62 | ~1000000 | 25 |
| Contrast | 2 | Medium (default) | 1 | 2.62 | ~1000000 | 25 |
| Contrast | 4 | Lowest | 0.5 | 2.62 | ~1000000 | 25 |

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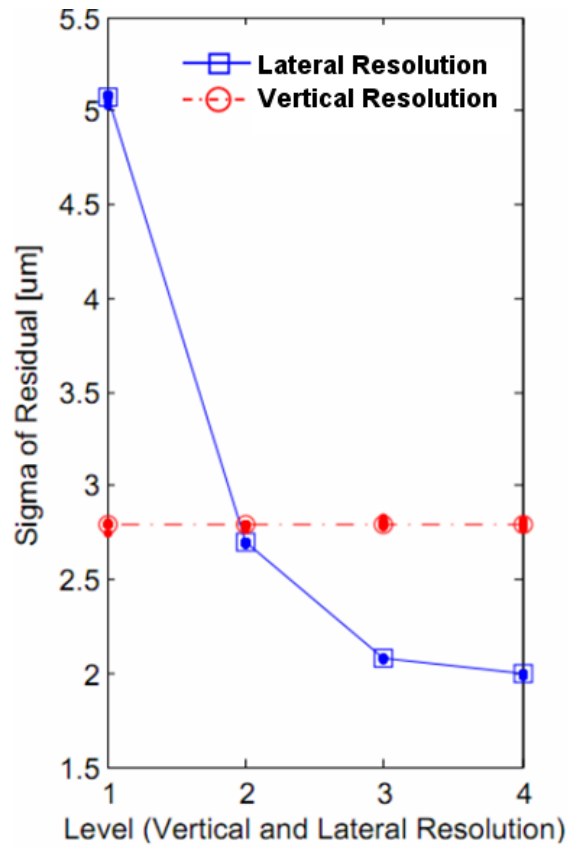


Figure 10: Effect of lateral and vertical resolutions.

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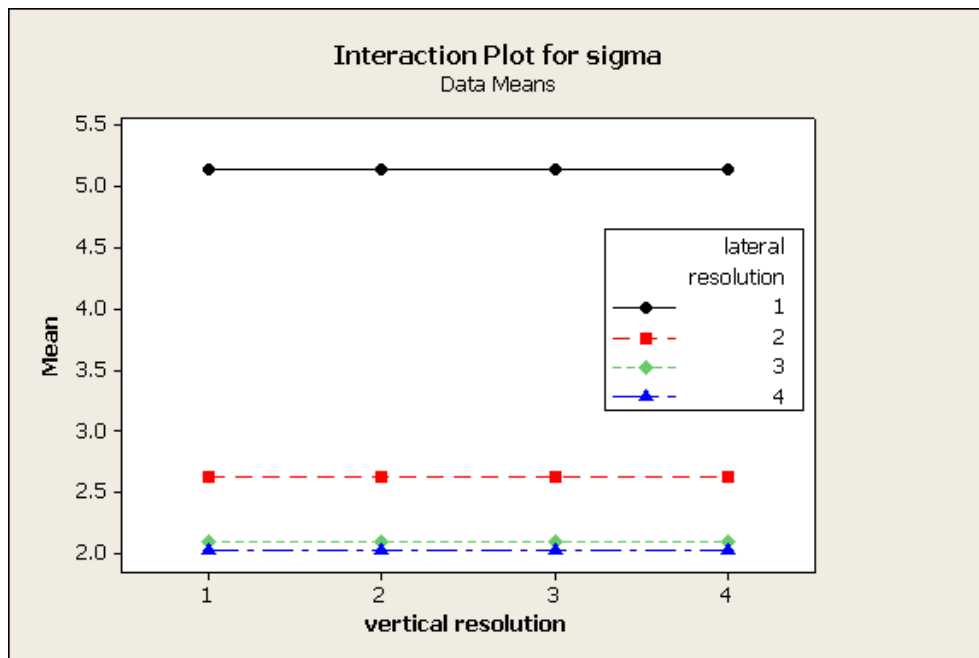
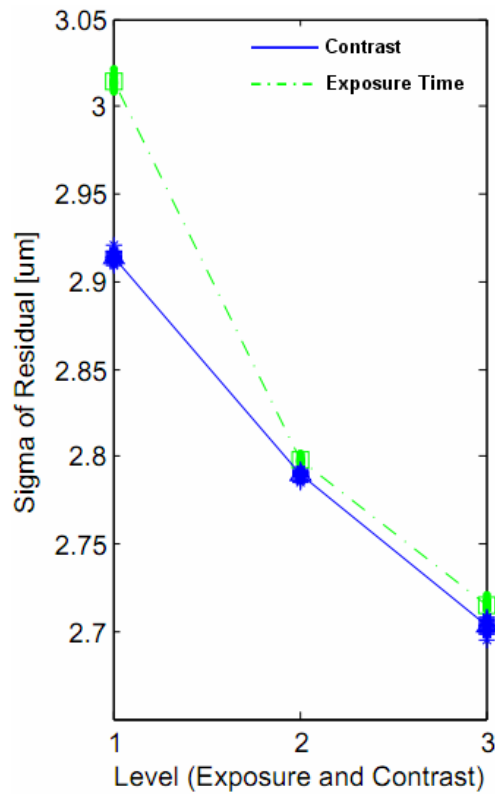


Figure 11: Interaction plot between lateral and vertical resolutions.

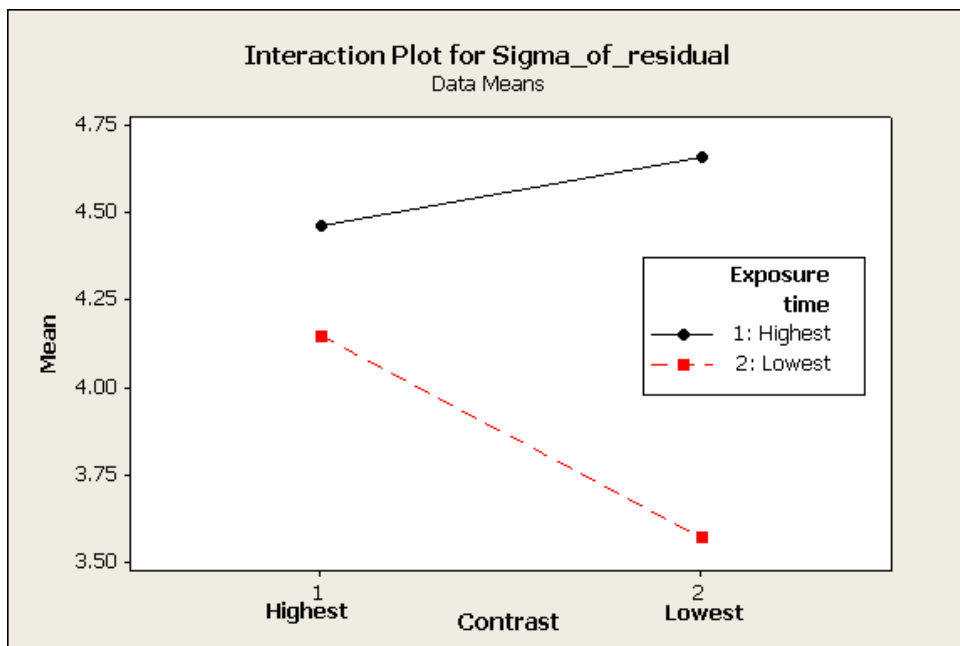
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Exposure time (brightness) and contrast effects were then considered. From this analysis, it is shown that exposure time and contrast are significantly affecting the sigma of residual σ . Figure 12 shows that σ decreases when both exposure time and contrast are set to lower values. Interaction between exposure time and contrast is also

503 found significant (figure 13). The range of σ for the contrast and exposure time settings
 504 are 0.2 μm and 0.3 μm , respectively.
 505



506
 507 Figure 12: Effect of different levels of exposure time and contrast.
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509
 510 Figure 13: Interaction plot between the exposure time and contrast.
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512 3.2.7 Long measurement (drift) behaviors

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 514 The variation of σ due to long measurement, both with and without stitching, has been
 515 investigated. Measurement time was considered because the FVM instrument

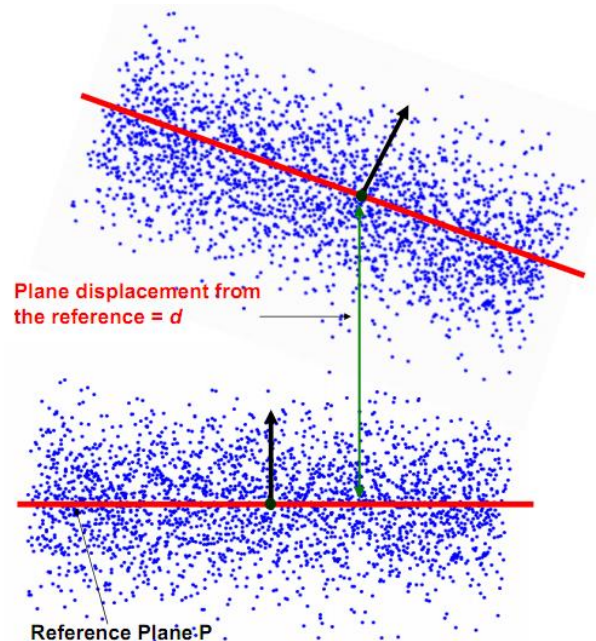
516 components drift can be a relevant uncertainty source. The titanium flat sample has been
517 used for measurements without stitching.

518 Measurements without stitching do not involve stage movements. Instead, for
519 measurements with stitching from four images, an ISO 3290-1 steel sphere was used.
520 The purpose of this type of measurements is to observe the behavior of the instrument
521 in continuous measurement involving stage movements. Both types of measurements
522 were carried out continuously without operator interventions. Thanks to a scripting
523 ability of the instrument, this continuous measurement can be automatically run by the
524 FVM instrument. The measurement used a 5× magnification lens with default lateral
525 and vertical resolutions.

526 For non-stitching measurements, a total of 30 runs (~1 million points obtained for
527 each measurement run) were carried out with a time span of around five hours. Sigma
528 of residual σ and flatness are calculated for each measurement. Range of σ for this
529 period of time is 0.0067 μm . Results of flatness measurements show a decreasing trend
530 up to the 10th measurement sequence. The flatness interval (95%) for the first 100
531 minutes of measurement is 1.25 μm . After this 100 minutes period, the interval becomes
532 0.62 μm .

533 To represent a systematic error, measurements of distances from i -th plane to a
534 reference plane (plane fitted from the first measurement) were conducted as can be seen
535 from figure 14. In this figure, the systematic error representation is defined as the
536 distance from the center point of the fitted plane of measurement i to the reference plane
537 (plane fitted from the points of the first measurement). They show that the variation
538 range (95%) of the distance during the first 19 measurements (the first 190 min.) is 0.16
539 μm , while after this period, it increases to 2.72 μm . Note that the value is shifted one
540 position to the left, since the 1st measurement is not included. Starting from the 20th
541 measurement, juggling phenomena of the measured distance to the reference plane of
542 the flatness can be observed. These results are presented in figure 15.

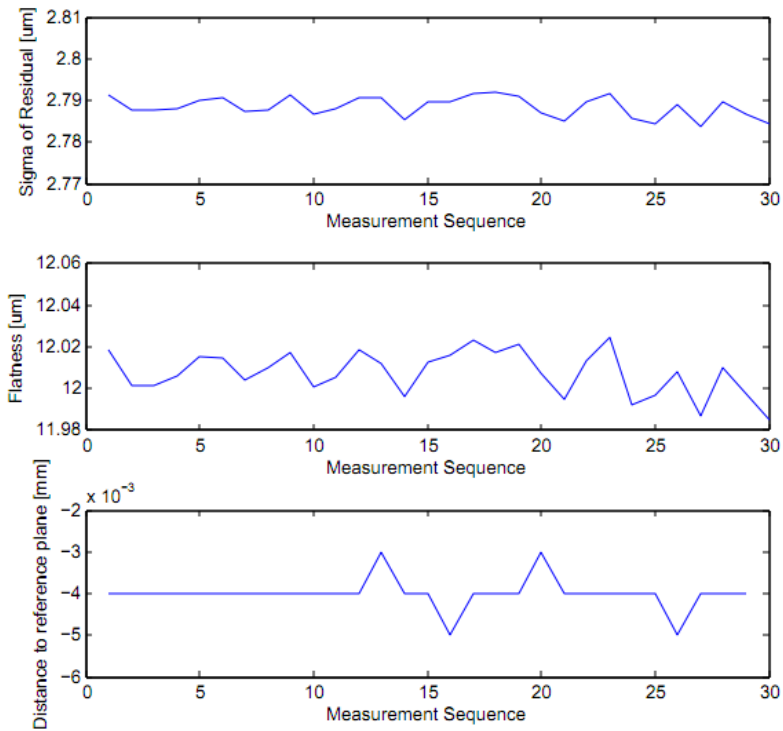
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545 Figure 14: Illustration of distance to reference plane.

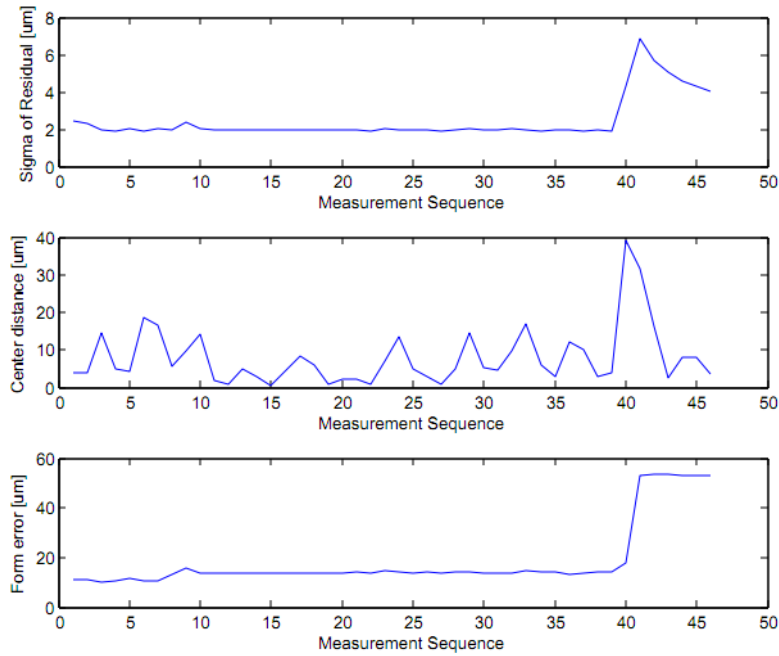
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Figure 15: Long continuous measurement behaviors by plane measurements (without stitching).

Measurements of a sphere with stitching were carried out for 45 runs (~3 millions of points for each measurement run) which correspond to a six hour period. Parameters calculated from the measurement include sigma of the residuals σ , the distance of two consecutive centers and the sphere form error. The sigma of the residuals is used to represent a random error. For a systematic error representation, distances between two consecutive centers are calculated. A stable variation was observed during the first 40 measurements (the first 320 minutes). A shifting is observed for σ after 320 minutes is around 3 μm and for form error is about 40 μm , while the shift between the center distances is about 25 μm . Figure 16 presents the plot of the measurement drift behavior for this type of measurement. The range of σ for the drift is around 2 μm .



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Figure 16: Long continuous measurement behavior by sphere measurements (with stitching).

3.3 Summary of the contributions

Finally, to summarize all the results from the uncertainty characterisation study, table 7 shows the range of the variation of σ for all the considered factors (worst-case scenarios). These values, that are considered relevant in each measurement task, are the s_i values included in the sill s_{sim} parameter used in the simulation model (equation 5).

Table 7: Summary of the influence of the factors.

| Factor | Effect | σ [μm] |
|-----------------------------------------|-----------------|----------------------------|
| Peak-Valley shape | Significant | 2.2 |
| Illumination type with lambert surface | Significant | 0.5 |
| Illumination type with specular surface | Significant | 1 |
| Lateral Resolution | Significant | 3 |
| Vertical Resolution | Not Significant | 0.01 |
| Exposure time | Significant | 0.3 |
| Contrast | Significant | 0.2 |
| Stitching | Significant | 0.9 |
| Magnification | Significant | 1.3 |
| Part orientation | Significant | 3 |
| Drift | Significant | 2 |
| Ambient light | Not Significant | 0.01 |

575 4. Validation

576 The ISO/TS 15530-4 standard [10] is the basis for the application and validation to
577 guarantee the traceability of a simulation-based uncertainty estimation in coordinate
578 metrology. As there are several deeply different coordinate measuring systems, the
579 ISO/TS 15530-4 standard cannot define a general methodology for simulating the
580 measurement and stating the uncertainty based on the simulation results. Instead, the
581 ISO/TS 15530-4 standard defines the general requirements for the simulation, and the
582 procedures for validating the uncertainty statements, thus guaranteeing the traceability.

583 The validation according to the ISO/TS 15530-4 standard includes both the
584 mathematical model and the model parameters. The ISO/TS 15530-4 states that:

585

586 “Performing a number of measurements on calibrated objects, the coverage of the
587 uncertainty ranges is checked. The plausibility criterion should be satisfied for an
588 appropriate percentage of the time (95% for $k = 2$); this criterion is that a statement of
589 uncertainty is plausible if: $|y - y_{cal}| / \sqrt{U_{cal}^2 + U^2} \leq 1$ ”.

590

591 In this method, one should then calculate a E_n value for each measurement run. E_n is
592 formulated as:

593

$$594 \quad E_n = |y - y_{cal}| / \sqrt{U_{cal}^2 + U^2} \quad (9)$$

595

596 where y is a measurement result, y_{cal} is the calibrated value of y , U_{cal} is the expanded
597 calibration uncertainty, and U is the expanded uncertainty obtained by simulation. If
598 the expansion factor k is equal to 2, a good agreement can be concluded if
599 approximately 95% of total measurements runs are characterized by $E_n < 1$.

600 Several case studies of geometric measurements are considered to validate the
601 proposed simulation method; they include form (flatness measurements) and size
602 measurements (diameter and height measurements). More complicated case studies can
603 be found in [17]. It is worth to note that although the components are not a micro-sized
604 component, the portion of features of the measured component and tolerances are at
605 micro-scale [1, 2]. In the case study, the variogram model, used for uncertainty
606 estimations by the proposed simulation, are selected based on the type of the material
607 of the cased study considered.

608

609 4.1 Flatness measurement

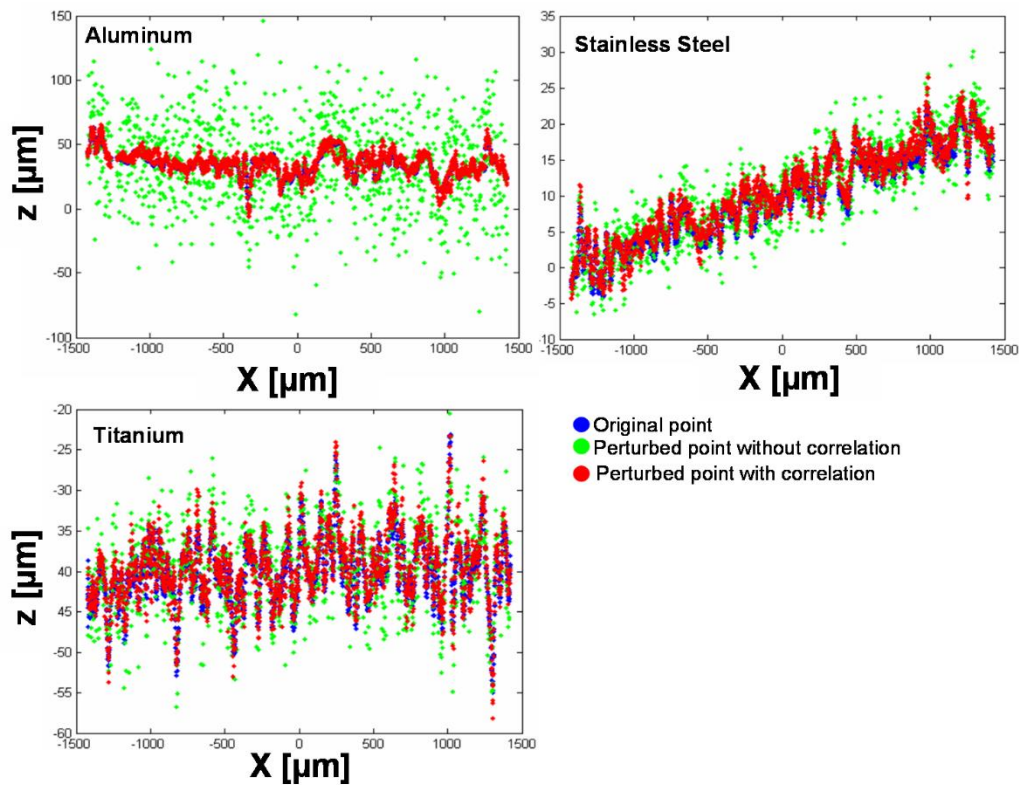
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611 The three calibrated samples originally adopted for the definition of the variogram
612 models were considered (see §3.1). The simulation is applied to points obtained from a
613 real measurement. Therefore, feature form deviation of the part is already included [20].
614 Figure 17 qualitatively shows that a variogram based simulation yields better results
615 compared to a simulation of uncorrelated points. The red line shows the simulation
616 result if the variogram model is applied: it is clear that it is close to the original data.
617 Instead, if the noise is simulated as pure white noise with a standard deviation equal to
618 the sill s of the variogram, the simulation result is far from the original data (green
619 points).

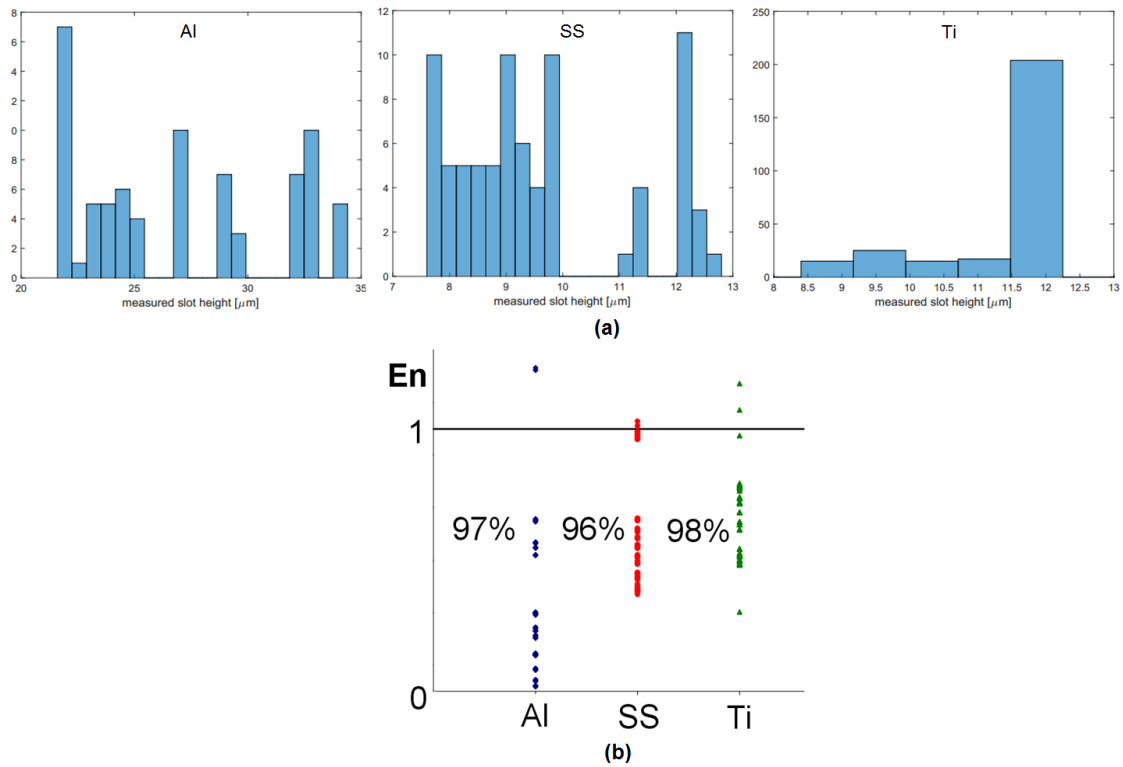
620 Numbers of 100 flatness measurement runs were carried out by changing the part
621 orientation (approximately perpendicular to the optical axis, 5° tilted clockwise and
622 anticlockwise) to represent an orientation error when placing the part. The measurement
623 parameters used followed those shown in Table 1 for each material type and orientation.
624 To evaluate the uncertainty, 500 simulation runs were carried out. The sill s parameter
625 of the simulation was modified according to Eq. (5) to consider the influence of the
626 various uncertainty factors in the real measurement situation of the flatness
627 measurement. Figure 18a shows results of the flatness measurements. It is worth noting
628 that the flatness is based on a min-max fitting. This kind of fitting in general generates
629 a non-Gaussian distribution of the measurement results.

630

631 The flatness samples were calibrated on a traceable tactile-CMM with $E_{0:MPE} = 2 +$
 632 $L/300 \mu\text{m}$ where L is the measured length in mm (the CMM is periodically performance
 633 verified). The calibrations follows a multiple-measurements strategy that vary the
 634 position and orientation of the sample during the calibration process to take into account
 635 the volumetric error of the traceable tactile-CMM. Calibration results of the flat samples
 636 are $y_{\text{cal}} = 25.1 \mu\text{m}$ and $U_{\text{cal}} = 1.6 \mu\text{m}$ for Al, $y_{\text{cal}} = 4.8 \mu\text{m}$ and $U_{\text{cal}} = 0.2 \mu\text{m}$ for SS,
 637 and $y_{\text{cal}} = 4.1 \mu\text{m}$ and $U_{\text{cal}} = 0.4 \mu\text{m}$ for Ti. The estimated U for Al, SS, and Ti are 14.0
 638 μm , 7.7 μm , and 10.1 μm , respectively. From calculation of each E_n value, the fraction
 639 of E_n values for which $E_n < 1$ for Al, SS, and Ti are 97%, 96%, and 98% respectively
 640 (Figure 18b), so the simulator can be considered validated in this case. From figure 18,
 641 some portions of E_n are larger than one. Having some portion of $E_n > 1$ suggest that the
 642 estimated uncertainty by the proposed simulation is not overestimating the expected
 643 uncertainty. Similar explanation for the E_n values are valid for all other presented case
 644 studies in this paper.
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 646



647 Figure 17: Plot of original points (blue) superimposed with the simulated points
 648 without considering (green) and with considering (red) the correlation among points
 649 for aluminum (Al), stainless steel (SS), and titanium (Ti).
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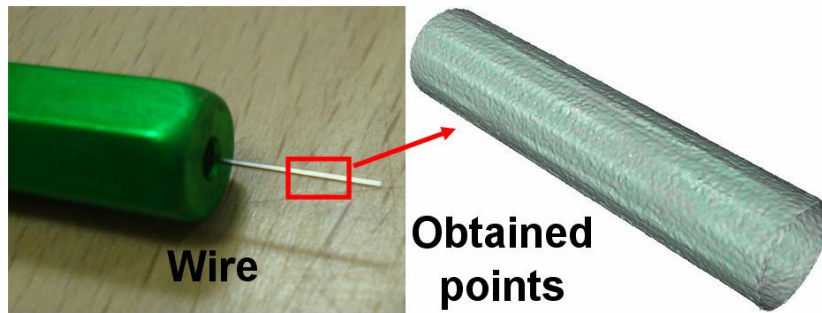


652
 653 Figure 18: Plot of (a) histogram of the flatness value and (b) E_n values for the flatness
 654 measurement of Al, SS, and Ti.
 655

656 4.2. Commercial micro-wire measurements

657 The measurement of a diameter (a dimensional characteristic) is presented in this
 658 case. An industrial micro steel wire with diameter of $310 \pm 2 \mu\text{m}$ was measured (Figure
 659 19). The wire is used as a plug-gage to measure the nozzle diameter of a water jet
 660 machine. Since the part is a commercial plug-gage, y_{cal} and U_{cal} are based on the part's
 661 nominal specifications. The y_{cal} is considered to be equal to $310 \mu\text{m}$. The U_{cal} of the
 662 plug-gage diameter is estimated as a type B uncertainty and is assumed to have a
 663 rectangular distribution. Hence, U_{cal} is equal to $2.31 \mu\text{m}$.

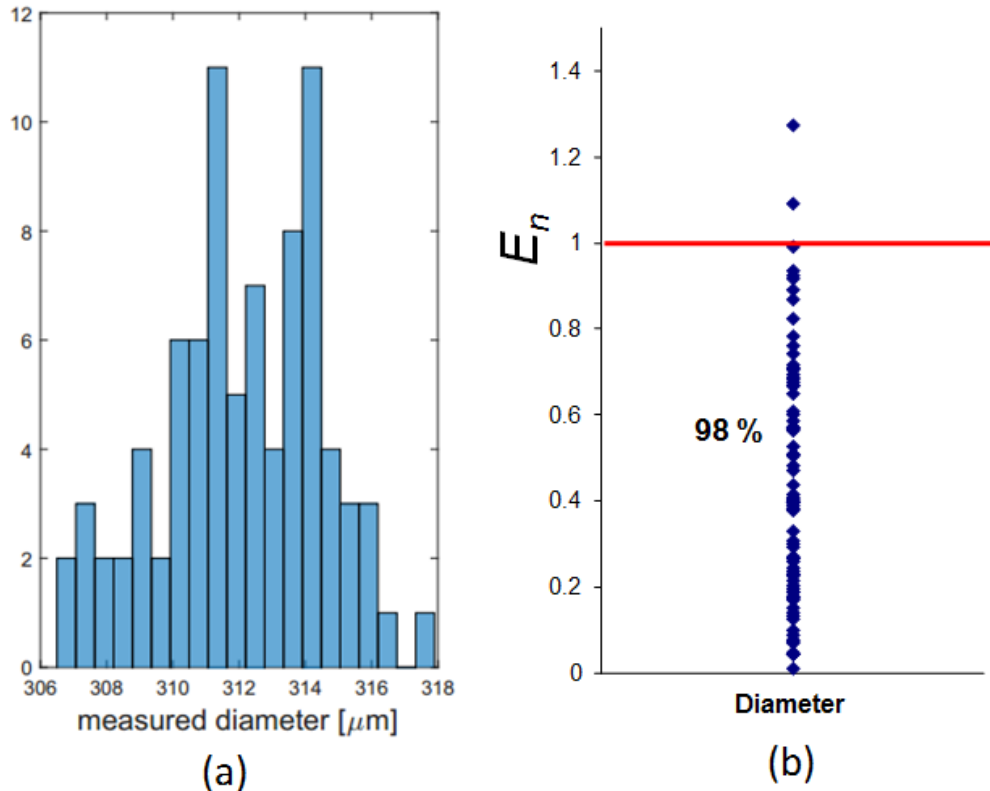
664 Before running the simulation, the procedure, explained in Section 2, to determine
 665 the variogram model was carried out for steel since the variogram model of the steel
 666 material used in this case study has not yet been determined. The selected variogram
 667 model is a Gaussian one with s , n , and r parameters equal to $34.4 \mu\text{m}$, $0 \mu\text{m}$, and 14.8
 668 μm respectively. The estimated U is $5.6 \mu\text{m}$ obtained from 500 simulation runs y . A
 669 total of 85 measurement runs y were carried out with the following measurement
 670 parameters: 193.2 ms (exposure time), 0.44 (contrast), $0.6 \mu\text{m}$ (vertical res.) and 3.9
 671 μm (lateral res.) by using $10\times$ objective lens. From the E_n calculation, a total of 98 %
 672 values have $E_n < 1$, thus ensuring validation. The histogram of the measurement results
 673 y and the E_n calculation for each measurement are shown in figure 20. In figure 20
 674 right, around 2 % of E_n values are more than one.
 675



Specification: dia. $310 \pm 2 \mu\text{m}$

Figure 19: The micro-wire.

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Figure 20: (a) Histogram of the diameter measurement results and (b) E_n values for the diameter measurement validation.

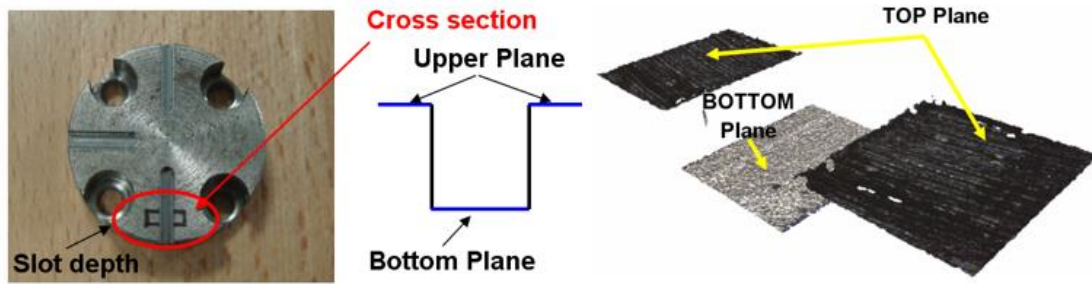
682 4.3. Step-height measurements of a slot-milled steel component

683

684 A measurement of the step-height of a slot-milled part is presented in this study. The
685 part was made of a steel material by using a precision micro-milling machine. The part,
686 the slot height definition and an example of the measured surface are shown in figure
687 21. Measurement parameters for the slot step-height measurement are exposure time =
688 $88.32 \mu\text{s}$, contrast = 0.2, lateral resolution = $7.83 \mu\text{m}$ and vertical resolution = $0.4 \mu\text{m}$
689 by using a $5\times$ objective lens.

690 The results of a calibration process using a traceable tactile-CMM are $y_{\text{cal}} = 698.7$
691 μm and expanded uncertainty $U_{\text{cal}} = 0.25 \mu\text{m}$. Total of 100 measurements runs y was
692 carried out. From around 500 simulations runs to estimate the uncertainty of the slot
693 measurement, an expanded estimated uncertainty U is obtained as $0.45 \mu\text{m}$. From a
694 total of 100 measurement runs y , 93% (almost 95%) of E_n values are less than 1, hence
695 the simulation and the uncertainty estimation are validated. Figure 22 shows the

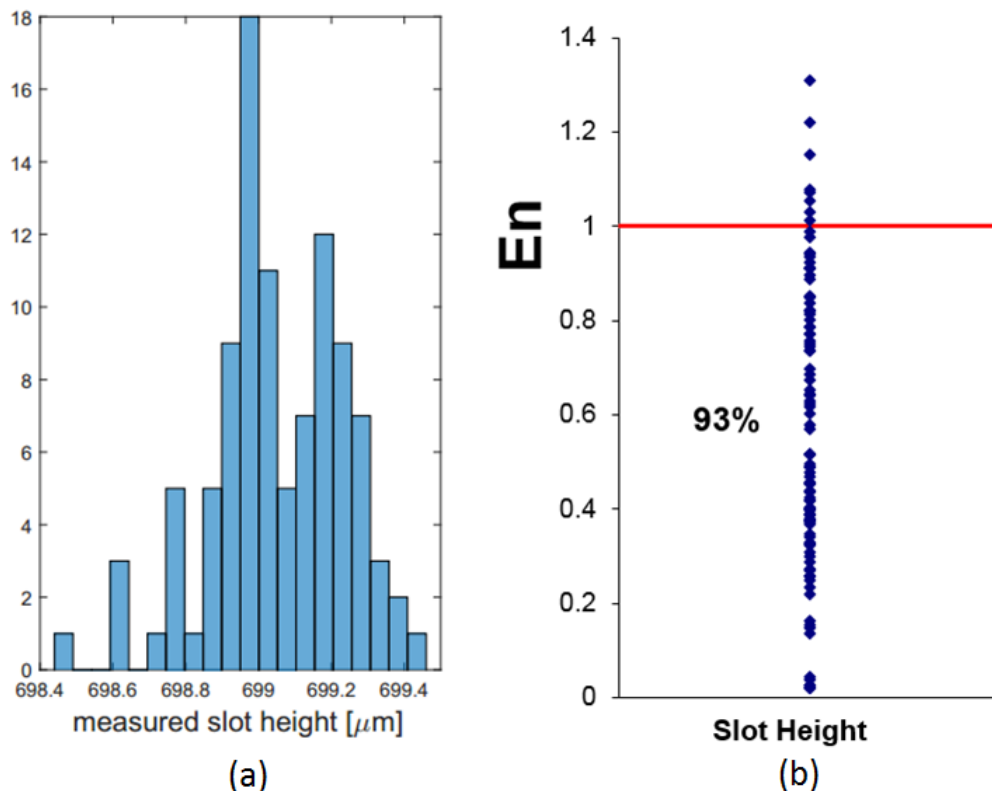
696 histogram of the measurement results and the E_n value calculation for each
 697 measurement.
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The measured slot The measured surface

Figure 21: The measured slot and its obtained surface.

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Figure 22: (a) Histogram of the height measurement results and (b) E_n values for the slot step-height measurement validation.

705 5. Conclusions

706 This paper presents a proposal of a simulation-based approach to estimate the task-
 707 specific measurement uncertainty of a 3DM performing geometric inspections. A case
 708 study regarding FVM is proposed. The case study is validated according to the ISO/TS
 709 15530-4 standard. The method considers the correlation among points obtained by the
 710 optical instrument since correlation naturally occurs among points measured
 711 sequentially or continuously. Variogram models are determined for each material to
 712 represent the property of correlations among points. In general, the correct type of
 713 variogram (Gaussian, exponential, spherical, etc.) is defined based on the gathered
 714 experimental data. In this work, we are suggesting and describing a possible approach

715 we developed and validated in a case study. The proposed approach can be applied to
716 other type of 3DM instruments and can be implemented and integrated into instruments
717 software system as a module.

718 Extensive uncertainty characterization has been carried out to identify and quantify
719 the uncertainty sources and incorporate them into the simulation parameters. The
720 validation is carried out with industrial case studies and the results show that the
721 simulated uncertainties have a good agreement with the real measurement.

722 The proposed simulation approached can be summarised as follows:

- 723 1. Define the variogram model and quantify the s , n and r parameters for each
724 material type. This step is carried out once for every different material.
- 725 2. Experimentally evaluate the additional uncertainty sources not considered in the
726 variogram, but influencing the measurement result. The uncertainty sources
727 quantification is carried out once for each type of instrument.
- 728 3. Measure the part to inspect, and compute the measured value y .
- 729 4. Having modified the value of s considering the additional sources of uncertainty,
730 apply the variogram model to generate an adequate number of simulation runs
731 and the related perturbed clouds of points, compute the simulated measured values
732 and, based on these values, estimate the expanded uncertainty U .
- 733 5. State the measurement result $y \pm U$.

734 Further works include building a database of optimal variograms for various types of
735 materials and applying the proposed method to estimate task-specific uncertainty for
736 surface texture measurements.

737

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739

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747

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