Object Shape Error Modelling and Simulation During Early Design Phase by Morphing Gaussian Random Fields

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Geometric and dimensional variations in objects are caused by inevitable uncertainties in manufacturing processes and often lead to product quality challenges. Failing to model the effect of object shape errors, i.e., geometric and dimensional errors of parts, early during the design phase inhibits the ability to predict such quality challenges. This consequently leads to expensive design changes after freezing of design. State-of-art methodologies for modelling and simulating object shape error have limited defect fidelity, data versatility, and designer centricity that prevent their effective application during the early design phase. To overcome these limitations, this paper presents a novel Morphing Gaussian Random Field (MGRF) methodology for object shape error modelling and simulation. The MGRF methodology models the spatial correlation in the deviations of the part from its nominal design using Gaussian Random Fields and then, utilises the modelled spatial correlations to generate non-ideal parts by conditional simulations. The MGRF methodology has (i) high defect fidelity enabling it to simulate various part defects including local and global deformations, and technological patterns; (ii) high data versatility allowing it to simulate non-ideal parts under the constraint of limited data availability and to utilise historical non-ideal part data of similar parts; (iii) designer centric capabilities such as performing ‘what if?’ analysis of defects of practical importance; and; (iv) the ability to generate non-ideal parts conforming to statistical form tolerance specification without additional modelling effort. The aforementioned characteristics enable the MGRF methodology to accurately model and simulate the effect of object shape variations on product quality during the early design phase. Practical applications of the developed MGRF methodology and its advantages are demonstrated using sport-utility-vehicle door parts and compared against state-of-art methodologies.

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1. Introduction

Object Shape Error Modelling and Simulation (OSEMS) plays a vital role in determining the quality and functionality of mechanical products and their assembly systems. Shape error arises due to various inevitable uncertainties in manufacturing processes which lead to the actual manufactured part exhibiting imperfect form, i.e., having geometric and dimensional errors. A model of the resulting true manufactured part with geometric and dimensional errors is called a ‘non-ideal part’ [1].

Object shape error, i.e., geometric and dimensional errors in non-ideal parts, leads to numerous quality related problems such as (i) high rate of re-work or scrap, (ii) inferior product functional performance, (iii) tooling failures, and (iv) unexpected production downtime which, in turn, reduces both product quality and production throughput [2]. The aforementioned critical issues necessitate accurate modelling and simulation of object shape error, especially during the early design phase. This is because accurate prediction of the effect of objects’ non-ideal behaviour on product quality during early design phase enables prevention of unnecessary design changes during later stages of production and aids achieving required product quality Right-First-Time (RFT). This, in-turn can lead to (i) reduction of New Product Introduction (NPI) time, and (ii) elimination of the significantly higher costs of rectifying a design fault in a product or assembly system during later stages of production [3,4].

The general requirements for OSEMS methodologies have been discussed in existing literature [5]. However, a detailed analysis of the requirements from an early design perspective has not been performed yet. Therefore, we first describe the essential requirements for OSEMS methodologies during early design; they can be broadly classified into the following categories:

1. Object fidelity — refers to the ability of the methodology to be applied to objects/parts with varying levels of surface
complexity. These surfaces, in increasing order of complexity can be classified into the following three types, (i) planar or 2D surfaces; (ii) 3D primitives such as spherical, cylindrical, and conical surfaces; and (iii) complex 3D free form surfaces.

While planar and 3D primitive surfaces are fundamental blocks essential for the functional description of many mechanical assemblies, complex 3D free form surfaces, due to their high functional and aesthetic utilities, are increasingly employed in automotive, aerospace, and optics industries [6]. Therefore, a methodology should be able to model shape error of all the three types of surfaces.

2. Defect fidelity — refers to the ability of the methodology to accurately emulate various types of part defects encountered during the manufacturing process. This requirement is vital to accurately model the assembly process and enable the diagnosis of various complex and ill-conditioned faults arising during the assembly process of compliant parts and to enable achieving the required assembly quality.

High defect fidelity can be achieved by (i) simulating shape errors at multiple spatial scales, i.e., local, and global deviations [7,8]; and (ii) simulating technological patterns, i.e., spatial deviation patterns specific to a given manufacturing process.

Global deviations are the non-ideal behaviour affecting a large area or the entire part. In contrast, local deviations are those that affect a small or localised region of the part. In sheet metal parts fabricated by forming, shape error caused by spring back could affect the entire part and can be classified as a global deviation. Whereas surface dents or flange deformations that typically affect a localised region can be classified as local deviations. The simulation of global and local deviations is important because some manufacturing processes require tighter dimensional quality requirement in a localised region or have variable tolerance requirements throughout the part. For instance, in a sheet metal assembly, the non-ideal behaviour of part flanges is critical as fastening/joining of parts takes place along the flange. Any variation in this region has a high probability of affecting key product characteristics and thus, needs to be simulated and analysed during design. This simulation of various types of global and local deviations is termed as simulation of design intent in this paper.

On the other hand, simulation of technological patterns enables the creation of a non-ideal part that captures the spatial deviation patterns specific to a given manufacturing process. The non-ideal part thus simulated is a better representation of a true manufactured part, and hence, can provide accurate assembly simulation and tolerance analysis results compared to non-ideal part with random form variations. Therefore, a methodology should possess high defect fidelity while simultaneously satisfying other criteria.

3. Data versatility — refers to the ability of the methodology to perform effectively at different levels of data availability and to handle the imprecision and uncertainty arising during various stages of NPI. Imprecision relates to the constantly evolving object geometry, especially during early stages of NPI. Whereas uncertainty relates to the various levels of part-to-part variation which occur during different stages, such as from initial prototyping to final product and full production.

For instance, during the NPI process of an assembly system development, the various stages are, engineering, manufacture and assembly, installing and commissioning, launch, and production. During this NPI journey from engineering to production stage, availability of measurement data or data from manufacturing process simulations from which the non-ideal behaviour of parts can be quantified varies from, (i) no data, (ii) historical data from similar/surrogate parts, (iii) preproduction data from same product, to (iv) data on production parts.

For a methodology to be data versatile it should be able to effectively handle this imprecision and uncertainty, and generate non-ideal parts at any of the above-described levels of data availability. This is especially the case during the early design phases where limited data is available (stages (i) through (iii) described in the previous paragraph) in order to prevent unnecessary design changes during later stages of production and eliminate the corresponding time and cost penalties associated with it.

4. Designer centricity — refers to the methodology’s ease of applicability, and the interpretability of its parameters by the designer. During early stages of design, ease of applicability can be understood as the ability to simulate technologically wanted design variations to perform several ‘what if?’ analysis with little or no additional modelling effort. Examples of ‘what if?’ analysis could include the ability to quantify the effect of the following non-ideal behaviours on assembly quality: (i) various levels of spring-back, (ii) specific local part deformations such as flange variations and dents, and (iii) part bending or twisting about a given axis. The ability to perform these ‘what if?’ analysis early during design with little or no additional modelling effort enables timely fault detection and helps prevent expensive design changes during later stages.

On the other hand, interpretability of model parameters criterion enables the designer to understand/evaluate the model parameters with ease and to manually tune them, especially when no historical or simulation data are available to aid optimum parameter identification. The interpretability of model parameters can be improved if (i) their dimensions are in the modelling space (i.e., the 3D domain of the part) as opposed to low dimensional or latent space, and (ii) they are physically meaningful. A methodology should possess the aforementioned qualities to be considered designer centric.

5. Support for tolerance analysis and synthesis — refers to the ability to generate non-ideal parts conforming to statistical form tolerance specification without additional modelling effort. In this study, we focus specifically on form tolerance for profile of a surface [9], as most other types of tolerance specifications can be simulated through rigid transformations or scaling of the resulting part. The ability to generate non-ideal parts that resemble real manufactured parts and conform to tolerance specifications enables performing accurate assembly process simulations and thus helps to allocate optimum tolerances early during the design.

6. Computational intensity and scalability — refers to the ability of the methodology to be (i) computationally less intensive, and (ii) scalable to assembly with large number of parts. While the necessity of being computationally less intensive is easily understood, the necessity to be scalable to large assemblies stems from the fact that most mechanical assemblies have a large number of parts – for instance an automotive body assembly process is a multi-level hierarchical process in which 200–250 sheet metal parts are assembled together to form the final product [10,11] – and the methodology should be capable of being applied to them. A key factor that can affect scalability is the total number of model parameters. This is
because assembly system optimisation incorporating compliant parts’ non-ideal behaviour is typically performed using computationally expensive Finite Element Method (FEM) simulations [12,13] and the number of FEM simulations required increases exponentially with the number of model parameters whose effect on product quality has to be determined. Thus, a design friendly model is one with a small number of model parameters which reduces the number of necessary computationally expensive FEM simulations.

Though numerous methodologies to model object shape error exist [8,14–28], they exhibit several limitations with respect to the aforementioned criteria such as (i) limited defect fidelity due to which they are unable to accurately simulate many true non-ideal part behaviours, (ii) limited data versatility which reduces their ability to operate effectively at different levels of data availability often found during early design phases, and (iii) limited designer centric capabilities making them less intuitive for designers.

To overcome these limitations, this paper presents the Morphing Gaussian Random Field (MGRF) methodology to model and simulate object shape error, primarily during early design phases. The contributions of this study are the development of (i) a high defect fidelity OSEMS methodology capable of simulating local and global deformations, and technological patterns; (ii) an OSEMS methodology that has high data versatility and can effectively simulate non-ideal parts at all levels of data availability; (iii) a highly designer centric OSEMS methodology capable of performing ‘what if?’ analysis, and with model parameters that are physically meaningful; and (iv) an OSEMS methodology capable of generating non-ideal parts conforming to statistical form tolerance specification without additional modelling effort.

The rest of the paper is organised as follows: In Section 2, we classify the existing OSEMS methodologies and analyse their applicability with respect to the criteria described in Section 1. In Sections 3 and 4 we describe the problem formulation and the developed MGRF methodology in detail, respectively. In Section 5, we demonstrate the capabilities of MGRF methodology in various practical scenarios using automotive door inner parts. In Section 6, we compare the MGRF methodology with state-of-art and discuss the computational requirements of the MGRF methodology. Finally, in Section 7 we discuss conclusions and future research.

2. Literature review

State-of-art OSEMS methodologies can be classified into three main categories (i) morphing based, (ii) deviation decomposition or mode-based, and (iii) Deep Neural Network (DNN) based. Morphing based methodologies model non-ideal parts by modifying either a parametric geometry represented by Bézier, NURBS, and B-spline; or discrete geometry represented by mesh or Cloud-of-Points (CoP). Deviation decomposition or mode-based methodologies model non-ideal parts by decomposing part deviations from measurement or simulation data into a linear combination of orthogonal modes, and are typically applied to discrete geometry representations. DNN-based methodologies use Generative Adversarial Networks (GANs) to generate 2D non-ideal part patterns and map them to 3D parts.

A key concept, in addition to the three categories of classification described above, is that of the Skin model. It is defined as a model of the physical interface between the workpiece and its environment [1] and is based on the tenants of GeoSpelling, a coherent uni-vocal language for non-ideal part specification and verification [29]. All existing OSEMS methodologies can be considered as different means to generate skin model shapes, i.e., unique finite skin model representatives comprised of deviations from ideal manufacturing and assembly process [23].

2.1. Morphing based OSEMS methodologies

Volume splines have been used to fit deformed or deviational point data to CAD and find the non-ideal part by minimising a sum of squared error functions in [15,17]. Hermite approximation was applied to reduce the high degree polynomial compositions when an explicit expression of the surface is needed during free-form deformation in [20]. A NURBS based interpolation of measurement data focused on the reconstruction of CAD geometry with form errors was proposed in [26]. While the afore-discussed techniques mainly focus on reconstruction of CAD geometry for accurate part representation, the Envelope-T model to simulate non-ideal parts for tolerance analysis was proposed in [8,28].

A morphing mesh methodology based on constrained deformation was employed to generate non-ideal part in [18]. Second order shapes such as paraboloid have been used to model the systematic deviations of discrete geometry representation of non-ideal parts in [19].

2.2. Deviation decomposition or mode-based OSEMS methodologies

Statistical Modal Analysis (SMA), a mode-based methodology was proposed in [22], where shape deviation is decomposed into a set of orthogonal patterns based on Discrete Cosine Transform (DCT). Geometric Modal Analysis (GMA), a technique utilising 3D-DCT capable of characterising shape variations in 3D surfaces, was proposed in [24].

Natural Mode Analysis, based on the decomposition of deviation data into natural modes of vibration, was developed in [16]. Metric Modal Decomposition (MMD), a methodology based on a variation of Natural Mode Decomposition, was proposed in [25]. Principal Component Analysis (PCA) is used to characterise part variation in [21]. A random field-based methodology to model and simulate part shape error was developed in [23].

2.3. Deep Neural Network (DNN) based OSEMS methodologies

DNN based OSEMS methodologies use GANs, a type of DNN architecture consisting of a pair of generator and discriminator networks, to generate 2D non-ideal patterns. The training data for this network consists of simulated patterns from mode based OSEMS methodologies and real part measurement data [30]. The non-ideal part patterns generated from this method are mapped onto a partitioned 3D-surface of a part to generate a non-ideal part instance. The 2D-non-ideal patterns generated by DNN based methodologies need to be classified into one of various systematic or random deviation patterns before non-ideal part instances are generated, this task is performed by using the AlexNet DNN architecture in [31].

2.4. Applicability of state-of-art OSEMS methodologies during early design stage

The state-of-art OSEMS methodologies have many advantages such as,

- Designer centricity and computational advantages of morphing mesh methodology due to its physically meaningful model parameters and low computational requirements [18].
- The ability to work under the constraint of limited or no data availability of a few morphing based methodologies [8,18,20,26,28].
- Support for statistical form tolerance without additional modelling effort by Envelope-T methodology [8,28].
• Technological patterns modelling capability of mode-based methodologies and DNN-based methodologies due to their ability to learn from measurement and simulation data [16,21–25,30,31].

However, they also entail many limitations such as,

• The morphing mesh methodology’s [18] inability to model technological patterns.
• Limited defect fidelity and designer centricity of morphing based methods [8,20,26,28] as they
  - Require setup and optimisation of many parameters such as degree of polynomial, location of knots, numbers of spline intervals and displacement vectors.
  - Lack the ability to model spatial deviation patterns.
  - Face non-trivial challenges to demarcate the region of control influencing the local deformation, as it depends on cell dimensions and spline degree which are difficult to predict and modify because it requires expert knowledge of the underlying mathematics making them less design friendly [32].
• Limited defect fidelity, data versatility and designer centricity of mode-based methodologies [16,21–25] due to their
  - Inability to model local deformations.
  - Model parameters typically being present in frequency space or other reduced dimension latent space.
  - High computational requirements.
  - Inability to perform effectively when measurement and simulation data are not available [5].
• Limited defect fidelity, data versatility and designer centricity of DNN-based methodologies [30,31] due to their
  - Inability to model local deformation.
  - Requirement of large amount of training data
  - Un-explainable (black-box) nature of model parameters and high computational requirements during training.

A summary of the aforediscussed analysis of the applicability of state-of-art OSEMS methodologies to early design phases according to the criteria detailed in Section 1 is presented in Table 1.

Therefore, to overcome these limitations we developed the MGRF methodology that satisfies all the criteria described in Section 1. A detailed description of the problem formulation and the developed MGRF methodology are presented in Sections 3 and 4, respectively.

3. Problem formulation

Representing the nominal coordinates of points on the surface of the part by $\mathbf{X}$, a $N \times 1$ matrix, where $N$ is the number of nodes in the mesh representation of the part. The non-ideal deviations of all mesh nodes of the part along the surface normal direction, represented by the $N \times 1$ vector $Z$, is modelled as a Gaussian Random Field (GRF), $f$. A GRF is a collection of random variables indexed by D-dimensional real numbers, i.e., $Z = \{z_\theta | x \in \mathbb{R}^D\}$, where any finite subset of $Z$ has a joint multivariate Gaussian distribution [33–36]. The GRF provides a means to generate spatially correlated random variables which are well suited to model non-ideal part behaviour, and overcomes the limitations of 1D-Gaussian and multi-Gaussian methods that could generate unrealistic shapes [23].

The covariance function which affect the shape and smoothness of the generated non-ideal part [35]. The mean function is defined as $E[f(x)]$, where $E$ is the expectation operator and can be estimated by fitting regression models [37]. Since an ideal part’s deviation from nominal is zero, in the present study mean function is taken to be zero without affecting the analysis [33]. In this paper, we model the non-ideal deviations as a second-order stationary GRF without any prior transformation. The second-order stationary assumption of the GRF implies that its covariance function only depends on the separation vector $x - x'$. For a function to represent the covariance between two input points, it has to be positive semi-definite [38]. Various types of covariance functions with different characteristics exist, and a detailed review is presented in [33].

The spatial pattern of the simulated non-ideal part and the smoothness of deviations from nominal depend on the parameters of the covariance function. To illustrate the effect of change in covariance function parameters on the simulated non-ideal part spatial patterns, we utilise the squared exponential covariance function represented by Eq. (1),

$$\text{cov}_{SE}(x, x') = \sigma^2 \exp \left[ -\frac{1}{2} \sum_{i=1}^{D} \frac{(x_i - x'_i)^2}{l_i^2} \right]$$

which is parametrised by $\theta = [\sigma, l_i]$, where $\sigma^2$ is the scaling factor, $D$ is the dimension of the input space, i.e., 2 for the illustration in Fig. 3 and 3 for the case of 3D-non-ideal part modelling. $l_i$ is the characteristic length scale along dimension $i$. The scaling factor is equivalent to the variance of the GRF and can be utilised to simulate non-ideal parts conforming to a given statistical tolerance specification as described in Section 4.2.2.

When the characteristic length scale is small, the deviations of two points which are at a distance larger than the characteristic length scale are weakly-correlated of each other, and the resulting non-ideal deviation pattern can simulate roughness, as illustrated in Fig. 1a. Similarly, when the characteristic length scale is large, two points with distance between them less than the characteristic length scale are highly-correlated. This leads to simulation of smoother form variation as shown in Fig. 1b. On the other hand, periodic errors can be simulated using Eq. (2),

$$\text{cov}_{\text{periodic}}(x, x') = \sigma^2 \exp \left[ -\frac{1}{2} \sum_{i=1}^{D} \left( \frac{\sin \left( \frac{\pi (x_i - x'_i)}{p_i} \right)}{l_i} \right) \right]$$

a modified squared exponential covariance function [39], which is modified by $\theta = [\sigma, l_i, p_i]$, where $l_i, \sigma_i$ and $D$ are similar to those described in (1), and $p_i$ represents the periodicity of the pattern along dimension $i$. A simulated periodic pattern from Eq. (2) is illustrated in Fig. 1c. Therefore, varying the parameters of the covariance function which characterise a GRF enable the simulation of multi-scale errors, such as roughness, waviness, and large scale form errors. The characteristic length scales influence the extent to which a given deviation affects (is correlated with) the neighbouring points along a given coordinate direction, and are conceptually equivalent to the domain of influence in the morphing mesh methodology [18] which defines the region of influence of the deviation.

Various covariance functions, such as periodic and squared exponential or two squared exponential covariance functions with different length and scale parameters can be combined to form a compound covariance function as in Eq. (3) [33],

$$\text{cov}_{\text{sum}}(x, x') = \text{cov}_{\text{small scale}}(x, x') + \text{cov}_{\text{large scale}}(x, x') + \text{cov}_{\text{periodic}}(x, x')$$

(3)
Table 1
Summary of the literature on object shape error modelling and simulation methodologies.

<table>
<thead>
<tr>
<th>Methodologies</th>
<th>Essential requirements for object shape error modelling and simulation during early design</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metric modal decomposition [25]</td>
<td>3D* G, TP, WoMD, DPL, No, CM, NP&lt;10</td>
</tr>
<tr>
<td>Statistical analysis [22]</td>
<td>2D G, TP, WMD, HD, DPL, No, CM, NP&lt;10</td>
</tr>
<tr>
<td>Second order shapes, PCA [19][21]</td>
<td>3D G, TP, WMD, HD, DPL, No, CM, NP&lt;10</td>
</tr>
<tr>
<td>Volume splines [19][17]</td>
<td>3D G, L, WMD, DPL, Yes, CM, NP&lt;10</td>
</tr>
<tr>
<td>Envelope-T [8][28]</td>
<td>3D G, L, WMD, DPL, No, CM, NP&lt;10</td>
</tr>
<tr>
<td>NURBS reconstruction [26]</td>
<td>3D G, L, WMD, DPL, No, CM, NP&lt;10</td>
</tr>
<tr>
<td>Natural mode decomposition [16]</td>
<td>3D G, TP, WMD, HD, DPL, No, CM, NP&lt;10</td>
</tr>
<tr>
<td>Morphing mesh [18]</td>
<td>3D G, L, TP, WoMD, HD, HD, DPL, Yes, CM, NP&lt;10</td>
</tr>
<tr>
<td>MGRF (This paper)</td>
<td>3D G, L, TP, WoMD, HD, HD, DPL, Yes, CM, NP&lt;10</td>
</tr>
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</table>

Legend for entries:
- 2D: 2D surface
- 3D*: 3D primitive surfaces such as cylinder, sphere etc.
- DPI: Dimensions of model parameters in Latent space
- HD: Dimensions of model parameters in Design space
- CL: Computational intensity low
- CM: Computational intensity medium
- CH: Computational intensity high
- CHT: High Computational intensity during model training
- HWMD: Without Measurement Data
- HD: Historical Part Data
- HD: Number of model parameters in the order of 10.
- SP2D: Surrogate/Similar Part Data
- NP: Number of model parameters in the order of 100, typically NURBS, B-spline or Reisier curve parameters, or number of modes.
- NP: Number of model parameters in the order of Millions, dependent on the type of Deep Neural Network architecture

Legend for Colours:
- Unacceptable
- Acceptable
- Good

Fig. 1. Illustration of multi-scale and pattern modelling abilities; the covariance function parameters are (a) \( \sigma_f, l \), small scale = \( \{1, (0.5, 0.5)\} \), (b) \( \sigma_f, l \), large scale = \( \{1, (5, 5)\} \), and (c) \( \sigma_f, l, p \), periodic = \( \{1, (5, 5), (3, 3)\} \).

where large scale and small scale subscripts are used to represent the two different characteristic length scales of a squared exponential covariance function (1). This property of covariance functions enables simulation of complex patterns in non-ideal parts. An illustration of a non-ideal pattern simulated from a combination of small scale (\( \text{cov}_{\text{small scale}} \)), large scale (\( \text{cov}_{\text{large scale}} \)) and periodic (\( \text{cov}_{\text{periodic}} \)) covariance function with parameter values as described in Fig. 1, is shown in Fig. 2.

A non-ideal part with a combination of different deviation patterns can be decomposed into its constituents by using the combined covariance function, and the optimum parameters can be automatically estimated by maximising the marginal likelihood as described in Section 4.1.2. This enables the covariance function to automatically model and extract complex non-ideal part deviation patterns [40]. Additionally, maximum likelihood estimates of the covariance function parameters, such as the characteristic length scales, have the asymptotic property of being equal to their true value as more sample points are collected [41]. The aforementioned properties make the modelling of non-ideal part deviations using covariance function appealing.

In this section, to simplify the exposition of the simulation of non-ideal parts, we utilise a 2-Dimensional (2D) part whose ideal form is the flat plate illustrated in Fig. 3a. A cross-sectional view of the flat plane is illustrated in Fig. 3b.

To simulate the non-ideal behaviour of a real manufactured part, we utilise a flat plate with simulated form error (exaggerated for illustration purposes) shown in Fig. 4. The spatial deviation pattern of a given part from its nominal design is
An illustration of a non-ideal part with complex pattern.

characterised by estimating the optimum values of the covariance function parameters ($\hat{\theta}$) that best describe it. The selection of the type of covariance function, i.e., using a simple covariance function as in (1) and (2), or a compound covariance function as in (3) is a modelling choice that depends on the spatial deviation pattern exhibited by the real manufactured part.

The number of parameters depends on the type of covariance function used. For instance, if covariance function (1) or (2) is used, $\theta$ is $\{\sigma_f, l_i\}$ or $\{\sigma_f, l_i, p_i\}$ respectively. On the other hand, if a compound covariance (3) is used, $\theta$ is $\{(\sigma_f, l_i)_{\text{small scale}}, (\sigma_f, l_x, l_y)_{\text{large scale}}, (\sigma_f, l_x, p_i)_{\text{periodic}}\}$.

Since on inspection it is evident that the simulated real part in Fig. 4 does not exhibit periodic, small scale or a combination of deviation patterns, a single squared exponential covariance function (1) is utilised to model its deviations, the corresponding $\theta$ is $\{\sigma_f, l_i\}_{\text{large scale}}$.

The methodology to obtain the optimum parameters’ value ($\hat{\theta}$) and generate non-ideal parts that exhibit similar spatial deviation patterns as the real manufactured part remains unchanged irrespective of the type of covariance function used and is described in detail in Section 4.1.

In this section we focus on illustrating the key concepts of unconditional simulation and morphing GRF through conditional simulation using the simulated 2D real part.

Unconditional simulation is a spatially consistent Monte-Carlo simulation with the goal to mimic spatial variation pattern as realistically as possible. Whereas conditional simulation, in addition to mimicking spatial variation pattern, constrains the simulated non-ideal parts to pass through given data points or fixed key points [34,36].

Unconditional simulation is obtained by sampling from the prior distribution of the GRF which has covariance function parameters that model the spatial deviation pattern of the real manufactured part [33,34]. It consists of a two step process: firstly estimating the optimum covariance function parameters ($\hat{\theta}$) of the GRF, secondly stochastically sampling multiple realisations of the GRF as schematically illustrated in Fig. 5 and described in detail in Section 4.2.2-(ii)(b).

Optimum covariance function parameters ($\hat{\theta}$) for the simulated real part in Fig. 4 are obtained by maximising their likelihood as described in Section 4.1.2. Accordingly, $\theta = \{\sigma_f, l_i\}_{\text{large scale}} = \{\sigma_f, (l_{x1}, l_{x2})\}_{\text{large scale}}$ was estimated to be $\{0.96, 3.38, 1.34\}$.

The obtained optimum values faithfully represent the simulated real part deviation pattern, where (i) the correlation along $x_1$ is high and a given point’s deviation strongly influences that of a point further along $x_1$, (ii) the correlation along $x_2$ is smaller causing the deviations of two points that are further apart to be weakly dependent on each other.

An illustration of two non-ideal parts generated for the simulated 2D real part in Fig. 4 by unconditional simulation for a statistical (97% confidence interval (CI)) profile tolerance of a surface of $\pm 2\%$ with symmetric tolerance zone is shown in Fig. 6. It shows that the simulated non-ideal parts emulate deviation patterns of the source part in Fig. 4, i.e., long characteristic length scale causing smooth deviations. Though the non-ideal parts generated by unconditional simulation emulate the spatial deviation patterns of manufactured part, they cannot simulate technologically wanted design variations to perform several ‘what if?’ analyses such as bending, twisting or part flange variations, because the generated non-ideal parts are equally likely to take any shape around the ideal surface.

The ability to incorporate user knowledge and simulate technologically wanted design variations is achieved by morphing the GRF. Key points ($X_k$) are specific points on the surface of the part whose deviation from nominal ($Z_k$) can be set by the designer to simulate parts conforming to given design intent. Key points ($X_k$) are chosen to be as uniformly spaced as possible and
cover the surface of the part as illustrated in Fig. 3a, a more detailed description of key points is presented in Section 4.2.1. Morphing is performed by manipulating a subset of these key points ($\tilde{X}_k$) and generating non-ideal parts that pass through them by utilising conditional simulation. When setting the deviation of a subset of key points ($\tilde{Z}_k$) the user has the ability to simulate a design intent as described in Section 1. This simple manipulation of a subset of key points ($X_k$) to characterise a design intent contributes to designer centricity. It also increases...
defect fidelity of MGRF methodology by enabling simulation of
design intent as demonstrated in Sections 5.1.1 and 5.2. The key
points selection and their deviation setting processes are further
detailed in Section 4.2.

Conditional simulation is performed by sampling from the
posterior distribution of the GRF which is conditioned (in a
probabilistic sense) to pass through the manipulated key-points
[33,34]. This is a stochastic process similar to sampling from a
conditional probability distribution. The samples obtained have
different values at all points except at fixed or conditioned points,
which in the present study are the manipulated key points.

The covariance function parameters used during conditional
simulation are same as those used in the unconditional simula-
tion and model the spatial deviation pattern of the real manu-
factured part. Conditional simulation is performed in this paper
as a two step process consisting of (i) first estimating the mean
part that passes through all the manipulated key-points thus
modelling the systematic deviations ($\bar{Z}$) and the design intent;
(ii) then generating multiple non-ideal parts that exhibit spatial
device pattern similar to real part and conform to design intent
by passing through manipulated key-points as described in detail
in Section 4.2.2 and schematically illustrated in Fig. 9.

An illustration of two non-ideal parts simulated through MGRF
along with the mean part for the 2D simulated real part in Fig. 4
by setting the deviation of three key points is shown in Fig. 7a.
All simulated non-ideal parts pass through the manipulated key
points, this process of simulating non-ideal parts that conform
to design intent by constraining them to pass through a few
manipulated key points is called MGRF.

Fig. 7b illustrates a sectional view of the ideal, mean and
non-ideal parts at the plane in Fig. 7a along with the 97% sta-
tistical tolerance bound for profile tolerance of a surface. The
tolerance bounds for constrained non-ideal parts is smaller than
that of unconditional non-ideal parts because the deviation of
non-ideal parts at the manipulated key points are fixed; this
leads to limiting the deviations of nearby points due to material
covariance [42], i.e., the physical limitation in part deviation due
to material properties of the part. The constraint eases as we
move away from the key point, therefore, the uncertainty in the
shape of the predicted non-ideal part is low near the key point
and increases as we move further away from it. This change in un-
certainty is captured by the posterior variance of the GRF [33,34].
A detailed explanation of the methodology to generate non-ideal
parts by MGRF is provided in Section 4.

4. Methodology

The MGRF methodology proposed to model and simulate
shape error of parts has two main stages (i) non-ideal part
modelling, and (ii) non-ideal part simulation. The non-ideal part
modelling stage estimates the optimal covariance function pa-
rameters of the GRF which models the spatial deviation pattern
of the given true manufactured part. The optimum parameters
estimated in the part modelling stage are utilised to simulate
multiple non-ideal parts that emulate the spatial deviation pat-
tern of the true manufactured part and conform to design intent
in the non-ideal part simulation stage. These two main stages are
explained in detail in Sections 4.1 and 4.2.

4.1. Non-ideal part modelling

Non-ideal part modelling stage estimates the covariance func-
tion parameters of the GRF characterising the spatial deviation
pattern of a given manufactured part. Representing by $\theta =\{(\sigma_f, l_i)_{\text{small scale}}, (\sigma_f, l_i)_{\text{large scale}}, (\sigma_f, l_i, p_i)_{\text{periodic}}\}$, the set of all co-
variance function parameters if Eq. (3) is used to model the
device pattern, the aim of non-ideal part modelling is to
find the optimum $\theta$, that best describes the given manufactured
part deviation. Non-ideal part modelling consists of (i) input
pre-processing, and (ii) non-ideal part deviation characterisation.
The non-ideal part modelling stage is schematically illustrated in
Fig. 8 and is explained in detail in Sections 4.1.1 and 4.1.2.

4.1.1. Input and pre-processing

The inputs for the proposed methodology are (i) the Com-
puter Aided Design (CAD) geometry or mesh file of the ideal part,
and non-ideal part data from real part measurement (typically CoP)
or simulation of current part, or (ii) historical data of a similar
part which consists of an ideal mesh file and real manufactured
part measurement data. The ability of MGRF methodology to use
historical data makes it suitable for non-ideal part modelling
during early design stages where measurement data availability
for current part could be scarce, thus contributing to its data
versatility. Section 5.2 explains the use of historical data in the
MGRF methodology in detail. Additionally, mesh element size
limits the kind of non-ideal behaviour that can be simulated,
for instance if the mesh element size is very large compared to
small scale characteristic length scale. Then, the non-ideal parts
simulated cannot display small scale effects in spite of being
modelled with the GRF.
Pre-processing involves calculating the surface normal deviation of the mesh nodes from available non-ideal part data. The mesh node coordinates of the nominal part represent the set of all points \( \mathbf{X} \) on the surface of the part. If measurement data are available, \( Z \), the deviation of each node from the design nominal in the surface normal direction is calculated by finding the distance between each ideal mesh node and the aligned CoP using routines provided in [43]. If data of non-ideal part deviations are available through manufacturing or assembly process simulation, for instance from FEM analysis, the node deviations from simulation can be projected along the surface normal direction to obtain \( Z \). Following the estimation of \( Z \), optimum covariance function parameters \( \hat{\theta} \) are obtained as described in the following section.

4.1.2. Non-ideal part deviation characterisation

The ability to mimic the spatial deviation pattern of the true manufactured part as closely as possible depends on the estimation of covariance function parameters \( \theta \), that best describe a given non-ideal part deviation. Optimum values of \( \theta \) are found by maximising the log-likelihood of covariance function parameters given the part surface normal deviation data \( Z \), estimated in Section 4.1.1. The log-likelihood function for a GRF is a function of \( \theta \) for a given non-ideal deviation \( Z \), and is estimated using Eq. (4) [33,41].

\[
\ln(L(\theta|Z)) = -\frac{N}{2}\ln(2\pi) - \frac{1}{2} \ln |\mathbf{C}(\theta)| - \frac{1}{2} Z^T \mathbf{C}(\theta)^{-1} Z
\]  

(4)

where \( \mathbf{C}(\theta) \) is the \( N \times N \) covariance matrix with entries obtained by evaluating the chosen covariance function between all possible pairs of nominal surface points, and \(|.|\) is the matrix determinant operator. For a compound covariance function each entry
in the covariance matrix $\Sigma(\theta)$ is the sum of individual covariance functions chosen to represent the compound covariance function evaluated between a pair of nominal surface points. While the values of $\theta$ do not directly appear in Eq. (4), they influence the values of the entries in the covariance matrix $\Sigma(\theta)$ and thus indirectly influence the minimum of the log-likelihood function.

Eq. (4) follows directly from the definition of the GRF in Section 3 which states that any finite collection of $Z$ has a joint multivariate Gaussian distribution. The method of obtaining the optimum covariance parameters by maximising the log-likelihood is robust and immune to over-fitting [41,44].

The computational complexity of calculating $\Sigma(\theta)^{-1}$ scales as $O(N^3)$, therefore, optimising the covariance parameters for large parts where $N$ is very large leads to computational challenges. To overcome computational challenges, in this paper, minimisation of the negative log likelihood function (equivalent to maximising log likelihood) is carried out by considering the non-ideal deviations of just the key points in Eq. (4), i.e., only utilising the non-ideal deviations $Z_k$ corresponding to location of key points $X_k$ defined in Section 4.2.1 to calculate $\Sigma(\theta)$.

Finally, the optimum values of $\theta$ minimising Eq. (4) are obtained by conjugate gradient method using the routines provided in [45]. This method of finding optimum values of the covariance function by minimising the negative log likelihood, eliminates the need for manual parameter guessing, and enables automatic deviation pattern modelling. For parts with more than 10000 key-points Full Independent Training Conditional (FITC) approach can be utilised and similar to the earlier case, the minimum of the negative log-likelihood function can be found by using the routines provided in [45].

Additionally, if a batch of part deviation data along with key parameters which influence the part deviation such as the manufacturing process parameters or the material composition are available, trends in covariance function parameters can be identified by fitting regression models or probability distributions to capture the functional relationship between process parameters and non-ideal part behaviour [46,47]. The developed functional relationship can then be used to simulate non-ideal behaviour of parts for which neither measurement nor simulation data is available for the current part. This capability of the proposed methodology to learn from historical data contributes to its data versatility and is demonstrated in Section 5.2.

The characteristic length scales of the covariance function as demonstrated in Section 3 describe the behaviour of the non-ideal part along different coordinate directions. Therefore, when covariance function parameters estimated using measurement data of historical similar parts are used to model non-ideal parts of current part it has to be ensured that the orientation of both parts match. This transformation is typically not necessary for automotive parts as they utilise the standardised vehicle coordinate system $(X_V, Y_V, Z_V)$, where the $X_V$ axis is parallel to the vehicle’s longitudinal plane of symmetry and points forwards. The $Y_V$ axis is perpendicular to the vehicle’s longitudinal plane of symmetry and points to the left and the $Z_V$ axis pointing upward [48].

Following the estimation of optimum covariance function parameters $\theta$, the simulation of non-ideal parts is performed as described in Section 4.2.

4.2. Non-ideal part simulation

The estimation of optimum parameters $\hat{\theta}$, as described in Section 4.1, enables simulation of non-ideal parts with spatial deviation patterns similar to the true manufactured part. The ability to simulate non-ideal parts which represent the designer’s intent and conform to given form tolerance specifications is achieved by MGRF through conditional simulation. Non-ideal part simulation consists of (i) key point selection, and (ii) MGRF to simulate non-ideal parts. These two steps are schematically illustrated in Fig. 9 and explained in detail in Sections 4.2.1 and 4.2.2.

4.2.1. Key point selection

Key points $X_k$ are specific nodes in the mesh representation of the nominal part such that $\{X_k \subset X | k \in 1, 2, 3, . . . , K\}$, where $K$ is the total number of key points. The generated non-ideal parts are constrained to pass through a subset of key points $X_k$, i.e., $\tilde{X}_k = \{X_{k} \subset X | p \in 1, 2, 3, . . . , \tilde{K}\}$, where, $\tilde{K}$ is the total number of manipulated key points. These are chosen to be in the region of interest, for instance on the flanges or around slots and holes. The optimal distance between key points is a function of the characteristic length scale parameter $\theta$ [49]. A large characteristic length scale implies a large region of influence for a given key point, therefore the key points can be spaced further apart. A large number of closely spaced key points provide the ability to precisely control the non-ideal behaviour of the part. However, as computational cost is cubic in the number of key points, it entails additional computational effort during estimation of optimal covariance function parameters. Following the selection of key points, non-ideal parts are generated by MGRF as described in Section 4.2.2.

4.2.2. MGRF to generate non-ideal parts

Simulation of non-ideal parts by MGRF consists of (i) key points deviation setting, to reflect design intent, and (ii) conditional simulation of non-ideal parts for a given setting of key points.

(i) Key points deviation setting:

Global and local deviation patterns are realised by manipulating the key points and setting the magnitude of their deviations. Manipulating a few key points simulates local deviation patterns, whereas, manipulating all or a large number of key points simulates global deviation patterns. This ability to simulate both global and local deviation patterns adds to the high fidelity of the MGRF methodology. The number of manipulated key points $K$ depends on design intent such as simulation of bending, local dent or flange geometric variation. The magnitude of deviations which we set at key points is represented by $Z_k$ (i.e., $Z_k = \{Z_k | k \in 1, 2, . . . , K\}$). The method of setting key point deviations is intuitive to the designer and various practical examples are illustrated in Section 5.1, this contributes to the designer centricity of the MGRF methodology. Once $Z_k$ are set, deviation of the entire part $Z$, corresponding to the manipulated key points’ deviation are estimated by conditional simulation.

(ii) Conditional simulation of non-ideal parts:

Conditional simulation of non-ideal parts is a two-step process of (a) predicting the mean part deviations ($\bar{Z}$) for given setting of key points’ deviations, and, (b) generating multiple non-ideal parts conforming to given form tolerance specifications and design intent. A detailed explanation of the steps for conditional simulation is given below as follows:

(a) Prediction of mean part deviation:

The decomposition of part form error into mean shape (systematic deviations, $\bar{Z}$) and correlated shape error (random form error, $\xi$) as represented by Eq. (5) is the standard procedure to generate skin model shapes [5,23]. In this paper the systematic deviations $\bar{Z}$ as described in Section 1 are further classified into local and global deviations that enable simulation of design intent.

$$ Z = \bar{Z} + \xi $$

(5)
The mean part deviations ($\bar{Z}$) for a given setting of key points, is estimated by Gaussian Process Regression (GPR) [33]. GPR is similar to the geostatistical approach [34]. However, GPR considers the probabilistic interpretation of the individual parameters of the covariance function [39], which aids in characterising the non-ideal part deviation as detailed in Section 4.1.

The mean non-ideal part after fixing the deviation of the manipulated key points ($\tilde{Z}_k$) is estimated by using the mean of joint posterior distribution of the GPR conditioned on the deviation of manipulated key points. Since any finite subset of $Z$ has a joint multivariate Gaussian distribution, the joint posterior distribution obtained by conditioning (i.e., fixing) the deviations at manipulated key points also has a Gaussian distribution. The mean of this distribution is given by Eq. (6) [33],

$$\bar{Z} = E(Z|\tilde{Z}_k, \hat{X}_k, \theta, \mathbf{X}) = C(\mathbf{X}, \tilde{X}_k)[(C\tilde{X}_k, \tilde{X}_k) + \sigma_n^2 I]^{-1} \tilde{Z}_k$$

(6)

where $\mathbf{X}$ is the $N \times 3$ matrix of nominal coordinates of all mesh nodes; $\hat{X}_k$ is the $K \times 3$ matrix of nominal co-ordinates of manipulated key points; $\tilde{Z}_k$ is the $K \times 1$ vector of manipulated key point deviations; $C(\mathbf{X}, \tilde{X}_k)$, is the $N \times K$ covariance matrix with the chosen covariance function evaluated between all pairs of points in $\mathbf{X}$ and $\tilde{X}_k$, similarly $C(\tilde{X}_k, \tilde{X}_k)$, is the $K \times K$ covariance matrix; $I$ is an identity matrix with size equal to the number of manipulated key points; $\sigma_n^2$, traditionally is the nugget effect or measurement error variance [33,34], which in this paper is set to zero so that the generated non-ideal parts pass through the manipulated key points; $\tilde{X}_k$, Eq. (6) gives $\bar{Z}$ the $N \times 1$ vector representing the mean surface that passes through the manipulated key points.

The prediction of the mean part using GPR has the following advantages: (i) it does not require guessing the degree and order of the regression, and, (ii) it does not limit the non-ideal behaviour of parts to second order shapes such as paraboloid as described in [21].

(b) Simulation of multiple non-ideal parts:

In this paper, multiple non-ideal parts are simulated by conditional simulations [34] with modifications to (i) simulate parts conforming to form tolerance specifications, and (ii) overcome computational limitations that entail non-ideal part simulation of large parts. The methodology utilises unconditional simulations to generate non-ideal parts conforming to given form tolerance specification and design intent. Therefore, firstly, the methodology to generate an unconditional simulation of spatially correlated random variables is detailed. Following which, the methodology to utilise the generated unconditional simulations for the simulation of non-ideal parts conforming to a given form tolerance specification and design intent is detailed.

The unconditional simulation of an $N \times 1$ vector $\xi_u$, with a spatial deviation pattern similar to the true manufactured part can be generated by sampling from the $N \times N$ covariance matrix $C(\mathbf{X}, \mathbf{X})$, obtained using optimum parameters $\theta$ estimated in Section 4.1. The sampling can be performed by the multiplication of a standard Gaussian random vector ($U$) with (i) Cholesky factor of the covariance matrix as in Eq. (7a), or, (ii) eigen-decomposition of the covariance matrix as in Eq. (7b) [50].

$$\xi_u = \mathbf{L}U \quad \text{ (7a)}$$

$$= \Phi \Lambda^\frac{1}{2}U \quad \text{ (7b)}$$

where $\mathbf{L}$ is the $N \times N$ lower triangular Cholesky factor of $C(\mathbf{X}, \mathbf{X})$, $\Phi$ is the $N \times N$ eigen basis matrix of $C(\mathbf{X}, \mathbf{X})$, and $\Lambda$ is the diagonal eigenvalue matrix of $C(\mathbf{X}, \mathbf{X})$. Multiple instances of $\xi_u$ can be obtained by generating independent instances of $U$ and substituting it in Eq. (7a) or Eq. (7b).

Cholesky decomposition or eigen-decomposition of the $N \times N$ covariance matrix, $C(\mathbf{X}, \mathbf{X})$, is computationally challenging, when $N$, the number of mesh nodes becomes greater than 10,000. To overcome this limitation, the eigen-decomposition is performed on the $K \times K$ covariance matrix $C_k$, obtained by limiting $\mathbf{X}$ in $C(\mathbf{X}, \mathbf{X})$ to the key nodes $X_k$, to obtain the key point eigen basis matrix, $\Phi_k$. The eigen basis matrix $\Phi$ for all mesh nodes of the part is estimated by interpolating the values at key nodes based on prior work of Wolff [49]. In this paper the interpolation of eigen basis $\Phi$ from $\Phi_k$, is performed by solving the Poisson problem described by Eq. (8) using FEM formulation utilising routines provided in [43]. The interpolation in Eq. (8) can also be performed using the discrete form of Laplace–Beltrami operator commonly used in computer graphics [51–53].

$$\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Phi = \Phi_k \quad \text{ (8)}$$

Typically the first $R$ columns of $\Phi$, $R \ll K$, account for most of the variance in data and $\xi_u$ can be generated using Eq. (9).

$$\xi_u = \Phi_k \Lambda^\frac{1}{2} U_k \quad \text{ (9)}$$

where $\Phi_k$ is the $N \times R$ interpolated eigen basis matrix, $\Lambda_k$ is the $R \times R$ diagonal matrix with elements equal to the first $R$ eigenvalues of $C_k$, and $U_k$ is the $R \times 1$ vector of independent standard Gaussian random variables. Thus, enabling the unconditional simulation of spatially correlated patterns for large non-ideal parts. Alternatively, if the mesh structure is uniform and the key points are regular large-scale non-conditional simulations ($N > 10,000$) can be obtained utilising FFT-based simulations, which provide an accurate reproduction of the covariance function and are computationally more efficient [34,54].

The conditional simulation of a non-ideal part conforming to form tolerance and design intent is obtained by first estimating the variance or the scaling factor parameter $\sigma_f$, of the covariance function that corresponds to a given form tolerance specification. As described in Section 1, in this paper, we demonstrate the simulation of non-ideal parts conforming to the specified form tolerance requirements for the profile of a surface [9], specifically the free state tolerance specification as described in [55]. Considering a statistical tolerance CI of $p\%$, Lower Specification Limit (LSL) and Upper Specification Limit (USL) of $t/2$, i.e., $|\text{LSL}| = |\text{USL}| = t/2$, we estimate $\sigma_f$ using
5.1.1. Non-ideal part modelling

The engineering phase of the NPI process. The two scenarios are able but historical data for a similar part is available, representing the NPI process of an assembly system development. Secondly, the case where measurement or simulation data for the current part is available, represents the engineering and assembly stage of the NPI process of an assembly system development. Secondly, we consider the case where data for the current part is unavailable but historical data for a similar part is available, representing the engineering phase of the NPI process. The two scenarios are explained in detail in Sections 5.1 and 5.2.

5. Applications in automotive assembly process

The MGRF methodology developed in this paper is demonstrated using sport utility vehicle door inner sheet-metal parts. The door inner is a vital part of the door subassembly which consists of window channel, halo, hinge, latch reinforcement, and seat belt reinforcement. The two door inner parts utilised in this section have 27,468 and 75,979 mesh nodes and demonstrate the scalability of the MGRF methodology to large parts. As described in Section 1, non-ideal behaviour of parts play a key role in determining quality of joining/fastening with other parts belonging to the subassembly. Therefore, its effect on assembly quality has to be quantified as early as possible through simulation studies.

In this section, defect fidelity, designer centricity, and ability to support tolerance analysis and synthesis are illustrated for two specific scenarios of data availability common during early design phases, demonstrating the MGRF methodology’s data versatility. Firstly, we demonstrate the application of MGRF methodology to the case where measurement or simulation data for the current part is available, representing the engineering and assembly stage of the NPI process of an assembly system development. Secondly, we consider the case where data for the current part is unavailable but historical data for a similar part is available, representing the engineering phase of the NPI process. The two scenarios are explained in detail in Sections 5.1 and 5.2.

5.1. Case 1: Measurement or simulation data for the current part are available

5.1.1. Non-ideal part modelling

Input and pre-processing: The inputs, in this case, are the CAD model of the ideal geometry of the part and measurement data. The CAD model of the part is converted to its mesh representation using Altair Hypermesh commercial software; the CAD along with its discrete meshed representation is illustrated in Fig. 10. The mesh representation of the door inner consists of 27,468 mesh nodes with an average mesh element edge length of 25.73 mm.

The true manufactured part’s measurement data in the form of CoP aligned with the CAD geometry was obtained as output from an optical 3D-surface scanner and is illustrated in Fig. 12a, it consists of 839,874 points with an average spacing of 30 μm between points.

\[
\sigma_T = \frac{|\text{USL}|}{S_2}
\] 

where $S_2$ is the Z-score corresponding to cumulative probability of $P \leq (1+p)/2$, i.e., the number of standard deviations by which a standard normal random variable ($\chi$) is above or below the mean and corresponds to a cumulative probability of $P(\chi \leq (1+p)/2)$. This can be obtained using cumulative standard normal table [46] or programmatically using many statistical software. Following the estimation of $\sigma_T$, steps described in detail in lines 3–10 of Algorithm 1 lead to non-ideal parts that conform to both form tolerance specifications and design intent.

Algorithm 1: Conditional simulation of non-ideal parts conforming to form tolerance specifications and design intent

1. Calculate Z-score $S_2$ for a standard normal distribution corresponding to cumulative probability $P \leq (1+p)/2$;
2. Calculate the standard deviation $\sigma_T$ of a zero mean normal distribution for which the probability of a random variable having value $\leq \text{USL}$ is $p$, by using Eq. (10);
3. Generate mean surface $\bar{Z}$ using GPR Eq. (6) by setting manipulated key point deviations to $\bar{Z}_k$ and estimating the $N \times \bar{K}$, $K \times \bar{K}$ covariance matrices using optimum covariance function parameters $\hat{\theta}$;
4. For each non-ideal part representative to be simulated do
   5. Generate scaled unconditional simulation $\xi_u$, by sampling from covariance matrix obtained by using optimised characteristic length scale parameters from $\hat{\theta}$ and setting $\sigma_T = \sigma_U$;
   6. Find the deviation values ($U$) at locations corresponding to manipulated key-points (axis points in case of bending) in $\xi_u$;
   7. Generate a surface $\tilde{Z}_U$ using GPR Eq. (6), with deviations at manipulated key points set equal to the values ($U$) found in line 6 and covariance function parameters set to $\hat{\theta}$; Note: $\xi_u$ and $\tilde{Z}_U$ are unconditional simulation and the corresponding mean surface generated to perform conditional simulations;
   8. Find the difference in deviation at each mesh node between the un-conditioned simulation generated in line 5 and surface generated in line 7, i.e., $\tilde{Z}_U - \xi_u$;
   9. Subtract the difference obtained in line 8 at each node with the corresponding node deviation of the mean surface $\bar{Z}$ generated in line 3 to obtain a non-ideal part conforming to given form tolerance specification and design intent, i.e. $Z = \bar{Z} + \xi = \bar{Z} - (\tilde{Z}_U - \xi_u)$;
10. end

Utilising this CoP data, the deviation of each mesh node in the surface normal direction is estimated as an average of the deviation of all the projected distances (in the node normal direction) of measurement points that lie within the footprint of the base of a cylinder of given area centred at the mesh node with the axis of the cylinder coinciding with the mesh node normal. All points that are at a distance larger than a given cut-off value are not considered while calculating the average, this helps with noise reduction/elimination. In this paper the appropriate area of the base of the cylinder, the cut-off distance were estimated from sensitivity studies and taken to be 4 mm² and 5 mm respectively. A schematic illustration of this is presented in Fig. 11. The estimation of these mesh node normal deviations $Z$ was performed using routines available in [43]. The colour map of the obtained surface normal deviation is shown in Fig. 12b.

Characterisation of non-ideal part deviation: Since no small scale variation or periodicity was observed in the measurement data, a single Matérn covariance function was used to characterise the
Fig. 10. (a) CAD geometry, (b) mesh representation with key nodes.

Fig. 11. Schematic illustration of estimation of node normal deviation.

Fig. 12. (a) measured Cloud-of-Points, (b) estimated part surface normal deviation. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
deviation field. The Matérn covariance function with smoothness parameter $\nu = 5/2$ \cite{11},

\[
\text{cov}_{\text{Mat}, \nu = 5/2}(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \left( 1 + \sqrt{5} \sum_{i=1}^{d} \frac{|x_i - x_i'|}{l_i} + \frac{5}{3} \sum_{i=1}^{d} \frac{(x_i - x_i')^2}{l_i^2} \right)
\exp \left( -\sqrt{5} \sum_{i=1}^{d} \frac{|x_i - x_i'|}{l_i} \right)
\]

where $|x_i - x_i'|$ refers to the absolute value of $(x_i - x_i')$, was utilised in this case study due to its computational advantages compared to the squared exponential function as described in detail in \cite{41}. The optimum characteristic length scales were obtained by maximising the likelihood \cite{4}, $C(\theta)$ for this part was the $1434 \times 1434$ matrix obtained by estimating the covariance function \cite{11} between all the key points $\mathbf{X}_i$. The optimisation was performed utilising the routines provided in \cite{56} and optimum characteristic length scales in $X$, $Y$ and $Z$ coordinate directions were estimated to be $168.73$, $7.74$ and $93.70$ mm respectively. The optimum values were estimated with $300$ iterations and $3$ restarts to guard against obtaining locally optimum estimates. The obtained optimum characteristic length scales reflect the true deviation pattern seen in Fig. 12b, where a given non-ideal deviation is highly correlated in $X$ coordinate direction compared to the deviations in $Y$ and $Z$ coordinate directions. This visual confirmation of the obtained characteristic length scales with the real part spatial deviation pattern is recommended to guard against consistency issues described in \cite{57,58}.

Additionally, depending on the requirements and an initial inspection of the input part spatial deviation pattern any of the covariance functions described in Section 3 or \cite{33,34}, can be plugged in without affecting the methodology described in this paper. Following the estimation of optimum covariance function parameters, the simulation of non-ideal parts is carried out as described in Section 5.1.2.

5.1.2. Non-ideal part simulation

Key points selection: The key points in this paper are a subset of all the mesh nodes of the part and are chosen to be evenly spaced by finding the points of intersection of the part and its voxelised bounding box with cubic voxels of size $20$ mm resulting in $1434$ key-points. The distance of $20$ mm between two key-points is smaller than the optimum characteristic length scales in $X$ and $Z$ coordinate directions enabling increased control on generated non-ideal part instances. The selected key mesh nodes for the part are coloured red and superimposed on the mesh representation in Fig. 10b.

MGRF to generate non-ideal parts: This section illustrates the designer centrivity of MGRF methodology through the simulation of non-ideal parts for the following ‘what if?’ scenarios: (i) global deformation patterns, (ii) local deformation patterns, and (iii) parts that conform to form tolerance specification for the profile of a surface. The aforesaid scenarios can be simulated by simple manipulation of key-points which adds to the designer centrivity of the methodology.

Firstly, global deformation patterns of the non-ideal part are simulated by manipulating a large number of key points according to the design intent. In this section, a bending of the part about axis A-A is simulated (Fig. 13a), giving rise to a maximum deviation of $\approx 3$ mm. The mean part shape simulating bending is found through GPR using \cite{6} by setting all key points to deviate proportionately to the perpendicular distance from axis AA to simulate a bending of $2^\circ$ with the furthest key point from axis being deviated by $\approx 3$ mm, i.e., $Z_0 = 1434 \times 1 \times 2^\circ$. The magnitude of bending set here to $2^\circ$ can be set to any realistic value that the designer wants to evaluate the effect of. Simulation can also be performed for a range of values to conduct preliminary sensitivity analysis. $C(X, X_0)$, $C(X_0, X_0)$ are $27468 \times 1434$, $1434 \times 1434$ covariance matrices obtained by evaluating \cite{11} between each pair of ideal mesh node location $X$ and manipulated key points $X_0$ and between each pair of manipulated key points $X_0$ respectively. The generated mean surface is illustrated in Fig. 13b.

Two non-ideal part representatives that conform to the design intent of simulation of local deformations and form tolerance specification for the profile of a surface with symmetric tolerance
zone \([9]\) of \(\pm 1\) mm (statistical tolerance CI of 95\%) are illustrated in Fig. 14(c) and (d). They were obtained by conditional simulation as described in Section 4.2.2-(ii)-(b) by setting parameter values similar to that of the global deformation case except that the manipulated key-points for unconditional simulation are same as that used to generate the mean local part.

Finally, non-ideal part representatives conforming to form tolerance specification for the profile of a surface with symmetric tolerance zone \([9]\) of \(\pm 2\) mm and statistical tolerance CI of 95\% without any global or local deformations are simulated. Such non-ideal part representatives are obtained by adding to the ideal surface the scaled unconditional simulations obtained as described in Section 4.2.2(ii)-(b) by utilising the parameters of the optimum covariance function \(\hat{\theta}\) in Section 5.1.1, but setting \(\sigma_f\) to \(\sigma_T = 1.0204\) obtained using (10) to estimate the \(1434 \times 1434\) covariance matrix \(C_X\) without performing any conditional simulation. Fig. 15 illustrates two such simulated parts. All the demonstrated non-ideal part simulations are almost real-time (\(\leq 0.36\) s) as described in Section 5.3 and illustrated in Fig. 21, demonstrating the computational effectiveness of MGRF methodology.

5.2. Case 2: Historical data of similar part available

5.2.1. Non-ideal part modelling

**Input and pre-processing:** The inputs, in this case are (i) the CAD model of the ideal geometry of the current part, and (ii) CAD model and measurement data of a similar part. We utilise the door inner part described in Fig. 10 as the historically similar part with data. The pre-processing is performed as described in Section 5.1.1, the CAD geometry and mesh representation of the new part for which no real manufactured part measurement data is available is illustrated in Fig. 16. The mesh for the current part consists of 75,979 nodes and the average mesh element edge length is 14.58 mm.

**Characterisation of non-ideal part deviation:** The optimum correlation function parameters obtained from historical data can be utilised for non-ideal part simulation of the part for which no data is available if the parts (i) are geometrically similar, (ii) have similar material composition, and (iii) are fabricated using the same manufacturing process. In addition to the above constraints, the parts should also have the same orientation, enabling the transfer of characteristic length scale parameters. In this case study, the transformation was not necessary as the parts utilise
Fig. 14. Illustration of local non-ideal part deformation (a) manipulated key points, (b) mean part, (c) and (d) simulated part instances.

Fig. 15. Illustration of non-ideal part simulation with surface profile tolerance specification of ±2 mm with symmetric tolerance zone.
the same coordinate system and have the same orientations, i.e., both parts are right side door inners of similar automobile models. To demonstrate the learning from historically similar part, the optimum parameters estimated in Section 5.1.1 are utilised to simulate non-ideal parts for the new part illustrated in Fig. 16.

Additionally, as described in Section 4.1.2, a functional relationship between process parameters and the optimum covariance function parameters can be modelled. The model can then be utilised to obtain optimum parameters in the future. A simple illustration of this characterisation is shown in Fig. 17, where 3-Dimensional Gaussian distributions are fit to the optimum characteristic length scales of two batches of manufactured parts with different materials. First batch (batch 1) consists of 38 parts with mean optimum characteristic length scales of 120.20, 11.89 and 90.88 mm along X, Y and Z coordinate directions respectively. Second batch (batch 2) consists of 32 parts with mean optimum characteristic length scales of 168.73, 7.74 and 93.70 mm along X, Y and Z coordinate directions respectively.

The characteristic length scales of parts from two batches form separate clusters differentiating them. A two tailed t-test with the null hypothesis that the characteristic length scales of the two batches belong to a Gaussian distribution with equal means was rejected with all p-values < 0.025. However, the same test performed on two groups obtained by splitting the characteristic length scales of each batch (i.e. individual batches were divided into two equal groups and separate t-tests were performed on each batch) failed to reject the null hypothesis of equal means with all p-values > 0.22, i.e. proved that each batch belonged to the same Gaussian distribution with equal means. This demonstrates that characteristic length scales can be used effectively as a means to model non-ideal part characteristics.

Finally, when no historical data are available the characteristic length scales can be manually set as they are easily interpreted as the distance until which the non-ideal deviation at surface point can influence its surrounding along a given coordinate direction. This capability adds to the designer centricity and data versatility of the MGRF methodology.

5.2.2. Non-ideal part simulation

The Key points selection and MGRF to generate non-ideal parts are performed as described in Section 5.1.2 with a voxel size of 20 mm resulting in 1325 key-points. To illustrate the simulation of global deformation patterns similar to the non-ideal parts in Fig. 13, we move all the 1325 key-points about axis A-A represented by the two highlighted key points in Fig. 18(a) in a manner similar to that described in Section 5.1.2. The key-points for representing the axis are chosen manually to emulate the non-ideal parts in Fig. 13 and are illustrated in Fig. 18(a), they cannot
be exactly similar due to the differences in part geometry, its mesh and number of key-points. The objective is to emulate the spatial deviation pattern and not the exact deviations.

The magnitude of deviation of manipulated key-points, optimum covariance function parameters ($\hat{\theta}$), setting for the number of basis vectors for $\Phi$, magnitude of form tolerance specification for the profile of a surface with symmetric tolerance zone are all set exactly equal to as in Section 5.1.2 to aid comparison. The simulated mean part and two non-ideal part instances for the new part with no measurement data but utilising historical data from part in Fig. 10 are illustrated in Fig. 18 (b), (c) and (d), respectively. It can be seen that they exhibit spatial deviation patterns similar to the historical part.

To simulate local deformation patterns similar to the non-ideal parts in Fig. 14, we move the key nodes highlighted in Fig. 19a by 3 mm. This includes 9 key-nodes in total, with 5, 3, and 1 key-node for bottom flange deviation, left flange deviation, and dent simulation respectively. These key points are chosen manually to emulate the deviation pattern in Fig. 14 to facilitate comparison. The simulated mean part and two non-ideal part instances for the new part with no measurement data but utilising historical data from part in Fig. 10 are illustrated in Fig. 19(b), (c) and (d), respectively. It can be seen that they exhibit spatial deviation patterns similar to the historical part.

Finally, two non-ideal part representatives conforming to form tolerance specification for the profile of a surface with symmetric tolerance zone [9] of ±2 mm (statistical tolerance CI of 95%) with no systematic deviations is illustrated in Fig. 20. These non-ideal parts are generated using the same specifications used to simulate the non-ideal part in Fig. 16. The non-ideal parts simulated in this section demonstrate that the spatial deviation pattern from historical data of a similar part can be transferred to the part with no data, a capability that is essential for non-ideal part simulation during early design stages.

5.3. Computational time analysis

The computational time for simulation of non-ideal part using MGRF methodology has fixed and variable components. The fixed component cost is incurred once per part and is the sum of time taken to estimate the optimum covariance function parameters, the time to interpolate $\Phi$ using Eq. (8) and the time to estimate the mean part for a key-points setting using (6). Whereas, the variable time component is the time taken to simulate each non-ideal part as described in Section 4.2.2-(ii)(b). The computational time presented in this section utilised Matlab 2018b software.
Fig. 19. Illustration of local non-ideal part deformation using historical data (a) manipulated key points, (b) mean part, (c) and (d) simulated non-ideal part instances.

Fig. 20. Illustration of non-ideal part simulation with surface profile tolerance specification of $\pm 2$ mm with symmetric tolerance zone simulated with historical data.
The time to estimate the optimum covariance function parameters depends on the number of key points and takes approximately 0.458, 1.741 and 9.044 s for 2345, 4027 and 8122 key points respectively for each optimisation iteration and is illustrated in Fig. 21. It shows the $O(K^3)$ increase in computational cost of optimal covariance function parameters with respect to the increase in number of key-points. Typically 200 (in some cases 300) such iterations are required for convergence. This convergence study should be performed more than once to ensure that we do not obtain locally optimal values. Therefore, optimisation approximately requires around 274.74–5426.28 s for one part and is to be performed once during the modelling stage.

The computational time for interpolation of $\Phi$ using Eq. (8) depends on the total number of mesh nodes and takes 1.936 s for a part with 27468 mesh nodes and 5.553 s for a part with 75979 mesh nodes, both times are estimated as the average of 5 repetitions. However, this interpolation cost remains almost unaffected by the number of key-nodes and increases from 1.9681 s for 2345 key-points to 2.331 for 8122 key-points for the part with 27468 mesh nodes as illustrated in Fig. 21.

The computational time to generate the mean part is cubic in the number of manipulated key points ($O(K^3)$) as seen in (6). To demonstrate its effect we present the computational time required for both global and local deformations of the part used in Section 5.1 for three different key-point configurations. The results summarised in Fig. 21 show that the local deformation simulation takes $\approx 0.16$ s for all three configurations of key-point as the number of manipulated key-points remains the same. On the other hand, the time required to generate the mean global deformation part increases with the number of key-points from 2.108 s for 2345 key-points to 17.8225 s for 8122 key-points as we manipulate all the key points to create the mean part to simulate bending.

The variable component relating to the simulation of each non-ideal part conforming to requirements is almost real-time, requiring 0.197, 0.228 and 0.368 s for each part with 2345, 4027 and 8122 key points respectively and is illustrated in Fig. 21. Per part simulation time is estimated from averaging the time to generate a batch of 20 non-ideal part instances five times.

6. Comparisons with state-of-art OSEMS modelling methodologies

Numerous OSEMS methodologies exist in the literature. However, as described in Section 2.4 random field methodology [23] and the morphing mesh methodology [18] meet most of the criteria applicable for early design stages. Therefore, this section, first compares the developed MGRF methodology with these two methodologies. Then, it demonstrates the limitation of deviation decomposition or mode based methodologies in utilising historical data from similar parts.

6.1. Comparison with random field methodology

The random field methodology [23] compared to the developed MGRF methodology as discussed in Section 2, has limitations such as the ability to model local deformations and simulate non-ideal parts conforming to statistical form tolerance specifications. However, it can model spatial deviation patterns in the manufactured part in a limited manner. This ability of random field methodology to model spatial patterns is compared with the MGRF methodology. State-of-art random field methodologies do not describe a technique to handle large parts, therefore to enable comparison the approximation technique described in Section 4.2.2 is utilised for both methodologies.

The deviation pattern in Fig. 12b is utilised as input. Optimum characteristic length for the random field methodology is obtained as described in [23] which utilises one characteristic length for all three coordinate directions. This limits the state-of-art random field methodology to model and simulate spatial patterns that are spherical. Unlike the random field methodology, the MGRF estimates them as described in Section 5.1.1 and has one characteristic length for each coordinate direction which enables better emulation of spatial deviation of real manufactured parts. Three non-ideal parts simulated using both methodologies are illustrated in Fig. 22, which shows that MGRF methodology simulates non-ideal parts that are more similar to the true pattern in Fig. 12b with part deviations exhibiting high correlation along X direction, whereas the GRF methodology is unable to faithfully reproduce the true spatial deviation pattern.

6.2. Comparison with morphing mesh methodology

The morphing mesh methodology [18] compared to the developed MGRF methodology as discussed in Section 2, has limitations such as the inability to incorporate measurement data, model deviation patterns and utilise historical data. However, the methodology is versatile, intuitive and computationally efficient [5], and can model local deformations. In this section, the ability of both methodologies to simulate local deformations is
compared. Since the estimation of the radius of influence parameter of morphing mesh methodology is non-trivial and chosen by the designer, the optimum characteristic length scale parameters obtained in Section 5.1.1 are utilised as radius of influence and the simulated non-ideal parts are illustrated in Fig. 23, which shows that both methodologies simulate local deviations similarly. However the morphing mesh methodology does not simulate spatial deviation patterns.

6.3. Limitation of deviation decomposition or mode based methodologies

Deviation decomposition or mode based non-ideal part modelling methodologies such as natural mode analysis [16] can generate modes without deviation data, but require measurement data to calibrate the magnitude of modes to match a given spatial deviation pattern [5]. However, since the mode shape depends on geodesic distances among the points on the surface [52], the mode shapes vary with geometry and meshing. The modes for two similar parts obtained according to natural mode analysis methodology [16], have been estimated using free boundary conditions for both parts compared in Fig. 24. The modes are ordered in descending order of magnitude. It shows that the mode shapes differ for each of the two parts and hence learning from one part cannot easily be transferred to the other part, limiting the utility of historical data.
Conclusions and future work

A novel MGRF methodology for OSEMS was developed in this paper. Overcoming the limitations of state-of-art methodologies, the MGRF methodology has the following contributions that enable it to effectively model and simulate object shape error during the early design stage: (i) it has high defect fidelity as demonstrated in Sections 5.1.2 and 5.2 where global deformations such as bending, local deformations such as dents and flange variations, and form error such as profile tolerance of a surface with symmetric tolerance zones, were simulated; (ii) it has high data versatility enabling it to effectively simulate non-ideal parts at all levels of data availability. This is demonstrated by the ability to model non-ideal parts when measurement data are available in Section 5.1.1, and when historical data are available in Section 5.2.1. When no data are available the model parameters can be set manually without ambiguity as their dimensions lie in the 3D domain of the part; (iii) it is highly designer centric, as it is capable of performing ‘what if?’ analysis by simple manipulation of key-points which is intuitive as demonstrated in Sections 5.1.2 and 5.2, and as the model parameters such as characteristic length scales are easily interpretable and are physically meaningful as demonstrated in Section 3; and (iv) it supports simulation of statistical form tolerance for surface profile without additional modelling effort such as rejection of simulated parts. This is demonstrated with the simulation of form tolerance for profile of a surface with symmetrical tolerance zone in Sections 5.1.2 and 5.2. All the aforementioned capabilities demonstrated through industrial case studies clearly illustrate the contributions of the MGRF methodology.

Though the MGRF methodology has many advantages it entails a few limitations, which are as follows: (i) non-ideal part deviations are assumed to be in the surface normal direction, this assumption could lead to inaccurate modelling of non-ideal behaviour in the regions of high curvature; and (ii) dependence on designer for key point deviations, this could lead to generation of unrealistic non-ideal part representatives. Though the ability to effectively utilise historical data has been demonstrated in this paper, a few research questions are yet to be addressed and will be considered in future work. For instance, when using historical data, a definition of part similarity in terms of topology and manufacturing process used to fabricate the parts, has to be developed.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The source-code and data to reproduce the developed MGRF methodology can be accessed online at [61].

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