

Framework for Integrating the Finite Element Method and a Statistical Learning Approach for Characterizing the Effect of Process Parameters on Mechanical Response

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Abstract

Reliable analysis and insights are needed to guide processing parameters for additive manufacturing (AM) based material designs to reduce the cost associated with a trial-and-error approach. This work demonstrates an integrated framework that combines thermomechanical simulation with a statistical framework as a tool for providing interpretable insights into the interplay between AM process parameters on metallic alloy printing. Specifically, a large number of simulations (192) were performed using processing parameters (laser power, laser scan speed, layer height, and cooling assumptions) to predict the stress and deformation outcomes for a nickel alloy, Inconel-625. Instead of traditional plots for post-processing, two unsupervised machine learning approaches were applied to the outcomes, namely the finite mixture models (FMM) and the finite mixture of regression models (MoRM). The FMM used a mixture of Gaussians and regression to cluster the regions based on von Mises stress and deformation outcomes to identify locations (within and across simulations) that behaved similarly. The MoRM approach used a mixture regression model with Gaussian error, which directly allowed for the effect of each manufacturing process parameter to be considered. The MoRM performed well at capturing the variance present within the simulations. This approach also identified areas of geometry that were sensitive to changes in the manufacturing parameters. For example, the stress clusters at the lower layers were robust to change, while those at the higher layers were sensitive to changes. For the deformation, the unsupported regions were the most sensitive to change, while the rounded areas tended to be robust. The underlying thermomechanistic interpretation supported these outcomes. The findings collectively demonstrated how an independent statistical approach can be used to provide insights across a large number of process parameters and simulation outcomes for identifying optimum process and printing outcomes.

Categories: Structural Analysis and Finite Element Analysis, Materials Engineering, Data Science and Analytics for Engineering

Keywords: finite element analysis, computer aided manufacturing, pattern recognition, unsupervised learning, cluster analysis

Introduction

The engineering design process is highly iterative, relying on the ability to rapidly create and improve prototypes to achieve a final product [1]. Additive manufacturing (AM) is an appealing method for rapid prototyping due to its comparatively low setup cost and its ability to manufacture sophisticated parts [2]. Traditional manufacturing methods, such as subtractive manufacturing or molding, are not ideal for prototyping. Molding requires considerable initial setup

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costs, and is preferred for large production runs after the final design is determined. Subtractive manufacturing, such as machining and laser cutting, also requires a high initial set-up cost. While subtractive manufacturing can be effective for creating precise parts, it is limited in creating specialized features, such as internal features, and results in a larger waste of material. This is especially prohibitive when the material used for manufacturing is not abundant. These drawbacks from alternative methods make AM an attractive option for quick prototyping and designing complex geometries with relatively less material waste.

However, despite these benefits of AM, including the relative ease of setup to produce parts, the process is slow. Furthermore, AM requires interplay with multiple process parameters, such as laser power, laser speed, and cooling rates, among a few, with limited knowledge on the effect of these parameters on final outcomes. These considerations typically require multiple trial-and-error attempts to achieve desired outcomes. Specifically, these parameters control internal defects and warping and roughness of parts, due to the thermal and residual stresses generated from repeated heating and cooling during manufacturing [3,4]. Accurate prediction and control of residual stresses are therefore essential for optimizing process parameters for a sound structural outcome. Experimentally, these stresses are challenging to measure during part production and include destructive (hole-drilling) and non-destructive methods (X-ray and neutron diffraction) that require specialized equipment [5,6]. Numerically, the prediction of residual stresses from welding stainless steel has been investigated through neural networks with success as a surrogate model [7]. Machine learning (ML) has also been used for the prediction of nonlinear material deformation in simulation [8]. While these models are useful for prediction in their given setting, they are difficult to interpret to achieve a desired result beforehand. Hence, moving forward, an alternative integrated and faster approach for evaluating the interplay between different process parameters and the desired product outcome is required.

Fully exploring the process parameter space through experiments is costly and time-prohibitive. Alternatively, the finite element (FE) analysis can address some of these challenges through thermomechanical simulation to evaluate the effect of various process parameters on the final outcome. However, due to the multiple parameters and complicated interplay between the process parameters, a large number of simulations would be required. Furthermore, a suitable post-processing technique is also needed on the large amount of data generated from the FE analysis to identify the underlying relationship connecting the predictions to AM process parameters. Thus, fully exploring the process parameter space would require an interplay between the large number of FE simulations and post-processing techniques. Here, we aim to provide a solution for post-processing of such a large parameter space for AM using a statistical technique.

There are seven distinct techniques for AM as defined by the International Organization for Standards [9]. As noted by Wang et al., there are three primary categories commonly used to investigate the effects of process parameters on mechanical properties [10]. These include powder bed fusion (PBF), directed energy deposition, and material extrusion. PBF methods consist of a rising and lowering platform that contains powder, and a laser that is focused to melt a thin layer of powder in accordance with the design [9,11]. Then the platform lowers with new material being rolled over the build area, and the process repeats. Directed energy deposition uses a focused laser to melt a powder stream or a wire, with the material being placed onto the surface as it is melted [9,12]. Material extrusion uses a nozzle to place the liquified material onto the platform or another layer of the design [9,13]. Each of these broad methods has more specific techniques within them; however, that is beyond the scope of this work. Instead, the focus is on the PBF method and on characterizing the amount of stress and deformation generated from the manufacturing process as a consequence of the process parameters.

ML is often used to assist in predicting residual stress and deformation, both experimentally and in simulations. However, many techniques are not focused on the interpretability of the machine learning process. Zhou et al. use random forests to identify optimal configurations of laser shock peening parameters to achieve desired residual stresses for enhanced surface properties [14]. Gu et al. considered the optimized composite design using ML [15,16]. Multiple designs were assembled into an 8×8 (or larger) grid using three different unit cells with variable anisotropic properties, and their mechanical performance was evaluated using various ML algorithms. Note that they used FE to generate their training dataset for ML. Their models were able to start from mostly random configurations and hone in on an optimized design.

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Rong-Li et al. utilize a genetic algorithm along with a small-capacity neural network to find the optimal process parameters that minimize the shrinkage associated with selective laser sintering [17]. Kappes et al. used 3600 physically printed samples of Inconel 718 to characterize the process parameters, primarily to investigate pore formation [18]. Parand et al. consider a database of multiple materials and multiple manufacturing techniques to explore the performance of different ML algorithms on predicting mechanical properties [19]. They found that ensemble methods tend to outperform the other methods considered, but they did not consider the methods proposed here.

We propose using data generated from FE analysis of the PBF AM technique of Inconel-625. ABAQUS FEA (Dassault Systèmes Inc., USA), a FE software [20], was used to simulate the AM process on a fixed geometry, corresponding with the experimental work of Suresh et al. [21,22]. We utilize a variety of finite mixture models to characterize the effects of process parameters on outcomes, as measured by von Mises stress and total deformation predictions. The considered models include a naive baseline and two cluster-based techniques: finite mixture models (FMM) and finite mixture of regression models (MoRM). The naive model is a multiple regression model that gives regression coefficients without the clustering considerations. The FMM and the MoRM are used for their clustering and for providing regression coefficients. FMM groups points into clusters and fits a multiple regression model within each cluster. The MoRM simultaneously forms clusters and estimates the regression coefficients. Finally, the regression coefficients are interpreted in the context of the clustering solution, with a proposed mechanistic basis for their prediction, as visualized in the clustering solution.

Materials And Methods

This section describes the data generation process for the FE simulations, along with the details of the statistical methods FMM and MoRM. We first present the data generation and geometry discretization for the FE model followed by both statistical methodologies utilized including the parameter estimation method (i.e., the expectation maximization (EM) algorithm). Finally, both the statistical method and FE analysis use discretization, either for clustering (statistical) or for geometry (FE). Thus, for the purpose of clarity, the term node(s) will be used for FE, and the term data point(s) will be used for the statistical methodology or models. Similarly, the term process parameter(s) is used to indicate manufacturing-related parameters to make a distinction from the statistical use of the term parameter.

FE-based dataset generation

In the FE analysis, the continuum geometry problem is reduced to finding problem-dependent solution values at a finite number of nodal locations. Thermomechanical considerations must be accounted for under the AM framework. For thermomechanical analysis, the primary quantities of interest include displacement (mechanical analysis), temperature (thermal analysis), and derived quantities such as stress and strain tensors. The stress (or strain) tensor is a second order tensor represented in a 3×3 symmetric matrix. The stress tensor provides a full representation of internal stresses due to resulting deformation and temperature distribution for a given material response and geometry. Equation (1) gives the stress tensor, where the diagonal terms represent three axial stress directions and off-diagonal terms represent the shear stresses.

$$\sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix}$$

The scalar quantity von Mises stress is derived from the stress tensor as given by Equation (2) and is used as a yield criterion for elastoplastic materials such as the metallic alloy used here.

$$\sigma_v = \sqrt{\frac{1}{2} [(\sigma_{11} - \sigma_{22})^2 + (\sigma_{11} - \sigma_{33})^2 + (\sigma_{22} - \sigma_{33})^2] + 3(\sigma_{12}^2 + \sigma_{13}^2 + \sigma_{23}^2)}$$

The total displacement and the Von Mises stress are used for the statistical analysis of the simulation outcome.

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The material chosen for all simulations was a powderized Inconel-625 with temperature-dependent elastoplastic material properties taken from literature [23-25]. We used properties extracted for temperature varying from room temperature of 23°C to 1000°C. The properties that were extracted for simulation from these stress-strain plots are shown in Figure 1 and Table 1. The geometry can be seen in Figure 2, showing a single-track rectangular box with rounded corners, with its meshed model and laser path for deposition visible.

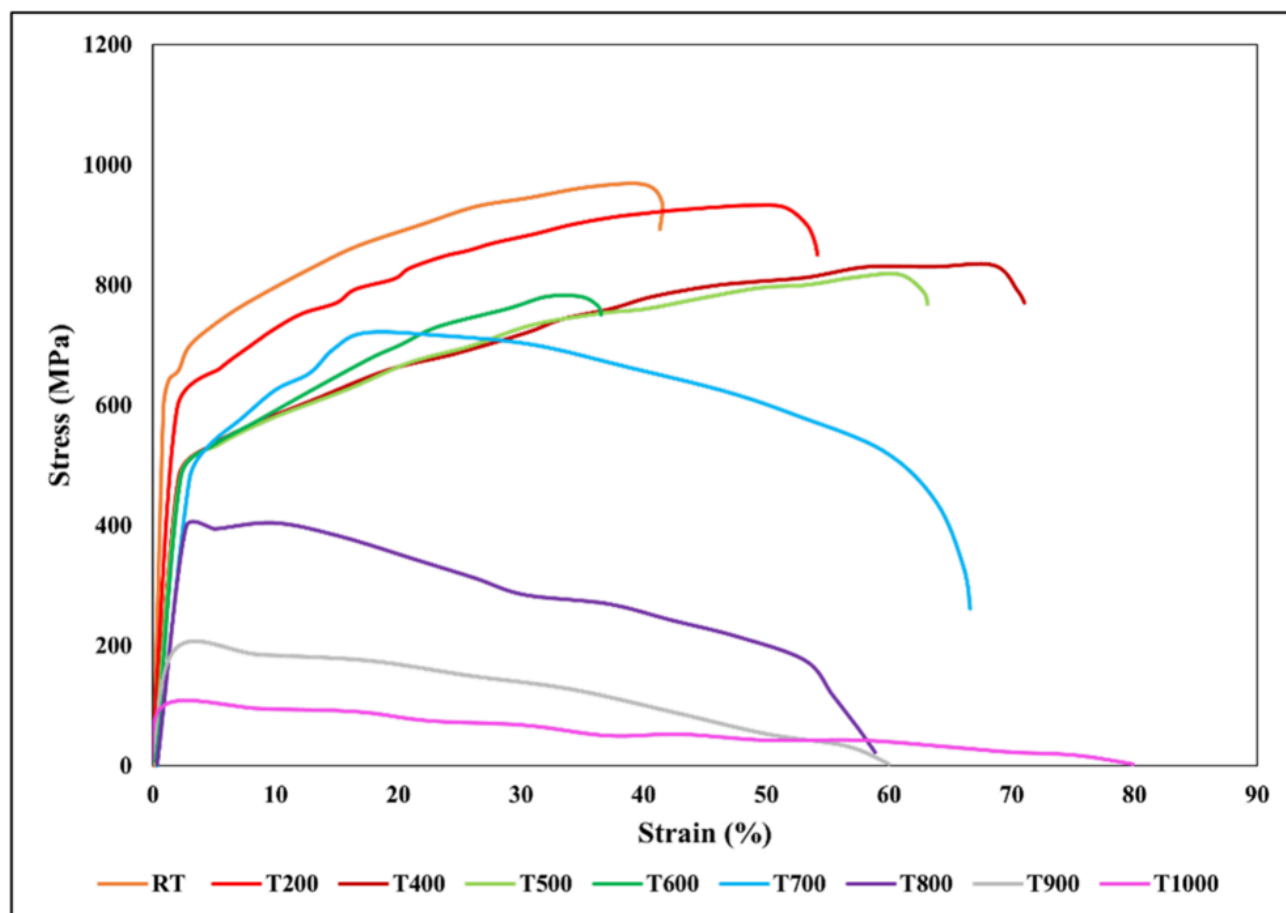


FIGURE 1: Temperature-dependent stress-strain profile for Inconel-625 ranging from room temperature, denoted RT, at 23°C through 1000°C

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T(°C)	E(GPa)	σ_y (MPa)	ϵ_p	T(°C)	$K(\frac{mW}{mm/^{\circ}C})$	C_p ($\frac{mJ}{Tonne./^{\circ}C}$)	α ($\frac{1}{^{\circ}C}$)
23	207.41	971	0.397	21	9.8	4.10×10^8	-
200	198.12	940	0.527	38	10.1	-	-
400	187.01	845	0.668	93	10.8	4.27×10^8	1.28×10^{-5}
500	180.96	829	0.607	204	12.5	4.56×10^8	1.31×10^{-5}
600	173.96	807	0.337	316	14.1	4.81×10^8	1.33×10^{-5}
700	165.84	722	0.177	427	15.7	5.11×10^8	1.37×10^{-5}
800	155.88	403	0.097	538	17.5	5.36×10^8	1.40×10^{-5}
900	144.08	199	0.099	649	19	5.65×10^8	1.48×10^{-5}
1000	132.28	104	0.019	760	20.8	5.90×10^8	1.53×10^{-5}
				871	22.8	6.20×10^8	1.58×10^{-5}
				982	25.2	6.45×10^8	1.62×10^{-5}

TABLE 1: Key material process parameters extracted for simulation corresponding to Figure 1

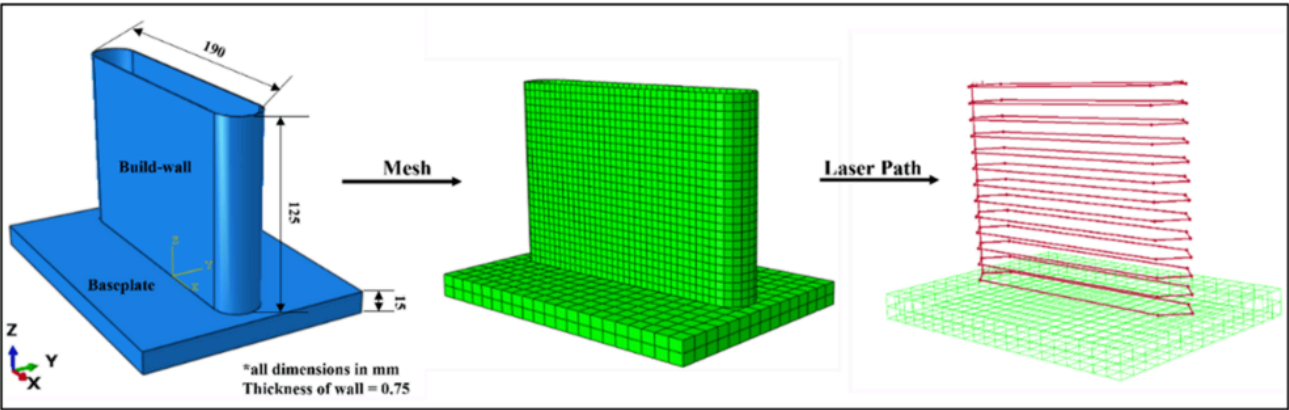


FIGURE 2: Single track geometry features, meshed model, and laser path used for the FEA framework. The node at the intersections of the mesh geometry are the points where the simulation outcomes were extracted

FEA, Finite Element Analysis

The model was based on a physical geometry reported in earlier work [21,22], which was generated by the directed energy deposition method using a single track with a laser of spot size of 1.1 mm. In other work, finer wall thicknesses of 0.2 mm to 0.7 mm have been achieved in laser-based methods (DED or laser-powder-bed fusion) [26]. Such fine dimensions are needed for applications such as heat exchangers. Hence, the chosen model geometry dimensions are physically relevant. For each layer, the laser makes one pass along the perimeter and ends when the laser returns to the starting point, with the build direction being the Z-axis. Correspondingly, for the FE discretization of the wall, a single line of 3D brick elements was used for each layer, as shown. The process is repeated until the total height of 125 mm is achieved to build the full geometry.

The base plate was fixed, and the substrate plate was tied together for thermal conduction between the two. The model was meshed using 8-node linear DC3D8 elements for thermal analysis and full integrated solid C3D8 for structural analysis using the same mesh topology. The outcomes for the nodes of each element, the stress tensor, and the displacement in the three Cartesian directions, were extracted at increments of 5 mm, resulting in 26 layers of outcomes. Each layer consists of 164 nodes, resulting in a total of 4264 nodes per simulation. Thus, considering the 192 process parameter configurations, there are a total of 818,688 nodal outcomes.

Each simulation was a unique combination of four process parameters, which are laser power (LP), laser scan speed (SS), layer height (LH), and different cooling assumptions (Cases). LP, measured in W, determines the intensity of the heat source, with larger values generating more heat. SS, measured in mm/s, has the effect of determining how long the heat source affects a portion of the powder. LH, measured in mm, determines how much material is rolled between each iteration of laser sintering. Note that it takes approximately 10 seconds to roll material over the powder bed between subsequent depositions. Cases consider cooling assumptions which include fast deposition with inadequate cooling with no cooling period (Case 1), a cooling period of 50 seconds (Case 2), Case 2 with convection heat losses (Case 3), and Case 3 with additional radiation heat losses (Case 4). The process parameters values were chosen to cover the space of feasible values, with values chosen summarized in Table 2. As stated earlier, the choice of model and process parameters was guided primarily by our earlier experimental work for PBF [21,22], which are within the literature range, but higher and lower than these values have also been used across different alloy types [26-28].

Laser Power (W)	Laser Scan Speed (mm/s)	Layer Height (mm)	Cooling Assumption
250	300	1	Case 1
500	600	3	Case 2
750	900	5	Case 3
1000	1200		Case 4

TABLE 2: Range of values for each process parameter used for simulation. Each unique combination was simulated to construct the dataset of 192 simulations

Data reduction

Iterative algorithms, such as the EM algorithm employed in this paper, struggle to incorporate all of these nodes in a computationally efficient manner. Thus, a method to incorporate the large-scale structural properties while reducing the computational burden is proposed. In short, the method averages the outcomes of nearby nodes within a simulation, which should behave similarly. As mentioned, each layer has 164 nodes, 82 of which belong to the inner portion of the

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layer, each with a corresponding pair on the outer surface. Since the wall thickness is extremely thin, we assume that the outcomes are similar and these pairs are averaged together, reducing the initial dataset size by half. The next step to further reduce the number of observations is to combine points that are nearby each other along the surface, which we call pixels. Each pixel results in one new averaged node that is made by averaging each of the selected nodes along each of the measured values. These pixels were created by considering a lateral slice (the same way a layer is created) of the geometry, and moving along the perimeter by picking a starting node according to any constant rule. We chose to use the point with the most negative y-coordinate and then the most negative x-coordinate. This is repeated at each layer and for a user-defined number of layers, at which point these nodes are grouped to form the respective pixels.

Three levels of pixelization were initially considered for analysis, which are denoted as coarse, moderate, and fine schemes. The coarse scheme is the most aggressive, with the most nodes per pixel, reducing the entire dataset down to 4608 data points. The moderate scheme is modest with its averaging, reducing the dataset down to 18816 data points. The fine scheme reduces the dataset down to 64896 data points. However, our analysis showed very limited differences in the results of the 25-fold cross-validation used to estimate out-of-sample error for the statistical methods across the different averaging methods. See the supplemental material for further details. A visualization of the moderate averaging scheme is shown in Figure 3. There are some obvious limitations to this approach. For example, nodes on the border between two pixels are likely to be more similar to each other than nodes across the pixel. However, this approach still captures the larger-scale geometric features and allows for cheaper implementation of statistical models. The modest scheme is shown in Figure 3, where adjacent nodes of the same color are in the same pixel.

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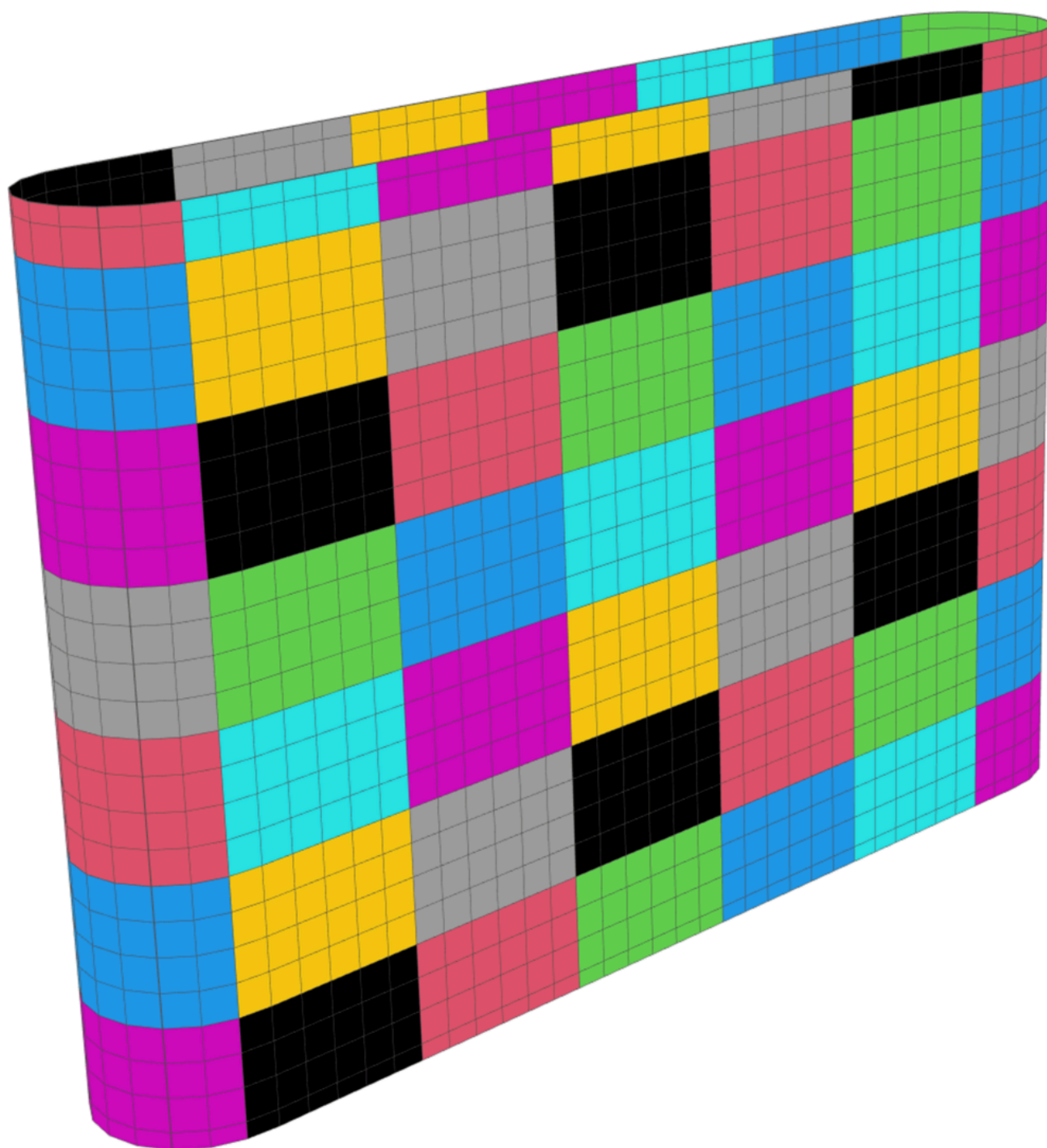


FIGURE 3: The considered geometry with only enlarged nodes. Nodes with the same adjacent coloring correspond to the nodes that were combined to create the reduced dataset

Models and estimation

Under the finite mixture framework, we assume that there is a collection of multivariate random variables, i.e., random vectors, $\mathbf{Y}_1, \dots, \mathbf{Y}_n$ distributed as a sum of weighted distributions. For example, the probability density function for $\mathbf{Y}_i$ is assumed to have the form $\sum_{k=1}^K \tau_k \phi(\mathbf{y}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ where $0 \leq \tau_k \leq 1$ is the k th mixing proportion and $\sum_{k=1}^K \tau_k = 1$, ϕ

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is the multivariate Gaussian density function, $\boldsymbol{\mu}_k$ is the k th mean parameter, and $\boldsymbol{\Sigma}_k$ is the k th variance parameter. This gives a K component multivariate Gaussian mixture model. In general, the probability density function does not need to be in the same category of distributions, but that is the typical use.

In the context of the problem, we are assuming that $g(\mathbf{Y}_1), \dots, g(\mathbf{Y}_n)$ are independent and identically distributed with density function given by $\sum_{k=1}^K \tau_k \phi(\mathbf{y}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ where $\mathbf{Y}_i$ is the i th random vector associated with the von Mises stress and the three spatial displacement components, and g is some monotone function or transformation. The Box-Cox transformation is utilized to determine the appropriate transformation [29]. Indirectly, distributional assumptions are being made about the random vector associated with the stress tensor through the von Mises stress, but those are not of interest explicitly. Under these assumptions, for a fixed K , we would like to obtain the maximum likelihood estimates. However, examining the form of the log-likelihood shows that it is difficult to directly maximize to obtain the parameter estimates in closed form. The log-likelihood is

$$\ell(\Psi) = \sum_{i=1}^n \log \left(\sum_{k=1}^K \tau_k \phi(\mathbf{y}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right)$$

where $\Psi = \{\tau_1, \dots, \tau_{K-1}, \boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_1, \dots, \boldsymbol{\Sigma}_K\}$.

To rectify the problem, we assume that there is a latent variable $Z_i \sim \text{categorical}(K, \tau_1, \dots, \tau_K)$ that determines class membership. That is, assume each realization originates from one of the components within the K term summation, and Z_i specifies which component the i th observation is being sampled from. The complete data is then constructed with the pairs of realizations of the random vector $\mathbf{y}_1, \dots, \mathbf{y}_n$ and the latent variables to get $(\mathbf{y}_i, Z_i)$ pairs. The latent class membership is the only term that is considered random here. Hence, the complete-data likelihood is constructed and maximized, and for the Gaussian mixture, closed-form parameter estimates can be obtained using the complete-data likelihood. It has been shown that maximizing the complete-data likelihood results in the maximum likelihood estimate of the original likelihood given proper initialization [30-32]. Note that the complete-data log-likelihood is written as:

$$\ell_c(\Psi) = \sum_{i=1}^n \sum_{k=1}^K I(Z_i = k) [\log(\tau_k) + \log(\phi(\mathbf{y}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k))]$$

where $I(\cdot)$ is the indicator function. Then, the EM algorithm is used to estimate the parameters [33].

The EM algorithm is an iterative approach that alternates between the expectation step (E-step) and the maximization step (M-step). Further, the EM algorithm has been shown to be effective as a way to account for missing data [33]. Recall that we are assuming that the class membership to the clustering solution is unknown or missing information. The E-step takes the conditional expectation of the complete-data log-likelihood given the previous iteration's parameter estimates are known. The estimation of the probability of class membership for the i th observation belonging to the k th cluster is denoted by π_{ik} . If we let s be the iteration number within the EM algorithm, the E-step assumes that the estimates for parameters at iteration $s - 1$ are known. The estimation of π_{ik} has closed form:

$$\pi_{ik}^{(s)} = \frac{\tau_k^{(s-1)} \phi(\mathbf{y}_i; \boldsymbol{\mu}_k^{(s-1)}, \boldsymbol{\Sigma}_k^{(s-1)})}{\sum_{m=1}^K \tau_m^{(s-1)} \phi(\mathbf{y}_i; \boldsymbol{\mu}_m^{(s-1)}, \boldsymbol{\Sigma}_m^{(s-1)})}$$

Note that the expectation of the log-likelihood given the previous parameter estimates is given as:

$$Q(\Psi | \Psi^{(s-1)}) = \sum_{i=1}^n \sum_{k=1}^K \pi_{ik}^{(s)} \left[\log(\tau_k^{(s-1)}) + \log(\phi(\mathbf{y}_i; \boldsymbol{\mu}_k^{(s-1)}, \boldsymbol{\Sigma}_k^{(s-1)})) \right]$$

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Then the M-step maximizes $Q(\Psi|\Psi^{(s-1)})$ directly with respect to each of the parameters in Ψ . Notice that when estimating τ_k , there is the additional restriction of $\sum_{k=1}^K \tau_k = 1$ for which a Lagrange multiplier is used. Then the estimation for the M-step of the sth iteration is given as

$$\tau_k^{(s)} = \frac{1}{n} \sum_{i=1}^n \pi_{ik}^{(s)},$$

$$\mu_k^{(s)} = \frac{\sum_{i=1}^n \pi_{ik}^{(s)} y_i}{\sum_{i=1}^n \pi_{ik}^{(s)}},$$

and

$$\Sigma_k^{(s)} = \frac{\sum_{i=1}^n \pi_{ik}^{(s)} (y_i - \mu_k^{(s)}) (y_i - \mu_k^{(s)})'}{\sum_{i=1}^n \pi_{ik}^{(s)}}$$

The EM algorithm iterates between the E-step and M-step until a predefined convergence criterion is met. Typically, the relative change in consecutive log-likelihood values is used as a convergence criterion given as $|\ell(\Psi^{(s)}) - \ell(\Psi^{(s-1)})| / |\ell(\Psi^{(s-1)})| < \epsilon$ where ϵ is a prespecified tolerance level.

Under the assumptions of the finite mixtures of (Gaussian additive error) regression models, we assume that there are several latent regression structures to explain the response y by the covariates X . For the current framework, y_i are realizations of the von Mises stress or the total deformation. Hence, the distributions we are considering are now univariate normal

$$\pi_{ik}^{(s)} = \frac{\tau_k^{(s-1)} \phi(y_i; \mathbf{X}_i' \boldsymbol{\beta}_k^{(s-1)}, \sigma_k^{2,(s-1)})}{\sum_{m=1}^K \tau_m^{(s-1)} \phi(y_i; \mathbf{X}_i' \boldsymbol{\beta}_m^{(s-1)}, \sigma_m^{2,(s-1)})}$$

The corresponding Q function that will be maximized in the M-step is as follows:

$$Q(\Psi|\Psi^{(s-1)}) = \sum_{i=1}^n \sum_{k=1}^K \pi_{ik}^{(s)} \left[\log(\tau_k^{(s-1)}) + \log(\phi(y_i; \mathbf{X}_i' \boldsymbol{\beta}_k^{(s-1)}, \sigma_k^{2,(s-1)})) \right]$$

The estimate for the k th mixing proportion at iteration s , $\tau_k^{(s)}$, remains unchanged from Equation (7). With the regression structure, the estimate for the mean at the i th observation and k th component is being estimated as $\mathbf{X}_i' \boldsymbol{\beta}_k$. The estimate for the k th component's regression coefficients at iteration s , $\boldsymbol{\beta}_k^{(s)}$, are found as:

$$\boldsymbol{\beta}_k^{(s)} = \left(\sum_{i=1}^n \pi_{ik}^{(s)} \mathbf{X}_i \mathbf{X}_i' \right)^{-1} \sum_{i=1}^n \pi_{ik}^{(s)} \mathbf{X}_i y_i$$

Lastly, the estimate for the variance is found as

$$\sigma_k^{2,(s)} = \frac{\sum_{i=1}^n \pi_{ik}^{(s)} (y_i - \mathbf{X}_i' \boldsymbol{\beta}_k^{(s)})^2}{\sum_{i=1}^n \pi_{ik}^{(s)}}$$

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For FMM, we start by determining which nodes behave similarly within and across simulations. To do this, we consider the von Mises stress and the three axes of spatial deformation. Using these variables, we need to estimate the number of clusters that are present. Here, we use the Bayesian information criterion (BIC) [34] to estimate the appropriate number of clusters, where we considered 2 to 11 clusters as feasible solutions. The R package `mclust` is used for parameter estimation [35]. The upper limit of 11 was chosen to correspond with intuition and some preliminary results from another approach not discussed in this work. Further, we did not want the number of clusters to be too large. Using the maximum a posteriori estimate as a hard classifier, each observation is assigned to the corresponding cluster.

After the best model was determined, a regression model was fit using 3 of the process parameters within each of the clusters. The cooling assumptions were removed as a covariate to reduce the number of parameters and due to errors in prediction during cross-validation. It was possible to form clusters that did not include all cases, but the validation set would attempt to put a new case into that cluster. That case had no coefficient associated with it, resulting in invalid predictions. Removing the cooling assumptions also had the effect of reducing the overall number of parameters by half.

Additionally, the Box-Cox transformation was performed within each cluster to see if it was appropriate to transform for g is [29,36]. The Box-Cox transformation considers the log-transform as well as the various powers of the response to see which best meets the assumption of the regression model. Each cluster had a different optimal transformation. However, a majority of the clusters found it was reasonable to use a log transformation. Hence, a log transformation is used for all clusters.

As a starting point for MoRM, the number of clusters determined from FMM is used. MoRM allows for clusters with small class membership to be removed automatically, thus reducing the number of clusters. For this work, the library `flexmix` in R was used [37]. The case variable is reintroduced as the possibility for invalid regression coefficients does not exist for MoRM. Continuing with the results from FMM, the log transform on the response was considered again to allow for reasonable comparisons between methods. Note that this approach is different from FMM since each cluster influences the estimation of the predicted value. Additionally, the clusters are formed simultaneously with the regression coefficients.

Results And Discussion

In this section, we perform data analysis based on the moderate averaging scheme and investigate the visualization of FE simulations. Both FMM and MoRM were fitted to the data using the von Mises stress and deformation as response variables, separately. This resulted in four different models' estimates, which will be presented below. Additionally, as a baseline comparison, a naive approach is considered that does not take any information from clustering solutions and fits a multiple regression model on the entire reduced dataset. There are two topics of interest. First, 25-fold cross-validation is considered to ensure that the model considered performs well out of sample. In this case, the same set of training and testing folds were used on each of the models, as well as the same regression model structure, which only includes LP, SS, and LH. Random nodes across all simulations are considered for the 25-fold train/test splits. That is, randomly selected node(s) from each of the simulations are held out rather than an entire simulation being withheld for one of the splits. For each fold, the computation time required $\mathcal{T}$, the number of parameters $|\theta|$ estimated, the total variability explained by the covariates R^2 , and the predicted residuals sum of squares (PRESS) statistics are computed.

For this analysis, a 12th Gen Intel(R) Core i9-12900H with 64 GB of RAM was utilized. Computation time was measured using the difference in time through the R function "`Sys.time()`" at the start and end of all tasks for each respective model. This was nested within the R libraries `parallel` and `foreach` to allow for parallel computation [38,39]. Each branch of the parallel computation evaluated each of the three models considered to reduce the bias of different performance on different cores. From the 25-fold cross-validation, the average and standard deviation of each of the statistics are reported in Tables 3 and 6. These will serve as metrics of model performance. Once cross-validation is complete, both the FMM and MoRM models are fitted to the entire dataset, and the estimated coefficients are given in Tables 4, 5, 7, and 8. For MoRM, the Cases variable is reintroduced to the regression formula, while FMM only includes LP, SS, and LH. As can be

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expected, the MoRM model was found to be the most flexible, outperforming both the FMM and the Naive models in all model performance metrics except computation time. Therefore, we further discuss the interpretation of the clustering solutions based on the MoRM for both the von Mises stress and deformation.

FE simulations

The FE results for von Mises stress for 16 of these simulations at various LP and SS settings with fixed LH and Case 1 is shown in Figure 4. The color gradient shows lower stress in blue colors and higher stress in red. It can be seen that stress tends to accumulate near the middle of the unsupported region of the geometry with high LP and slower SS. Intuitively, one would expect increasing the LP and reducing SS to result in increased von Mises stress, which aligns with the visualization.

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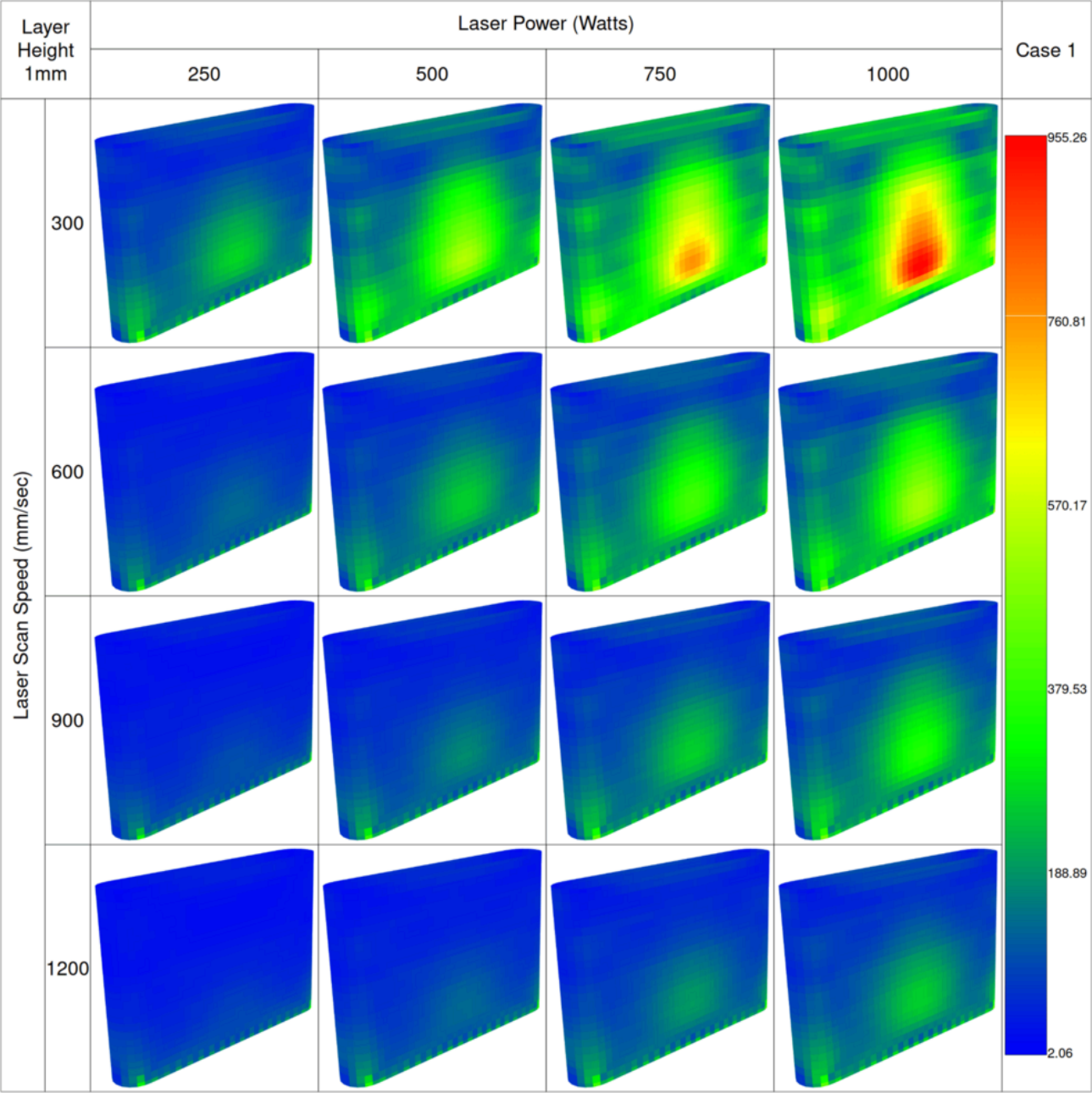


FIGURE 4: Resultant FE simulations visualizing the intensity of von Mises stress by varying LP and SS while keeping the LH and Case fixed at 1 mm and Case 1

FE, Finite Element; LP, laser power; SS, laser scan speed; LH, layer height

von Mises stress analysis

First, we consider the 25-fold cross-validation for model assessment. For the cross-validation, all models will not include the Cases variable since FMM can create invalid estimates for prediction to ensure fair model comparison. The naive model performed poorly within training and for testing data, with out-of-sample PRESS statistics of 1064.48 and R^2 of 0.22 on average. FMM showed model improvements with an average PRESS statistic of 258.30 and R^2 of 0.812. MoRM showed considerable improvements with an average PRESS statistic of 28.62 and R^2 of 0.979. This shows that considering both clustering and regression simultaneously can achieve considerable model prediction improvements.

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The computation time for FMM and MoRM is comparable at 27.9 seconds and 29.4 seconds, while the time for the naive approach is negligible. MoRM does have an advantage in that it utilizes the number of components from FMM as its starting points and then has the ability to remove underutilized clusters. These broad results are summarized in Table 3.

	Naive	FMM	MoRM
PRESS	1064.48 (45.44)	258.30 (33.52)	28.62 (4.66)
R^2	0.22 (0.001)	0.812 (0.02)	0.979 (0.003)
$ \theta $	4.0 (0)	43.6 (1.10)	56.36 (4.61)
$\mathcal{T}$	0.01 (0.002)	27.86 (7.11)	29.434 (3.17)

TABLE 3: Average values and standard deviations (in parentheses) of the various performance metric for each model when studying von Mises stress

PRESS, predicted residuals sum of squares; FMM, finite mixture models; MoRM, mixture of regression models

The models were then fitted on the full dataset. For MoRM, we can reintroduce the Cases variable. That is, we are interested in the following formula for FMM:

$$\log(\text{von Mises}_i) = \beta_{0,k} + \beta_{1,k}\text{LP}_i + \beta_{2,k}\text{SS}_i + \beta_{3,k}\text{LH}_i$$

where β_k denotes the coefficients associated with the k th cluster and for MoRM the formula is

$$\log(\text{von Mises}_i) = \sum_{k=1}^K \pi_{ik} \left[\sum_{j=0}^3 \beta_{j,k} I(\text{Case}_i = j) + \beta_{4,k}\text{LP}_i + \beta_{5,k}\text{SS}_i + \beta_{6,k}\text{LH}_i \right]$$

Using BIC, the optimal number of clusters for the FMM was found to be 11. The regression model fits, and the corresponding estimated coefficients are presented in Table 4. Consider nodes that belong to Cluster 1 and refer to Table 4, row 1. Holding the other process parameters constant, increasing LP by 1 W corresponds to an expected increase in the log von Mises stress by 0.001, and increasing SS by 1 mm/s corresponds to a decrease in the log von Mises stress by 0.0019. Likewise, increasing LH by 1 mm corresponds to an expected decrease in log von Mises by 0.6.

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Cluster (k)	$\hat{\beta}_{1,k}$	$\hat{\beta}_{2,k}$	$\hat{\beta}_{3,k}$	$\hat{\beta}_{0,k}$
1	0.001	-0.0019	-0.6003	5.9011
	(2e-04)	(3e-04)	(1e-01)	(2e-01)
2	-0.0004	0.0013	0.3344	5.2911
	(2e-04)	(3e-04)	(1e-01)	(2e-01)
3	-0.0004	0.0014	0.2447	5.2746
	(2e-04)	(3e-04)	(1e-01)	(2e-01)
4	-0.0007	0.0016	0.5148	4.9355
	(2e-04)	(3e-04)	(1e-01)	(2e-01)
5	-0.0008	0.0018	0.5565	4.5938
	(2e-04)	(3e-04)	(1e-01)	(2e-01)
6	-0.0007	0.0016	0.4899	4.5699
	(2e-04)	(3e-04)	(1e-01)	(2e-01)
7	-0.0001	0.0012	0.39	3.5192
	(2e-04)	(3e-04)	(1e-01)	(2e-01)
8	-0.0002	0.0013	0.3671	3.952
	(2e-04)	(3e-04)	(1e-01)	(2e-01)
9	-0.0002	0.0013	0.3812	3.9085
	(2e-04)	(3e-04)	(1e-01)	(2e-01)
10	-0.0005	0.0016	0.4722	2.8361
	(2e-04)	(3e-04)	(1e-01)	(2e-01)
11	0.0002	0.001	0.4145	1.8052
	(2e-04)	(3e-04)	(1e-01)	(2e-01)

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TABLE 4: Coefficients for FMM using the von Mises stress as the response. Each row corresponds to a cluster

FMM, finite mixture models

For example, consider a node in Cluster 1 where the corresponding process parameters are 250 W, 300 mm/s, 1 mm, with any cooling assumptions. Using FMM, the expected von Mises stress for those nodes with these process parameters would be 145.12 MPa. If we were to increase just LP to 500 W instead of 250 W, the expected von Mises stress is now 184.25 MPa. The interpretation is similar for the remaining clusters using FMM.

The emEM initialization scheme is used, which considers 500 short EM-algorithm runs with a loose convergence criterion for initial cluster values ranging from two clusters up to eleven, i.e., the number of clusters from FMM [40]. The model with the smallest BIC from each batch of 500 short runs is restarted until a stricter convergence criterion is met. The final model is then chosen from these ten candidate models that converged with the strict convergence criterion based on BIC. The final model had eight components, originally containing eleven. The results from the MoRM are presented in Table 5. For example, consider nodes that have their largest posterior probability belonging to Cluster 5 according to MoRM and refer to Table 5, row 5. Increasing LP by 1 W and holding the other process parameters constant will lead to an increase in the log von Mises Stress by 0.0005 (0.05% increase in von Mises stress). Similarly, increasing LH by 1 mm corresponds to a decrease in log von Mises stress by 0.1287 on average (a 12.9% decrease in log von Mises). The cooling conditions (Case 1-4) have a different interpretation as factor variables. For Cluster 5, if the node considered has corresponding process parameters belonging to Case 1, there would be an intercept term of 5.21. But if the node instead belonged to Case 3, the intercept term would be 3.45 instead. For this cluster, the lowest von Mises stress is associated with Case 3, meaning that including the conductive heat losses drastically reduces the amount of stress experienced for nodes predominantly in this cluster.

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Cluster	$\hat{\beta}_{4,k}$	$\hat{\beta}_{5,k}$	$\hat{\beta}_{6,k}$	$\hat{\beta}_{0,k}$	$\hat{\beta}_{1,k}$	$\hat{\beta}_{2,k}$	$\hat{\beta}_{3,k}$
1	0.0015	-0.001	-0.312	2.8643	4.9835	1.6467	4.1859
	(1.00e-05)	(9.10e-06)	(2.10e-03)	(1.50e-02)	(1.30e-02)	(1.30e-02)	(1.30e-02)
2	0.0007	-0.0005	-0.1697	4.4774	4.7648	2.3823	3.8972
	(2.30e-06)	(1.90e-06)	(3.90e-04)	(2.70e-03)	(2.70e-03)	(2.80e-03)	(2.70e-03)
3	0.0008	-0.0006	-0.4797	5.769	5.3315	3.4792	4.9917
	(2.80e-06)	(2.30e-06)	(4.60e-04)	(3.00e-03)	(3.10e-03)	(3.10e-03)	(3.30e-03)
4	0.0002	-0.0002	-0.0504	4.7147	5.1103	4.2331	4.7543
	(4.50e-06)	(3.60e-06)	(7.60e-04)	(5.30e-03)	(5.20e-03)	(5.10e-03)	(5.20e-03)
5	0.0005	-0.0005	-0.1287	5.2108	5.2198	3.4495	4.4944
	(3.70e-06)	(3.00e-06)	(6.40e-04)	(4.20e-03)	(4.30e-03)	(4.40e-03)	(4.30e-03)
6	0.001	-0.0011	-0.3506	4.5621	5.194	2.5207	3.917
	(8.30e-06)	(7.20e-06)	(1.50e-03)	(9.70e-03)	(9.70e-03)	(9.80e-03)	(9.70e-03)
7	0.0012	-0.0015	-0.2358	5.3116	5.4569	2.7555	3.7996
	(1.00e-05)	(8.20e-06)	(1.70e-03)	(1.10e-02)	(1.20e-02)	(1.20e-02)	(1.20e-02)
8	0.0022	-0.0016	-0.2692	3.5763	4.6138	1.9434	3.2618
	(6.60e-06)	(5.70e-06)	(1.20e-03)	(8.10e-03)	(7.90e-03)	(7.40e-03)	(7.50e-03)

TABLE 5: Coefficients for MoRM using the von Mises stress as the response. Each row corresponds to a cluster but each observation potentially has some weight in each cluster

MoRM, mixture of regression models

Deformation analysis

Similarly to von Mises stress, we considered a 25-fold cross-validation for model assessment using deformation as a response. Again, not all models will include the Cases variable since FMM can create invalid estimates for prediction to ensure fair model comparison. The results of model performance were similar. The naive model performed very poorly, with significant improvements seen from FMM and even more from MoRM. The full results of model performance metrics are shown in Table 6. Again, model performance can be improved considerably by allowing for more flexibility using the mixture model framework. The computation time for FMM is now only 10 seconds compared to the 36 seconds required by MoRM.

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	Naive	FMM	MoRM
PRESS	1376.59 (60.58)	450.38 (66.86)	86.11 (12.31)
R^2	0.085 (0.001)	0.705 (0.035)	0.943 (0.008)
$ \theta $	4.0 (0.000)	44 (0.0)	64.52 (1.66)
$\mathcal{T}$	0.01 (0.002)	10.029 (2.13)	35.85 (2.40)

TABLE 6: Average values and standard deviations (in parentheses) of the various performance metric for each model when studying deformation

PRESS, predicted residuals sum of squares; FMM, finite mixture models; MoRM, mixture of regression models

Again, the models were then fitted on the full dataset, and for MoRM, we reintroduced the Cases variable. In the case of FMM, the following formula is of interest

$$\log(\text{Total Def.}_i) = \beta_{0,k} + \beta_{1,k}\text{LP}_i + \beta_{2,k}\text{SS}_i + \beta_{3,k}\text{LH}_i$$

where β_k denotes the coefficients associated with the k th cluster and the formula associated with MoRM is

$$\log(\text{Total Def.}_i) = \sum_{k=1}^K \pi_{ik} \left[\sum_{j=0}^3 \beta_{j,k} I(\text{Case}_i = j) + \beta_{4,k}\text{LP}_i + \beta_{5,k}\text{SS}_i + \beta_{6,k}\text{LH}_i \right]$$

Using the entire dataset, we determined that 11 clusters are optimal for FMM using BIC. Consider nodes that belong to Cluster 1 and refer to Table 7. Holding the other process parameters constant, increasing LP by 1 W results in an expected increase in the log of total deformation by 0.0006. Similarly, increasing SS by 1 mm/s corresponds to an expected decrease in the log of total deformation by 0.0021. Increasing LH by 1 mm corresponds to an expected decrease in the log total deformation by 0.515. Interpretations of each regression model within each cluster can be done using these coefficients with respect to the total deformation.

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Cluster (k)	$\hat{\beta}_{1,k}$	$\hat{\beta}_{2,k}$	$\hat{\beta}_{3,k}$	$\hat{\beta}_{0,k}$
1	0.0006	-0.0021	-0.5147	1.6939
	(2e-04)	(4e-04)	(1e-01)	(3e-01)
2	-0.0008	0.0024	0.5361	0.2451
	(3e-04)	(4e-04)	(1e-01)	(3e-01)
3	-0.0005	0.0021	0.3065	0.9941
	(3e-04)	(4e-04)	(1e-01)	(3e-01)
4	-0.0004	0.002	0.4033	-2.5991
	(3e-04)	(4e-04)	(1e-01)	(3e-01)
5	-0.0003	0.0018	0.3562	-0.9676
	(3e-04)	(4e-04)	(1e-01)	(3e-01)
6	-0.0006	0.0021	0.4488	0.0113
	(3e-04)	(4e-04)	(1e-01)	(3e-01)
7	-0.0001	0.0016	0.3319	-2.7125
	(3e-04)	(4e-04)	(1e-01)	(3e-01)
8	-0.0002	0.0018	0.317	0.0066
	(3e-04)	(4e-04)	(1e-01)	(3e-01)
9	-0.0002	0.0018	0.3091	-0.0099
	(3e-04)	(4e-04)	(1e-01)	(3e-01)
10	-0.0005	0.0021	0.4818	-0.7319
	(3e-04)	(4e-04)	(1e-01)	(3e-01)
11	-0.0006	0.0021	0.4802	-1.2373
	(3e-04)	(4e-04)	(1e-01)	(3e-01)

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TABLE 7: Coefficients for FMM using the total deformation as the response. Each row corresponds to a cluster

FMM, finite mixture models

For MoRM, we use the same setup with the emEM algorithm that was used for von Mises stress. Coincidentally, it also found that eight clusters were optimal using BIC for the best 10 candidate models. Consider nodes that have their largest posterior probability belonging to Cluster 4 of MoRM and refer to Table 8. Holding the other process parameters constant, increasing LP by 1 W corresponds to an increase in the log total deformation by 0.001. That is, the distance those nodes would be displaced would increase as the LP increases. Similarly, increasing SS by 1 mm/s while holding the other process parameters constant corresponds to an expected decrease in the log total deformation by 0.0008. Increasing LH by 1 mm corresponds to a decrease of 0.2154 in the log total deformation on average. Again, the interpretation for Cases is different as they are factor variables. If the nodes in Cluster 4 use Case 1 for their simulation, the intercept term in the regression model would be 4.3091. If those nodes instead use Case 2 for their simulation, the intercept term would instead be 5.2533. This means that the additional cooling time relates to an expected increase in the total nodal deformation, which is consistent with results found when considering von Mises stress as the response variable.

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Cluster	$\hat{\beta}_{4,k}$	$\hat{\beta}_{5,k}$	$\hat{\beta}_{6,k}$	$\hat{\beta}_{0,k}$	$\hat{\beta}_{1,k}$	$\hat{\beta}_{2,k}$	$\hat{\beta}_{3,k}$
1	0.0012	-0.0011	-0.3069	4.5899	5.1844	2.608	3.9692
	(2.00e-05)	(1.67e-05)	(3.55e-03)	(2.26e-02)	(2.31e-02)	(2.30e-02)	(2.26e-02)
2	0.0011	-0.001	-0.2531	4.256	4.9462	2.6766	3.9411
	(1.77e-05)	(1.49e-05)	(3.09e-03)	(2.18e-02)	(2.10e-02)	(2.13e-02)	(2.10e-02)
3	0.0011	-0.001	-0.2925	4.4831	5.157	2.8624	4.1764
	(1.80e-05)	(1.48e-05)	(3.14e-03)	(2.18e-02)	(2.13e-02)	(2.16e-02)	(2.13e-02)
4	0.001	-0.0008	-0.2154	4.3091	5.2533	2.9724	4.4085
	(2.89e-05)	(2.46e-05)	(5.23e-03)	(3.51e-02)	(3.50e-02)	(3.31e-02)	(3.47e-02)
5	0.0012	-0.0011	-0.3338	4.8297	5.3778	3.0732	4.3379
	(2.22e-05)	(1.81e-05)	(3.81e-03)	(2.36e-02)	(2.61e-02)	(2.60e-02)	(2.61e-02)
6	0.001	-0.0008	-0.2356	4.3245	5.0917	3.0183	4.147
	(2.48e-05)	(2.10e-05)	(4.29e-03)	(3.07e-02)	(2.85e-02)	(2.85e-02)	(2.84e-02)
7	0.0011	-0.001	-0.2678	4.6028	5.0942	2.9699	4.0481
	(2.04e-05)	(1.68e-05)	(3.57e-03)	(2.25e-02)	(2.37e-02)	(2.40e-02)	(2.42e-02)
8	0.0012	-0.0011	-0.3002	4.481	5.2059	2.7196	4.0983
	(1.64e-05)	(1.36e-05)	(2.84e-03)	(1.94e-02)	(1.90e-02)	(1.94e-02)	(1.94e-02)

TABLE 8: Coefficients for MoRM using the total deformation as the response. Each row corresponds to a cluster, but each observation potentially has some weight in each cluster

MoRM, mixture of regression models

Discussion

Recall that for the MoRM with von Mises stress as a response, we found eight clusters to be optimal. Since clusters have different regression coefficients, this will result in cluster-dependent expected outcomes for each node. We can observe a pattern where each cluster corresponds with a set of layers from the geometry of the FE results, which was seen in Figure 4. The plots shown in Figure 5 highlight this trend, with the opacity being proportional to how often that node appeared in the given cluster across the 192 simulations. The clusters tend to correspond to the simple geometric features present in the geometry, with the differences in the influence of process parameters being expressed in the differences in regression coefficients.

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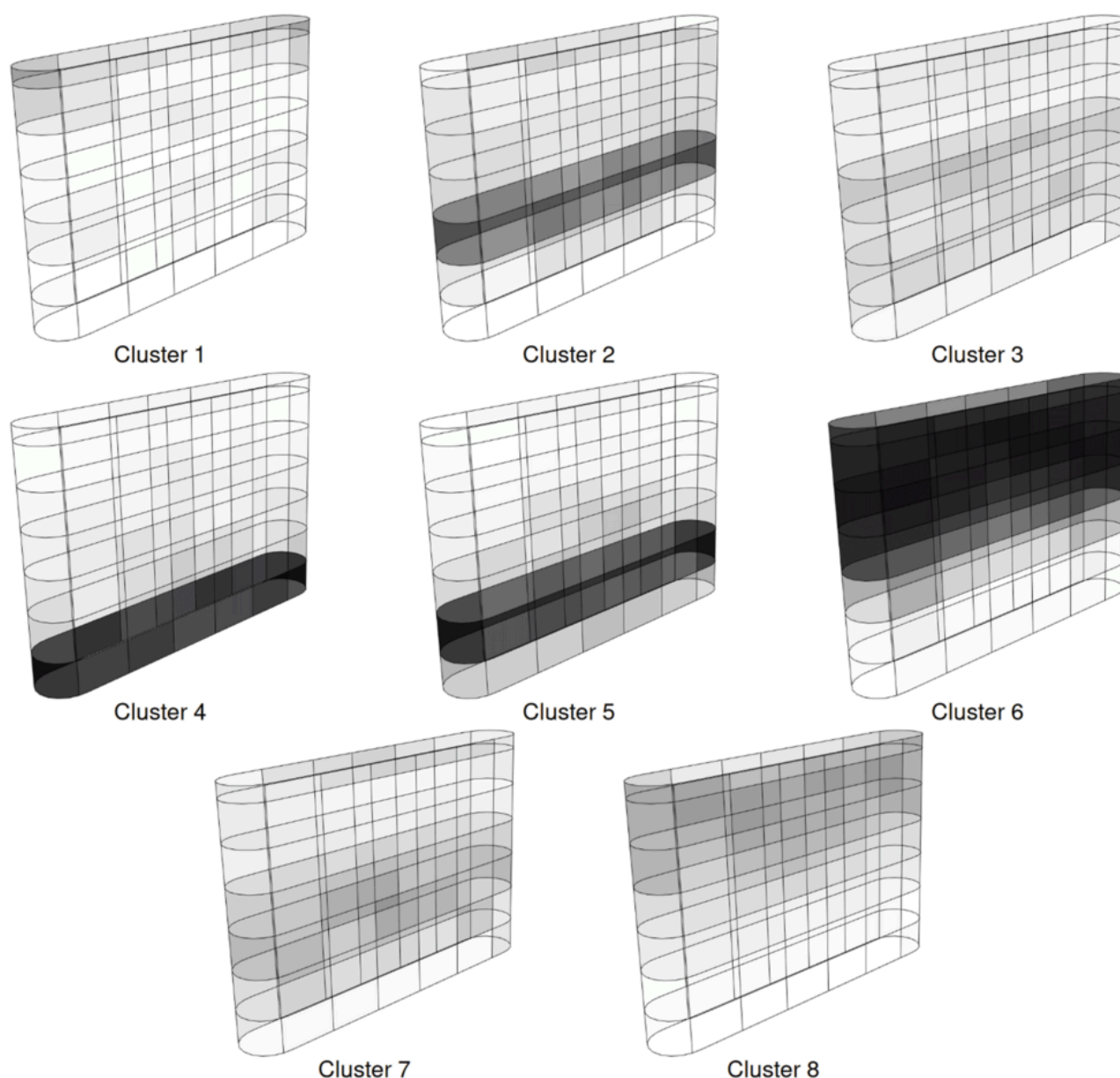


FIGURE 5: Proportion of nodes assigned to the cluster corresponding to its position for the von Mises stress. Proportion is shown by the opacity of the pixels

In particular, Cluster 1 appears to have most of its node membership in the top layer of the geometry. Cluster 2 predominantly has nodes from the ninth to twelfth layers of the print, and Cluster 3 has nodes from the fifth to sixteenth layers of the print. Cluster 4 contains many of the nodes from the bottom four layers of the print. Cluster 5 contains nodes from the fifth to the eighth layers primarily. Cluster 6 was a considerably larger cluster, collecting many nodes from the top half of the print. Cluster 7 tends to have a few nodes from everywhere except the bottom four layers. Cluster 8 mostly has nodes from the top ten layers of the print. Each cluster tends to follow the print lines closely, but not perfectly.

When considering the von Mises stress, it is intuitive that the clustering solutions form along the layer of the print. The clusters that appear more transparent tend to capture useful deviations around these more intuitive clusters and associated regression coefficient estimates. The magnitude of the regression coefficients associated with process

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parameters varied among clusters, suggesting which parameter had the most effect on the corresponding cluster. For example, Cluster 8 is primarily associated with the top half of the print also has regression coefficients that are larger in magnitude for LP and SS than any other cluster. This implies that for many of the simulations, this area is more sensitive to changes in manufacturing parameters. On the other hand, Cluster 4 has very small regression coefficients for LP and SS, which matches with the bottom four layers of the print, which we also observed to be less sensitive across simulations. These stress clusters' low sensitivity to changes matches the underlying physics and physical boundary constraints. This section is connected to a base, which enhances heat conduction and imposes geometrical restrictions on deformation.

An eight-cluster model was found to be optimal for MoRM total deformation. Similar to previously, the opacity of each of the sub-figures in Figure 6 corresponds with how often those nodes have maximum posterior probability within that cluster. The pattern here now corresponds with the broad level geometric features of the part rather than the layers directly.

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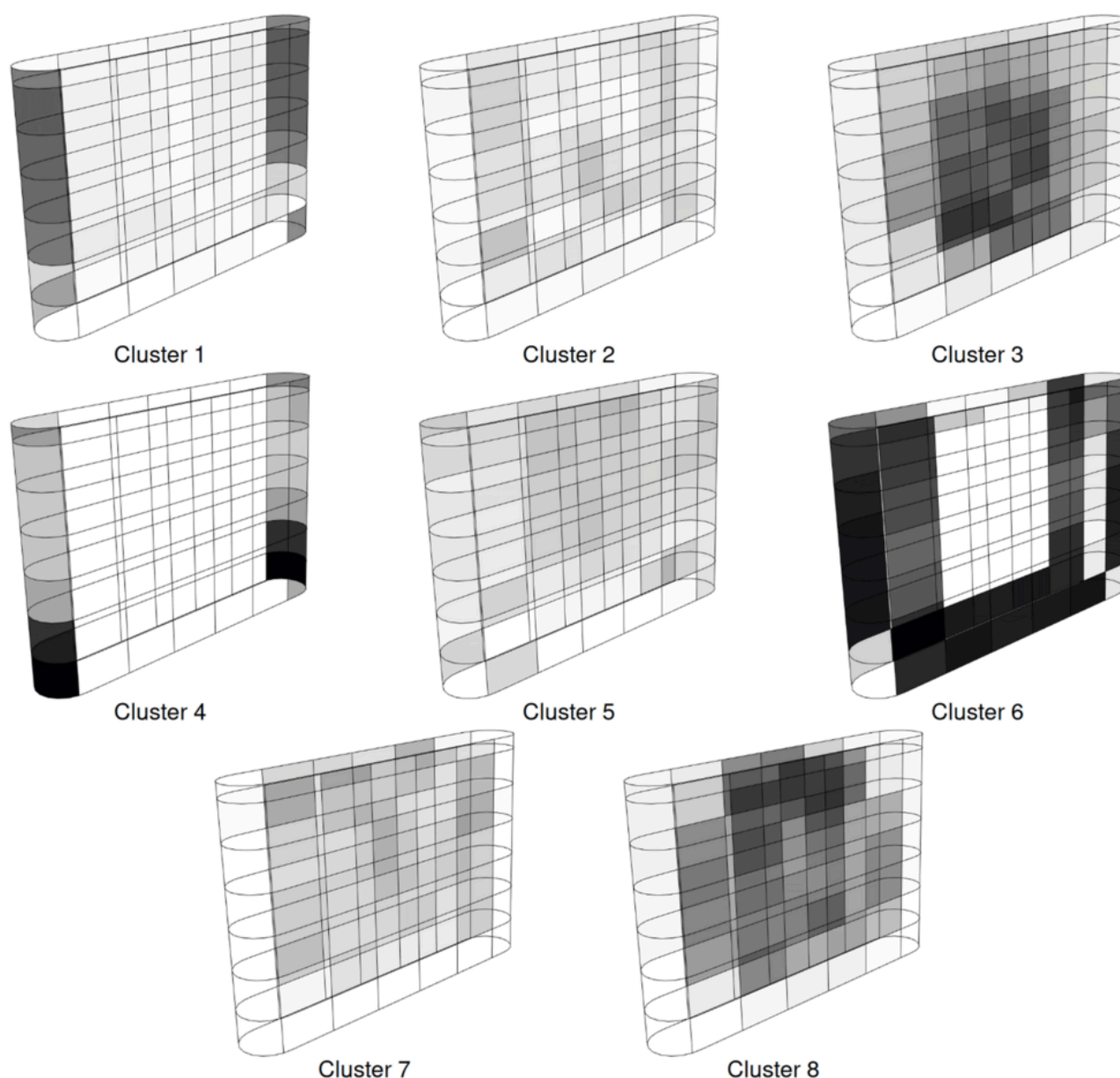


FIGURE 6: Proportion of nodes assigned to the cluster corresponding to its position for the total deformation model. Proportion is shown by the opacity of the pixels

Cluster 1 of Figure 6 shows the higher levels of the curved section. Clusters 2, 5, and 7 are made up of a few nodes that form the middle unsupported region of the geometry. Clusters 3 and 8 further focus that towards the very middle of the unsupported region. Cluster 4 is primarily the lowest portion of the curved section, with some higher layers included as well. Cluster 6 appears to form an outline of the shell except for the top middle of the geometry.

There is a similar relation with the underlying structure and physics for the total deformation as discussed earlier for stress. The inner piece of the long edge is expected to be the most sensitive to changes to process parameters, as it is unsupported. Similarly, the semicircles would be expected to be the least sensitive to changes, especially near the bottom, due to physical support as well as a metal base allowing higher heat conductivity. Cluster 4 has the smallest

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magnitude coefficients, showing that the semi-circles are indeed the least sensitive to changes in LP and SS. Although the difference between the largest coefficient and the smallest coefficient within a process parameter is small. The remaining clusters individually have comparable magnitudes in LP and SS, but there are changes in the coefficient for LH.

Overall, while there is not always one-to-one overlap, the general trends of clustering and regression coefficient are linked with the underlying thermomechanical responses and constraints, reinforcing the localized influences of process parameters in the fitted model. The clustering results can thus offer valuable insights into the spatial heterogeneity of stress and deformation in AM parts to inform manufacturing for targeted optimization strategies.

Limitations and future work

The focus of the paper is on providing a comprehensive statistical framework for the analysis of larger FEM data sets beyond general plots and analyses that are typically used in engineering literature. Hence, the paper did not comment deeply on the FEM model of the material system used for data generation itself, but on the format of the data and the outcome variables of von Mises stresses and deformation typically used in such analysis. The method developed and presented here can be applied to other similar thermomechanical FEM datasets beyond AM-based analysis.

However, future work can focus on FE modifications to address the current work and improve the underlying data. For example, the current model and parameter choice were guided by a related experimental work [21,22]. Future work can expand on the process parameter choice, such as scan speed, laser power, and laser spot size, both to add further granularity to the parameter space and to create a larger range of the parameter space that has been reported across different metal alloys. Metal AM processes are constantly evolving, and these changes may also be needed to address future developments in that space.

Similarly, FEM parameters can be improved. One such limitation is the finest layer height of 1 mm taken in the underlying analysis, which, though shown to be physically relevant for Inconel alloys to increase print speed, is coarser than typically used [41]. In the ABAQUS simulation version used here (Abaqus 2021, Build 2020 03 06-08.50.37 167380), the layer deposition was achieved through the "activating" of elements using model change options. So, essentially, deposition depth was connected with the mesh size. A finer depth in the micrometer range can be achieved through significant mesh refinement (i.e., 100X finer than the current), followed by mesh sensitivity and computational resource optimization studies in the future. On the other hand, in the context of the paper's primary goal, the chosen layer height enabled a larger parameter space to be included. Future work can extend and explore the model predictive capability with finer layer thickness to capture finer thermal and residual gradients.

Overall, the statistical method proposed in the paper continues to be useful and can be applied with the above proposed future modifications to the current FEM analysis, as well as to other FEA models and outcomes.

Conclusions

This work analyzes the complex association between AM process parameters and thermomechanical outcomes, tracked via prediction of von Mises stress and total deformation using finite element simulations. The process parameters varied across the simulations were LP, SS, LH, and different cooling assumptions, resulting in a total of 192 simulations. To mitigate the effects of the mesh choice of FEM, the nodal outcomes from FEM were averaged with their neighbors, which also eased the computation burden. Instead of a traditional and time-consuming approach using standard X-Y plots for results interpretation, here, two statistical algorithms, namely the FMM and MoRM, were used for post-processing.

Using the PRESS statistic as a measure of how much error the predictions from the statistical model differ from original simulations, the PRESS statistic for MoRM was an order of magnitude smaller than FMM in the deformation (86.11 vs 450.38) and stress (28.62 vs 258.30). Based on these outcomes, the study focused on MoRM for further consideration. The MoRM model identified eight stress clusters and eight deformation clusters across models to capture the combined effect of process parameters on the manufactured part. Additional insights were noted. For example, the effect of increasing LP by 1 W was approximately negated by increasing SS by 1 mm/s on both the stress and deformation. While increasing LH decreased stress and total deformation, the effects of increasing the cooling time and

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the cooling assumption varied depending on the cluster location. The most sensitive area was the unsupported region near the top center of the geometry, while the most robust was the bottom rounded corners. Overall, MoRM captured the heterogeneity of the considered geometry and its associated process parameter associations through differences in the regression coefficients. These outcomes observed independent of a mechanistic view also aligned with the underlying mechanistic reasons for the response, providing greater confidence in the predictions.

There are a few limitations to this work at present. The methods for reducing the dataset in the statistical framework reduced the data's granularity and may not capture spatial relations perfectly. The assumption that the averaged observations are independent and identically distributed should be adjusted to account for spatial correlation. The nodal averaging scheme addresses this concern on a small scale but removes the relationship between adjacent nodes that belong to different pixels. This work was also limited to one geometry and material, and could be expanded to other geometries and material combinations. The process parameters can also be further expanded to match industry-standard values for different alloy types.

In summary, the work demonstrated an independent statistical framework for post-processing of large datasets from FEM outcomes. It successfully demonstrated a clustering approach for identifying critical areas for stress and deformation consistent with the physical outcomes. By doing so, it provided guidance for future process changes. For example, the areas with the most deformation (Cluster 8) can be reduced by lowering the laser power, increasing the scan speed, increasing the layer height, and increasing the cooling time. The association between process parameters and stress and deformation varied across different areas of geometry. The clusters and associated estimated regression coefficients can be used to determine the best values to use for preferred outcomes when analyzing large datasets and to provide a data-guided approach for AM processes.

Additional Information

Author Contributions

All authors have reviewed the final version to be published and agreed to be accountable for all aspects of the work.

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Disclosures

Human subjects: All authors have confirmed that this study did not involve human participants or tissue. **Animal subjects:** All authors have confirmed that this study did not involve animal subjects or tissue. **Conflicts of interest:** In compliance with the ICMJE uniform disclosure form, all authors declare the following: **Payment/services info:** This research was supported by the South Dakota State University Research Scholarship Challenge Fund 2021 and the NASA EPSCoR Additively Manufactured GRCop-42 Extended Investigation. **Financial relationships:** All authors have declared that they have no financial relationships at present or within the previous three years with any organizations that might have an interest in the submitted work. **Other relationships:** All authors have declared that there are no other relationships or activities that could appear to have influenced the submitted work.

Data Availability Statements

The datasets (and/or code) supporting this study are available from the corresponding author upon reasonable request.

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