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Convolutional Neural Network for geometric deviation prediction in Additive Manufacturing

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Abstract

The geometrical quality of AM products is an indispensable concern when conducting Design for Additive Manufacturing (DfAM), since it dominates the geometrical consistency between the manufactured samples and the design intent and has an impact on the functionality of the products. Therefore, effective prediction of the geometric deviations prior to the mass production will provide useful information for designers in order for design optimization. Data-driven methods open up new possibilities to gain high-fidelity prediction based on existing observable data. In this paper, a Convolutional Neural Network based deep learning method is proposed which enables the prediction of deviations for different shapes and process settings. A data augmentation technique is also introduced to generate samples for network training based on a small number of available data. Through a case study, it's demonstrated that the trained network manages to accurately predict the geometric deviations of shapes manufactured with varied size and process parameter settings. The predicted deviations could substantially benefit DfAM in evaluation of geometrical consistency. Moreover, reverse compensation can be accordingly applied to the CAD model prior to the manufacturing process, thus increasing the geometrical accuracy of the manufactured parts.

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Keywords: Design for Additive Manufacturing; Geometric deviation modeling; Deep learning; Convolutional Neural Network

1. Introduction

Additive manufacturing (AM) has brought a great impact to the manufacturing industry with its novel layer-per-layer building strategy enabling the mass production of parts with more complex shapes and internal structures. Despite its profound industrial potential, the related standards and methodologies regarding design, tolerancing and quality control remain to be exploited and have drawn the interest of many researchers and practitioners. The thermal-mechanical properties of AM process, as well as its almost fully automatic execution with little human intervention, may induce undesirable geometrical uncertainties on the manufactured parts. Therefore, prediction of the geometric deviations in the design stage is an important concern in order to gain effective Design for Additive Manufacturing (DfAM). With the predicted information, designers could evaluate the geometrical consistency of the manufactured products with the design intent and accordingly derive pre-compensation plans to improve the geometrical quality.

The rapid growth of data science technologies have unveiled the potential to solve engineering problems with the power of data. Data analytics methods have been employed in different fields such as economics [7] with the use of artificial neural networks to predict market prices, and in the medical field [8] where convolutional neural networks have been used to segment medical images or in the language processing field [11] where recurring Long-Short Term Memory (LSTM) neural networks are now commonly used to predict the next words in a sentence. In the topic of deviation modeling for AM, the highly non-linear relationships among the deviations and their sources are hard to capture with traditional analytical methods, and the promising learning algorithms will be of significant help. Artificial Neural Network has been adopted in several works to evaluate thermal deformation [3] and surface quality [12] with respect to FDM process parameters. An unsupervised machine learning approach is used in [4] to characterize the geometric accuracy by recognizing clusters from the point cloud that are linked to certain process conditions, thus significantly reducing the amount of data required for the characterization. In [13], a transformation perspective coupled with a multi-task trans-

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fer learning algorithm is proposed to model and predict the in-plane shape deviations. The layer-wise deviations towards the build direction (out-of-plane deviation) are also investigated in [14, 15] with respect to a set of process parameters. Whereas, the respective modeling of in-plane (2D) and out-of-plane (3D) deviation makes it hard to integrate both models and yet a comprehensive predictive model that could be applied for different shapes is absent.

The use of deep learning techniques can also be anticipated, which, however, remains unexploited under this topic. Therefore, a deep learning method based on Convolutional Neural Network (CNN) will be proposed to enable the prediction of geometric deviations in the Selective Laser Melting (SLM) process. This method considers the shape, size of the part and also process parameters, which is quite comprehensive compared to existing works that only cover one or two aspects. Following the Introduction Section, Section 2 discusses details of the CNN algorithm for deviation prediction, the network architecture and training data structure are explained. To collect enough data for network training, Section 3 presents a data augmentation strategy using Statistical Shape Analysis (SSA) of AM simulation data. A case study is provided in Section 4 to validate the performance of the network and the conclusion is drawn in Section 5.

2. Deviation prediction with Convolutional Neural Network

CNN is a well-known deep learning algorithm that has gained mass adoption in computer vision and natural language processing to tackle problems such as face recognition, image classification, human pose estimation, etc [6, 5, 10]. Following a multi-stage architecture, CNN has proved its effectiveness in capturing the features of the input data. A typical CNN consists of an input layer, an output layer and several hidden layers that are divided into stages with each stage comprising a combination of layers of four types: the convolution layer, the non-linearity layer, the pooling layer and the fully-connected layer.

Take a typical image classification problem as an example, the input is a processed image with N pixels in width and height and 3 in depth representing the RGB color channels. So the input can be seen as an $N \times N \times 3$ matrix containing the color intensity values. The output is a vector indicating which class the image could be classified into. With appropriate design of the network architecture, CNN can also be used to tackle regression problems. The objective of using CNN in this paper is to achieve the prediction of geometric deviations in AM considering the effect of influential factors, including process parameters, part size and layer height, on parts of different shapes. Therefore, a multi-channel input has been designed as shown in Fig. 1, with each channel represented by an $N \times N$ 2D matrix. The first channel is the geometry channel conveying the 2D shape of the layer, in which elements are assigned 1s if their locations are occupied by the layer geometry and 0s otherwise. In the 2nd to 4th channel, a constant matrix is assigned as the corresponding process parameter values under which the part is manufactured. The parameters considered in this paper are layer thickness ($\boldsymbol{p}^1$), laser scan speed ($\boldsymbol{p}^2$) and laser power($\boldsymbol{p}^3$). Similarly, the 5th and 6th channel each contains a constant matrix representing the part size ($\boldsymbol{p}^4$) and layer height (h). Therefore, the total size of input parameters sums up to $N^2 + 5$. The output of the network is a 3-channel deviation field corresponding to the deviation in X, Y and Z axis.

The main structure of the network is divided into two stages, in each stage convolution and pooling operations are conducted to obtain a detailed feature map. The convolution layer performs as a filter that convolves the input across its height and width with small feature images, producing a 2D activation map of the filter which tells the network to activate the filter when it detects this specific feature at some spatial position of the input. In a convolution layer, N_f filters $\boldsymbol{F}^c \in \mathbb{R}^{s^c \times s^c \times d}$ are used to convolve with the input $\boldsymbol{I} \in \mathbb{R}^{s^i \times s^i \times d}$, where s^c is the size of the filter and d is the depth which is consistent with the input depth. The input of the convolution layer can either be the input image or the output of the previous layer. By specifying two extra parameters: stride S and padding P, the feature map $\boldsymbol{M}_i \in \mathbb{R}^{s^m \times s^m}$ after convolution using filter $\boldsymbol{F}^i$ is obtained as Eqn.(1), where $s^m = (s^i - s^c + 2P)/S + 1$, $*$ is the convolution operator and $\boldsymbol{b}_i^c$ is the bias vector.

$$\boldsymbol{M}_i = \boldsymbol{I} * \boldsymbol{F}_i + \boldsymbol{b}_i^c, i = 1, 2, ..., N_f \tag{1}$$

Convolution layers are stacked together in both stages extending the number of features to 192, each followed by batch normalization and a non-linearity layer which applies non-linear activation functions on the neurons. In this paper the canonical ReLU (Rectified Linear Unit) function is used to perform element-wise activation on the input, this function is represented as Eqn.(2) and has the form as illustrated in Fig. 2.

$$f(x) = \max(0, x) \tag{2}$$

At the end of each stage, a pooling layer is inserted to perform down-sampling, thus reducing the parameter count and computational cost as well as controlling over-fitting. Common forms of the pooling layer are max pooling and average pooling, the former of which is used in this paper. Given a specified pooling filter size s^p and the striding parameter S, the pooling layer uses a $s^p \times s^p$ block to scan each depth slice of the input progressively and takes the maximum value in each scanned block while discarding other elements.

Fully connected (FC) layers are located at the end of the network to enable high-level reasoning by connecting all neurons in the previous layer to each neuron in current layer[2]. Right before the FC layer, features in the previous convolution or pooling layer need to be flattened to a single vector as the FC input. Three FC layers are specified in this architecture, two reducing the number of features and the other producing the regression output of the network, all of which take the following

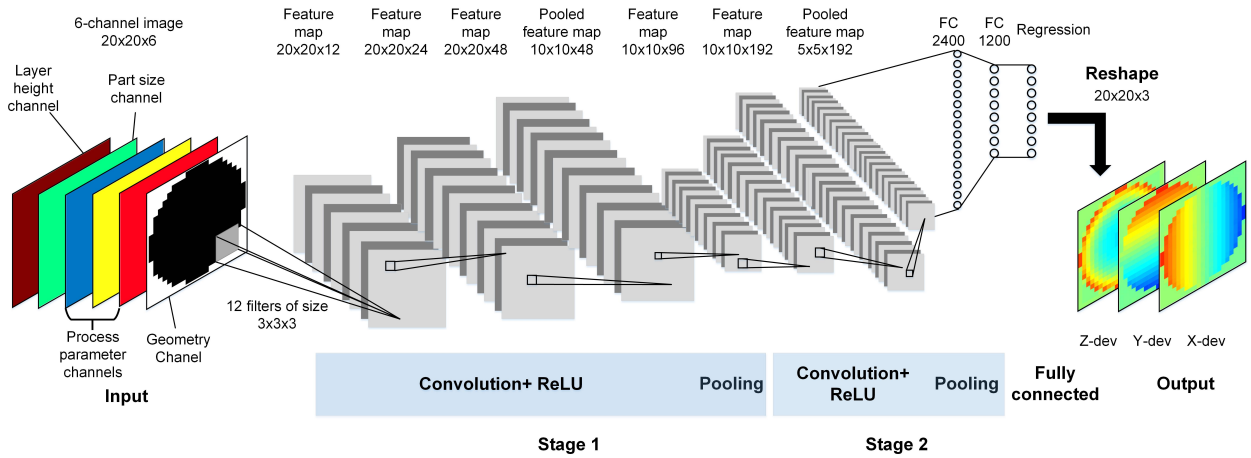

Fig. 1. The CNN architecture

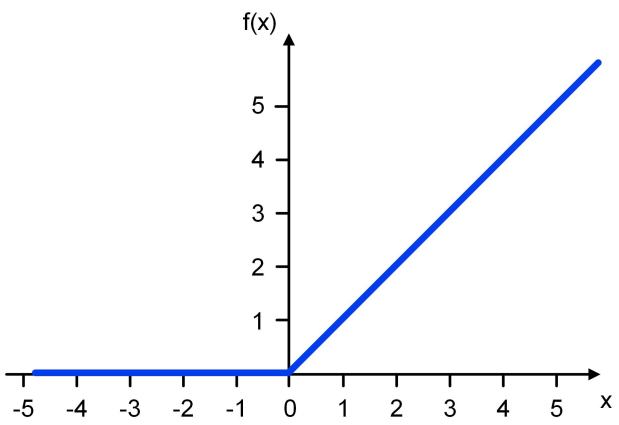

Fig. 2. The ReLU function

linear form, where $\boldsymbol{x}, \boldsymbol{y}$ are input and output vectors, $\boldsymbol{W}$ is the weighting vector and $\boldsymbol{b}^{fc}$ is the bias vector.

$$\boldsymbol{y} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}^{fc} \tag{3}$$

The output vector is further reshaped as an $N \times N \times 3$ matrix as the predicted X-,Y- and Z- deviation profiles on the 2D layer. Training of the network aims at finding optimal values of parameters, including $\boldsymbol{b}^c, \boldsymbol{W}$ and $\boldsymbol{b}^{fc}$, by minimizing a loss function. Since we are actually dealing with a regression problem, the half mean squared error (MSE) between the actual and predicted deviation values at all $3N^2$ locations of the 3 deviation profiles is used to define the loss as Eqn.(4).

$$J(\boldsymbol{b}^c, \boldsymbol{W}, \boldsymbol{b}^{fc}) = \frac{1}{2} \sum_{i=1}^{3N^2} \frac{(\boldsymbol{y}_i - \hat{\boldsymbol{y}}_i(\boldsymbol{b}^c, \boldsymbol{W}, \boldsymbol{b}^{fc}))^2}{3N^2} \tag{4}$$

Tensorflow [1] is utilized to establish the proposed network. And the Adam optimizer is chosen for network training, which decreases the training loss by searching in the parameter space. The hyper-parameters, such as filter size and number, stride, padding and pooling shape, are carefully selected to reach a balance between computational cost and prediction accuracy. Also, to avoid over-fitting and increase learning speed, a piecewise dropping mechanism is used which drops the learning rate by 50% every 20 epochs, starting from an initial value of 0.001.

As is known, deep learning necessarily requires a large amount of training data to ensure robust prediction. However, the time-consuming manufacturing, measurement and simulation process hardly allow the collection of sufficient data in an academic research. Therefore, in order to obtain a high-quality network, a data augmentation strategy is needed to generate new data samples based on existing ones without a significant loss of accuracy. In this context, a method based on Statistical Shape Analysis will be proposed in the next section enabling the quick augmentation of training data based on a small number of AM simulations.

3. Deviation data pre-processing and data augmentation with Statistical Shape Analysis (SSA)

The growth of data-driven models for design and quality control for AM has posed the demand for a substantial amount of data for model training and validation, which is quite challenging in view of the costly manufacturing and measurement processes. Therefore, AM simulation technologies are emerging aiming at providing quick and accurate prediction of the possible outcomes of AM processes for both industrial and academic applications. A number of AM simulation packages offer the functionality to predict the in-process and post-process geometric part deviations by considering thermal and mechanical effects. Moreover, the deviations of each 2D layer can be obtained from the simulation results, which is beyond the capability of traditional measurement techniques. In this regard, a proprietary software package named Ansys Additive® is used

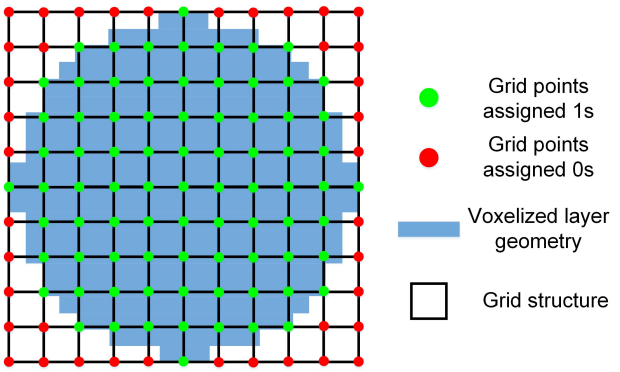

Fig. 3. Determination of the input geometry channel

in this paper for deviation data collection. The aforementioned process parameters are specified and a number of simulations are run for parts of different shapes and sizes. The software receives STL files as input and outputs a voxelized part model. The predicted deviations in $X-$, $Y-$ and $Z-$ axes are associated with each voxel. Given the specified layer height, the layer-wise deviation data can be conveniently retrieved from the voxel points lying on each 2D layer.

The input and output of the CNN architecture as shown in Fig. 1 call for a regular data structure resembling the image, which means that the deviation data of parts with different shapes and sizes needs to share a common $N \times N$ grid structure. Therefore, a mapping of the data is needed. For each 2D layer data of a specific part, a bounding square is determined which fully encloses the whole geometry of the layer. Then, the square is divided into a regular grid given the grid size. Since the deviation data are associated with each voxel point, we should figure out a way to map the data from voxel points to the grid points, and it is necessary to determine the input geometry channel from the grid structure. A straightforward solution is to find the boundary of the layer geometry and all the grid points lying on or within the boundary are considered to be occupied by the geometry and are assigned 1s, while other grid points are assigned 0s, as shown in Fig. 3. The values on the grid points together form the 2D matrix as the geometry channel in the network input. The data mapping can be done with interpolation techniques, here the cubic interpolation is used which considers the continuity in the distribution of data. The mapped grid data can be represented as another 2D matrix and element-wise multiplication of this matrix and that of the geometry channel is done to ensure that grid points lying out of the shape boundary are eliminated. Performing the interpolation respectively for $X-$, $Y-$ and $Z-$ deviations, three deviation fields are obtained for each simulated layer, regardless of the layer height, as well as the size and shape of the actual part. Such information is, however, considered at the network input as influential factors. If we consider the voxel points lying on the layer as a nominal 2D shape, by adding deviations on the three axes, a 3D deviation profile of the layer is obtained. The next step is to conduct SSA on the deviation profile with respect to the five control parameters $(\boldsymbol{p}, h)$ for data augmentation.

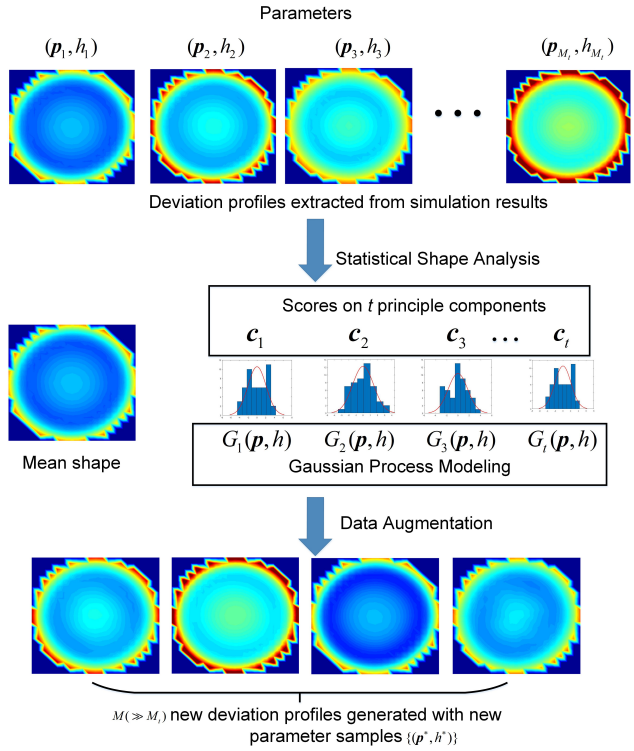

Fig. 4. Data augmentation with Statistical Shape Analysis and Gaussian Process

For each part with a specific shape, a design of experiment (DoE) is conducted to draw M_p samples of the process parameters $\boldsymbol{p}$ and accordingly M_p simulations are run. From the simulation result of each part, a given number of M_l deviation profiles are extracted with the corresponding layer height values h. Therefore, a total number of $M_t = M_p * M_l$ deviation data are collected together with the control parameters $(\boldsymbol{p}, h)$. These data serve as the basis for data augmentation. SSA has been used in our previous research [14] as a dimension reduction technique to extract main deviation modes (principal components) from the layer-wise deviation data and to map the original deviation profiles into the reduced t-dimensional space as a set of scores $\boldsymbol{c} = c_1, c_2, .., c_t$. Gaussian Process (GP) models $c_t = G_t(\boldsymbol{p}, h)$ are then established to represent the relationship between the parameters $(\boldsymbol{p}, h)$ and scores $\boldsymbol{c}$. Therefore, with the trained GP models, a large number $(M \gg M_t)$ of new deviation profiles can be generated with new combinations of $(\boldsymbol{p}, h)$, thus the available data for CNN can be substantially augmented. Figure 4 provides an overview of the data augmentation process. Due to the page limit, the details about SSA and GP modeling will not be discussed in this paper. Readers who are interested in these techniques may refer to [14] for more information. It is also worth noting that, the generality of SSA is quite limited by the shape. So here the SSA-GP technique is just used to augment the available deviation data for each input shape, and to assist the CNN in the pre-processing stage. Moreover, though the deviation data are collected from simulations, a vision can be made that, in an industrial application where manufactured samples are readily available, the model can be enriched.

NO.	Part size (mm)	Layer thickness (um)	Laser power (W)	Scan speed (mm/s)	Type
1	15	85	280	2400	Training
2	18	90	190	1600	Training
3	21	40	230	1300	Training
4	24	60	160	1700	Training
5	27	35	180	2100	Training
6	30	75	200	1000	Training
7	33	50	220	1900	Training
8	36	65	270	2200	Training
9	39	30	260	1400	Training
10	42	80	290	1800	Training
11	45	70	170	1100	Training
12	48	45	250	1200	Training
13	51	95	240	1500	Training
14	54	55	210	2000	Training
15	57	100	150	2300	Training
16	20	50	195	3000	Test (Cyl)
17	21	40	230	1300	Test (Sqr)

Table 1. Parameter values determined by DoE for simulation

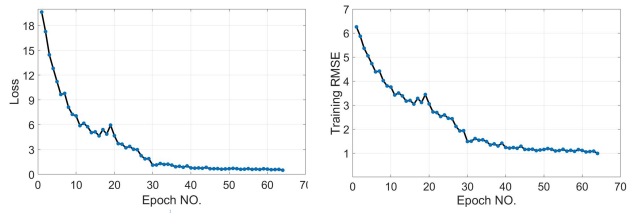

Fig. 5. The total loss and training RMSE in the training process

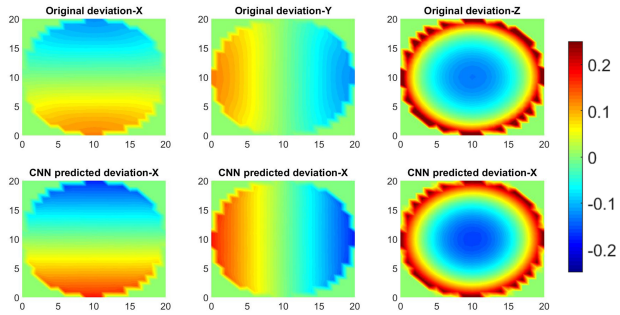

Fig. 6. Comparison between the original deviation profile and the CNN prediction on cylindrical shape

4. Case study

To illustrate the effectiveness of the proposed method, a case study is provided in this section regarding AM parts of a square shape and a cylindrical shape. For each shape, a Design of Experiments (DoE) procedure is performed using the Latin Hypercube Design (LHD) method to sample 15 levels of parameters within a reasonable range, more explanations to the selection of these parameters can be found in [15]. Based thereon, $M_p = 15$ simulations are run to generate the training data for SSM and data augmentation. Two extra simulations are conducted following two randomly generated parameter samples to test performance of the trained network on the cylindrical shape and square shape respectively. The parameter setting of each simulation can be found in Tab. 1, in which the Type column denotes whether the data belongs to the training or test set. The part size column indicates the size of the simulated part, standing for the side length for square shape and the diameter for cylindrical shape. All parts are designed with the height as 5mm.

A thermal-mechanical simulation is conducted under each parameter setting as listed in Tab. 1, while keeping the same setting for all other parameters, including baseplate temperature (353K), hatch spacing (100um), material (Inconel 718), etc. The resulting deviations in X, Y and Z axes are sampled in a layer-wise manner with a 1mm-interval in the build direction and in each layer the data are mapped into a 20×20 regular grid, resulting in $M_l = 6$ layers for each part. A total number of $M_t = 15 \times 6$ deviation profiles are obtained and used for data augmentation. Through SSA, the mean shape of the deviation profiles is found together with their scores in the reduced PCA space. The first $t = 4$ principle components manage to explain 98.944% of the variance in the original deviation data of the square part, and 98.467% in that of the cylindrical part. Based on the parameter values and scores, 4 GP models are trained respectively to capture the non-linear relationship between them. With the trained GP models, $M = 1200$ more parameter combinations are sampled using LHD and the corresponding deviation profiles are predicted.

In the next step, the data for network training are organized. The formulation of the input geometry channel has been discussed in Section 3, while the other channels are assigned the newly generated parameter values in data augmentation. The output deviation fields are also obtained from the predicted deviation profiles. The data are split into training and validation datasets following the 5-fold measure. We use a mini-batch strategy, which splits the total samples into 66 separate batches, each containing 30 pieces of data. In each iteration, the network parameters are updated by feeding one batch. After all the samples are fed, we complete one epoch of training and the whole training process is repeated for 64 epochs. The training progress is illustrated in Fig. 5 showing the changes in total loss and the RMSE of training data in each epoch. The blue dot denotes the median value of evaluations on all iterations of an epoch. It can be seen that, as the training process proceeds, the loss and RMSE both reach low levels around 50 epochs and show no significant fluctuations after that, which means the parameters are already well learned for prediction. Therefore, we take the network parameters at the 50th epoch (training checkpoint) for prediction.

The performance of the trained network is validated on the two parts (NO.16 and NO.17) held as test set. For the cylindrical shape, the X-,Y-,Z- deviation profile of the top layer of test part NO.16 is illustrated in Fig.6 as compared to the simulation result. For the square shape, the bottom layer of test part NO.17 is illustrated in Fig.7.

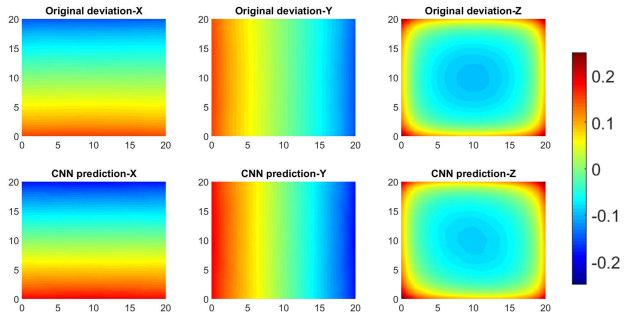

Fig. 7. Comparison between the original deviation profile and the CNN prediction on square shape

Though slight differences exist for the X- and Y- deviation of cylindrical shape and the Z- deviation of square shape, the CNN prediction has captured the major distribution of deviations on the test layer. The performance maintains at a high-level also for other test parts according to our experiment, which will not be demonstrated here due to the page limit. The trained CNN has managed to effectively predict deviations across the two different shapes by considering their sizes and process parameters. With more training data from other shapes and parameter settings available, the predictive capability of the network could be significantly enhanced.

5. Conclusion

In this paper, a new deep learning method has been developed for the geometric deviation modeling of AM processes. With the power of data, CNN has unfolded new possibilities to investigate the effect of manifold influential factors on the resulting geometric deviations. Based on the predicted deviations, the deformed part surface can be constructed from the nominal STL representation by deviating the layer boundary points, thus assisting DfAM in evaluation of geometrical quality. The pointwise reverse compensation can also be performed to obtain a compensated STL model so as the manufactured part surface will be closer to the design intent.

This method has the potential to be more powerful by being trained with more deviation data from a variety of shapes. The incorporation of more realistic measurement data will undoubtedly improve the predictive performance in practical industrial applications. This poses a need, however, for more advanced measurement techniques such as Computed Tomography (CT) in order to gain layer-wise data. Moreover, new process parameters can be taken into account by increasing the input channels and conducting more simulations under such parameters. It's also worth noting that, if simulation tools that goes beyond simple FEA are available, for instance generative design, then this work can consider more design constraints and requirements that could be incorporated as new parameters. Another promising research direction is towards the Digital Twin [9] for Additive Manufacturing with data analytics as the building block aiming at developing high-fidelity digital models driven by multi-domain data from the product life-cycle.

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