Validating Results of 3D Finite Element Simulation for Mechanical Stress Evaluation using Machine Learning Techniques

Alexander Smirnov\textsuperscript{1a}, Nikolay Shilov\textsuperscript{2b}, Andrew Ponomarev\textsuperscript{1c}, Thilo Streichert\textsuperscript{3}, Silvia Gramling\textsuperscript{3d} and Thomas Streich\textsuperscript{3e}

\textsuperscript{1}SPIIRAS, 14th Line, 39, St. Petersburg, Russia
\textsuperscript{2}ITMO University, Kronverksky pr., 49, St. Petersburg, Russia
\textsuperscript{3}Festo SE & Co. KG, Ruiter Str., 82, Esslingen, Germany

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Abstract: When a new mechanical part is designed its configuration has to be tested for durability in different usage conditions (‘stress evaluation’). Before real test samples are produced, the model is checked analytically via 3D Finite Element Simulation. Even though the simulation produces good results, in certain conditions these could be unreliable. As a result, validation of simulation results is currently a task for experts. However, this task is time-consuming and significantly depends on experts’ competence. To reduce the manual checking effort and avoid possible mistakes, machine learning methods are proposed to perform automatic pre-sorting. The paper compares several approaches to solve the problem: (i) machine learning approach, relying on geometric feature engineering, (ii) 2D convolutional neural networks, and (iii) 3D convolutional neural networks. The results show that usage of neural networks can successfully classify the samples of the given training set.

1 INTRODUCTION

When a new mechanical part is designed, it has to be tested for durability in different usage conditions (‘stress evaluation’). In order to save on time and expenses, the model is usually checked analytically before real test samples are produced. However, automated simulations sometimes deliver results that require expert knowledge for interpretation. Currently, experts validate if the results are reliable and detect the nonreliable ones (fig. 1, a). This is a time-consuming and prone to errors process.

In case of finite element simulations (Reddy, 2009), nonreliable results (“failures”) can arise from, for example:

- Overlapping components in the imported CAD file,
- Contact of different (rigid) components or
- Equal treatment of tensile and compressive stress.

In order to reduce the manual checking efforts and also to avoid checking mistakes, training of machine learning models that allow automatic pre-sorting is proposed within the scope of this research study (fig. 1, b).

The challenge of this classification task is that the simulation results are given as unstructured 3D point clouds, so common frameworks for processing regular data, e.g. for image recognition, cannot be applied directly. That is why different problem specific approaches have to be studied.

The research question considered in the paper is if the classification of reliability (automated validation) of the 3D finite element simulation results can be done using AI and which AI approaches can provide for acceptable results.

The paper compares three approaches to solve the

The paper is structured as follows. The next section defines the problem at hand. It is followed by the state of the art review. Sections 4-6 represent the AI training and classification results for the above mentioned techniques. The results are compared and discussed in section 7. The conclusions summarize the findings and outline the future research directions.

2 PROBLEM DEFINITION

The source data for the classification problem is stored in VTU mesh files (Kitware Inc., 2005) with different number of points per inch depending on the curvature of a particular fragment of the model (less points on smooth surfaces and more points for curves). An average number of vertices in a model is around 5000 but it differs significantly from model to model. Due to symmetry, models are given as 1/4 part or 1/2 part of a component. If the components had no symmetry properties, the model would have represented the whole part.

The locations of the vertices of a sample are set before the simulation is conducted. The output of the simulation are so-called safety factor values for each vertex. This safety factor (SF) value is defined as the relationship between an allowable mechanical load and a given mechanical load. That means, the higher the SF, the more stable the simulated component is. That is why the SF is used as a metric to decide if a component fulfills the mechanical requirements of the development process. Therefore, the minimal SF value has to lie above a certain threshold. Validation of the reliability of this minimal SF is the problem at hand. In order to automate it, within the scope of this research work machine learning models have been developed to validate if this minimum is reliable or not. The reliability check is then applied iteratively: If the global minimum is not reliable, the second lowest local minimum is validated and so on until a reliable minimum is found. This SF minimum has to lie above the threshold to be mechanically stable. Otherwise, the construction needs to be re-engineered.

In the dataset of this research study, the label refers to the global minimum, so only the global minimum is classified. Since the global minimum is the easiest to find and the patterns for classification are the same for other local minima, this study is focused on the classification of the global minimum.

The test set consisting of 814 simulation results was manually classified by an expert based on the evaluation of the reliability of the global minimum so that 304 samples were considered as reliable (“reliable samples”), and 510 samples as nonreliable (“nonreliable samples”). The nonreliable samples are split into 3 types of failures (failure modes): 142, 115, and 253 samples respectively. However, in the presented research only two labels are
used: reliable and unreliable. Classification of samples into failure modes is still the subject of future research.

3 STATE-OF-THE-ART REVIEW

The considered task is rather unique, and no “of the box” solutions or methods have been found. As a result, the paper presents approaches for classifying models of 3D objects. One can read on advances in 3D object classification in (Ahmed et al., 2018; Ioannidou et al., 2017). Based on these, all approaches to 3D object classification can be split into the following groups:

- Architectures exploiting descriptors extracted from 3D data,
- Architectures exploiting RGB data,
- Architectures exploiting 3D data directly.

The first group of approaches is not directly related to 3D object classification but follows the generic approach of feature selection and application of various models to the features and their combinations (L. Ma et al., 2018; Wahl et al., 2003). These models are less computationally expensive and are preferable for tasks where they can be applied successfully. However, they often cannot work well for distinguishing between some complex shapes.

The second group of approaches is based on application of various techniques to generating 2D images out of 3D objects and their further classification. These approaches can also be split into two groups: (i) analysing various views, projections, and cuts, and (ii) analysing images with depth information. The advantage of these approaches is the possibility to use well-studied 2D classification techniques without the need to develop a new 3D model. However, extensive application of such techniques caused appearance of specialized multi-view models (Su et al., 2015; Yavartanoo et al., 2019; Zhou et al., 2020). The cut-based approaches are most often used in medical domain since many medical data, for example, tomography results, were originally represented as cuts (Deng et al., 2018; Lu et al., 2018; Z. Ma et al., 2018), however they are applied in other domains as well (Qiao et al., 2018).

Analysing images with depth information (often referred as RGB-D) is a very popular group of approaches. They also had the advantage of applying state-of-the-art 2D classification techniques to classifying 3D objects but developed into a separate group classification models (Feng et al., 2016; Schwarz et al., 2015).

Direct analysis of 3D data can also be approached from different perspectives. Classification of meshes (Hanocka et al., 2019) and irregular point clouds (Charles et al., 2017; Y. Wang et al., 2019) are characterized by speed and absence of the need of computation-intensive pre-processing since usually engineering and design data (e.g., CAD models) are stored in this form. Approaches based on analysis of regular point clouds (voxel-based models) provide better results “out-of-the-box”, for the price of additional data pre-processing (Maturana & Scherer, 2015).

In the presented research one approach from each group was tested: classification based on geometrical feature engineering, 2D convolutional neural network (Resnet18) for depth images, and 3D convolutional neural network VoxNet. A number of models for irregular point clouds have also been tested, but so far their result were much worse than those presented so they are not considered in the paper.

4 CLASSIFICATION BASED ON GEOMETRIC FEATURES

4.1 Approach Description

The first approach is to build a classification model that relies on geometrical feature engineering. As the definition of the error modes is connected to some geometric properties of the SF minimum point and its neighbourhood, a set of features was proposed describing the geometry of the neighbourhood of the SF minimum. In particular, the features describe the complexity of the SF minimum neighbourhood, including two interpretations of mesh complexity:

1. Structural complexity, related to the number of nodes and faces in the mesh.
2. Geometric complexity, describing how similar the surface is to a “simple” shape (e.g., plane).

Structural complexity is quite easy to formalize and evaluate. We created two groups of features: cells_no_X (number of mesh cells in the SF minimum neighbourhood of the given radius in millimetres) and points_no_X (number of mesh nodes in the SF minimum neighbourhood of the given radius in millimetres). The corresponding features are calculated by intersecting the input mesh with a sphere of the particular radius positioned to the SF minimum point and finding the properties of the resulting mesh.

It is not clear in advance what is the size of the SF neighbourhood that is the most informative to the reliability classification. In order to understand that,
each feature was generated w.r.t. different sizes of neighbourhood (sphere radiuses). For example, we created the features “number of nodes in 1 mm radius neighbourhood” (points no_1), as well as in 2 mm (points no_2), 3 mm (points no_3) radius neighbourhoods and so on. It applies to all the features (representing both structural and geometric complexity).

The notion of geometric complexity is not so straightforward to formalize. Therefore, several features were introduced.

The first is the volume of the minimal oriented bounding box of the neighbourhood of the specified size (obb_volume_X). The intuition behind this feature is that flat or slightly bent surfaces have a bounding box with zero or close to zero volume, while for curved surfaces the bounding box will be (almost) close to a cube having relatively large volume. Minimal oriented bounding boxes are estimated with a help of trimesh library (Dawson-Haggerty et al., n.d.).

The second group of features is generalized variance of face normals (in the neighbourhood of the specified size – gen_var_X), estimated according to the following formula:

\[ GV(X) = \frac{1}{|X|} \sum_{i=1}^{|X|} (X_i - \bar{X})^2, \]

where \( X \) – a set of vectors normal to mesh faces (each vector is 3-dimensional), and \( \bar{X} \) – is the mean normal.

The next group of features is the neighbourhood convexity, estimated using the tangent plane, containing the minimum SF point. In particular, there are two groups of features, calculated using this tangent plane. Features convexity1_X are defined as the mean value of the plane equation for the neighbourhood points, while convexity2_X features are defined as the logarithm of the ratio of the number of points in the positive subspace w.r.t. the tangent plane, to the number of points in the negative subspace.

The features of the next group are rooted in the notion of surface curvature. Specifically, we use the notion of discrete gaussian curvature measure as defined in (Cohen-Steiner & Morvan, 2003) and implemented in trimesh library. This gives two groups of features gauss_curv_X (the sum of the discrete gaussian curvature of the nodes in the specified neighbourhood) and gauss_curv_avgd_X (mean discrete gaussian curvature of the specified neighbourhood).

All the described groups of features characterize the SF minimum neighbourhood of the given size in millimetres. The last group of features describe the closest possible neighbourhood of the SF minimum node, given by the mesh structure – nodes reachable from the SF minimum by one and two ‘hops’. This gives features edgeness_min_1nbr, edgeness_max_1nbr, edgeness_min_2nbr, and edgeness_max_2nbr. In the name of these features min and max correspond to minimal and maximal values of the cosine of the angle between the normal of faces situated in the given neighbourhood, and 1nbr and 2nbr suffixes correspond to the neighbourhoods reachable in one and two hops from the minimum SF point respectively. The complete list of features is provided in the table 1.

### 4.2 Feature Importance Analysis

Feature importance analysis shows how informative each feature is in the process of classification. In this problem, the role of feature importance analysis is at least twofold:

1. The features are very similar, they all try to capture convexity in some sense. Which one is better?
2. What neighbourhood size is the most informative? This knowledge can help to keep the model small and thus to speed up the processing. Besides, understanding the size of the informative neighbourhood may help to select neighbourhoods used to train other ML methods.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Neighbourhood sizes, mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>cells_no_X</td>
<td>10, 8, 6, 5, 4, 3, 2, 1</td>
</tr>
<tr>
<td>points_no_X</td>
<td>10, 8, 6, 5, 4, 3, 2, 1</td>
</tr>
<tr>
<td>obb_volume_X</td>
<td>10, 8, 6, 5, 4, 3, 2, 1</td>
</tr>
<tr>
<td>gen_var_X</td>
<td>10, 8, 6, 5, 4, 3, 2, 1</td>
</tr>
<tr>
<td>convexity1_X</td>
<td>5, 4, 3, 2, 1</td>
</tr>
<tr>
<td>convexity2_X</td>
<td>5, 4, 3, 2, 1</td>
</tr>
<tr>
<td>gauss_curv_X</td>
<td>5, 4, 3, 2, 1</td>
</tr>
<tr>
<td>gauss_curv_avgd_X</td>
<td>5, 4, 3, 2, 1</td>
</tr>
<tr>
<td>edgeness_min_1nbr</td>
<td>-</td>
</tr>
<tr>
<td>edgeness_max_1nbr</td>
<td>-</td>
</tr>
<tr>
<td>edgeness_min_2nbr</td>
<td>-</td>
</tr>
<tr>
<td>edgeness_max_2nbr</td>
<td>-</td>
</tr>
</tbody>
</table>

To estimate feature importance we used null importance method (Altmann et al., 2010; Grellier, 2018) in conjunction with feature importance estimation procedures typical for the tree-based learning algorithms.

The idea is as follows. The machine learning algorithm leveraged for reliability classification is a decision tree-based gradient boosting implemented in CatBoost library (Yandex, 2020b). Decision tree-based learning algorithms have an internal ability to
estimate feature importance, i.e. the impurity measure (information or Gini) gain, which is obtained by the splits that use the particular feature (Y. Y. Wang & Li, 2008). Gradient boosting on decision trees implemented in CatBoost is not an exception, as it also estimates the importance of the input features by how on average the prediction changes if the feature value changes (Yandex, 2020a). However, feature importance estimation is not always indicative of the actual importance of the feature, especially in multidimensional spaces and in the presence of noise. The main problem is that it is usually not clear what level of impurity gain corresponds to some real patterns in the data, and what gain can be learned even from the noise.

The null importance method provides some kind of a ‘reference point’ in assessing the importance. The rationale behind the method is following. Let’s consider a slightly modified learning dataset, where feature \( f \) is replaced with its random permutation \( f^* \). A learning algorithm can be applied to the modified dataset and an importance of \( f^* \) can be estimated in a usual way. Further, as we repeat this process several times, for each feature we can build an importance distribution (null importance distribution). That distribution essentially provides the required ‘reference point’ – if sampling the importance of the feature \( f \) in its original ordering is likely to be sampled from this distribution then the feature is actually no more important than the random noise. On the other hand, if the importance of the feature in its original ordering is greater than the importance of most of the permutations of this feature, it actually carries some information about the target. This also gives a way to measure the importance, e.g., by considering the ratio of the importance of the original feature ordering to the 3rd quartile of the null importance distribution. Table 2 shows top 10 features estimated by the described procedure. It can be seen from the table that only 5 features have importance greater than the 3rd quartile of the null importance distribution. The most important features are various convexity indicators applied to the SF minimum neighbourhoods of the radius 3 mm and 4 mm. Smaller and larger neighbourhoods are not so important.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Importance</th>
</tr>
</thead>
<tbody>
<tr>
<td>convexity1 4</td>
<td>5.5</td>
</tr>
<tr>
<td>convexity1 3</td>
<td>4.6</td>
</tr>
<tr>
<td>convexity1 5</td>
<td>4.0</td>
</tr>
<tr>
<td>convexity2 4</td>
<td>3.8</td>
</tr>
<tr>
<td>convexity2 3</td>
<td>3.8</td>
</tr>
<tr>
<td>convexity2 5</td>
<td>2.2</td>
</tr>
<tr>
<td>oobb volume 2</td>
<td>1.8</td>
</tr>
<tr>
<td>gauss curv avgd 2</td>
<td>1.3</td>
</tr>
<tr>
<td>convexity2 2</td>
<td>0.97</td>
</tr>
<tr>
<td>convexity2 1</td>
<td>0.95</td>
</tr>
</tbody>
</table>

Table 2: Top 10 features according to the null importance method.

5 CNN-BASED CLASSIFICATION OF DEPTH IMAGES

The second approach is based on the representation of the 3D models as 2D depth images and further classification by a convolutional neural network. In certain sense this representation can be considered as surface model, where coordinates of an image point correspond to the coordinates of the surface point along two axes, and the depth colour can be considered as the coordinate along the third axis.

Generation of the depth images has been done via the following procedure. First, the fragment of a given diameter around the analysed point (the point with the minimal SF, fig. 2, a and b). Experiments were carried out with radiuses of 2, 3, and 4 mm, however for simplicity 3 mm radius is considered in the descriptions below.

Then, the fragment is rotated so that the normal of the analysed point would be oriented along axis Z (pointing to the viewer in fig. 2, c).

In the presented example, one can see that in some complex shapes, there can be fragments obstructing the analysed point, and, as a result, it is not possible to see the shape around it. For this purpose, a procedure has been developed for removing such obstructing fragments. It consists of two steps: (1) remove all points whose normals are oriented to opposite direction (cosine between the normals of analysed point and checked point is negative); (2) remove all fragments that are not connected to the fragment containing the analysed point. The resulting fragment is shown in fig. 2, d.

Finally, the depth map is built via measuring distances between the fragment and nodes of a 224x224 grid located on a flat surface, which is perpendicular to the normal of the analysed minimum and positioned 3 mm away from it (fig. 3). The closer points are lighter (the points located 0 mm away from the grid are white), and the further points are darker (the points located 6 mm away from the grid are black). The resulting image is shown in fig. 2, e.

Since CNNs are usually oriented to object recognition, they do not work very well with colour shades, but with borders. For this reason, the contrast
of the generated images was increased. However, it was done in such a way that the analysed point always coloured as 127 (“located” 3 mm away from the grid). At the same time closer and further parts are “zoomed” proportionally to the closest and furthers points (fig. 4). We understand that the procedure of increasing contrast produces a risk of losing information about curvature, however, this was not a case for the considered training set.

Resnet18 was chosen as a classification model. Resnet18 is a 18 layers deep residual CNN for image classification (He et al., 2016). Experimentation showed that usage of pre-trained network did not give any advantage during training, so the network with randomly initialised weights was used. The following training parameters were applied for training:

- Additional linear layer was added with sigmoid output at the network output for binary classification;
- Error function: cross entropy;
- Used augmentations (for training set only) are horizontal flip and 15 rotations by 22,5 degrees (31 augmentations for each sample);
- Learning rate 1.0e-6 (no learning rate degrading);
- Batch size: 32.

The network was implemented in TorchVision library (Facebook Inc., 2020) ver. 0.6.0. One training procedure (1 fold and 50 epochs) on the Intel Xeon server with Nvidia Geforce 2080 RTX GPU took about 35 minutes. The training results are presented in fig. 5-7.

For the comparison with other techniques, the following numbers of epochs have been chosen for each of the radius that let one to avoid overfitting: 2 mm – 20 epochs (no more significant improvement), 3 mm – 14 epochs (further training causes overfitting), and 4 mm – 8 epochs (further training causes overfitting).

One can see that classification of samples with the radius of 2 mm produces the best results, however, there is a concern that in the future analysing such small fragments of the parts can produce false results. On the other side, fragments with the radius of 4 mm are not classified well and the model becomes overfitted already after 10 epochs, with the loss function values being higher than those for smaller fragments. As a result, for future research the classification of fragments with radiuses of 2 and 3 mm were selected.

### 6 3D CNN-BASED CLASSIFICATION OF VOXELIZED MODELS

The third implemented model is an adaptation of a 3D CNN to the reliability classification problem. The
Figure 5: Training results of Resnet18-based depth image classification of 2 mm radius fragments.

Figure 6: Training results of Resnet18-based depth image classification of 3 mm radius fragments.

The rationale is that two-dimensional representation (even with the depth map) misses some details of the part (e.g., it cannot distinguish between solid and hollow parts), and 3D model makes the difference between the inside and outside of the part more obvious. It is self-evident, that 3D representation contains much more detail about an object. The reason why neural networks for processing 3D data receive relatively less attention is that in most cases there are just no accurate 3D data. For example, in object detection problem, 3D representation typically should be constructed from 2D data or LiDAR data and this reconstruction is a problem itself. However, in the area of manufacturing (CAD/CAM systems) precise 3D models are available, which makes 3D neural networks (and 3D CNN, in particular) a reasonable choice. We have adapted VoxNet architecture described in (Maturana & Scherer, 2015). Original VoxNet is designed for object recognition problem and has softmax output layer (with the number of output units equal to the number of classes of objects). As reliability classification is binary classification problem, we changed the softmax output layer to a dense layer consisting of one unit with sigmoid activation function. We used the same input size as the original model: 32x32x32 (fig. 8). Overall, the
Figure 7: Training results of Resnet18-based depth image classification of 4 mm radius fragments.

Figure 8: Example of a voxelized neighbourhood of a SF minimum.

adapted VoxNet implementation has the following structure:

1. 3D convolution layer with filter size 5, strides 2, normal padding and Leaky ReLU activation function with alpha 0.1.
2. 3D convolution layer with filter size 3, strides 1, normal padding and Leaky ReLU activation function with alpha 0.1.
3. 3D max pooling layer with pool size 2 and strides 2.
4. Reshape to flat vector (of size 6*6*6*32).
5. Dense layer with 128 units and ReLU activation.
6. Dense output unit with sigmoid activation.

The network is trained with the Adam algorithm for minimization of binary cross-entropy as a loss function.

The data preparation procedure is the following. The part model is rotated to align the direction of the normal at the point of the examined SF minimum with Z axis. Then, the neighbourhood of the examined SF minimum node is transformed into a voxel model 32x32x32 so that the minimum SF point corresponds to the centre of the cube (voxel with coordinates [17; 17; 17]). The size of each voxel is 0.1 mm$^3$, therefore, a whole voxelized neighbourhood has dimensions 3.2x3.2x3.2 mm. An example of a pre-processed network input is shown in fig. 8. While the position of the normal at SF minimum is determined by the pre-processing step, the part may still be rotated around Z axis resulting in different models and potentially different results. To achieve the invariance to this rotations, we used an augmentation scheme, according during the training voxelization of 16 rotations of each model around Z axis were considered, and for each rotation, also one flipping. Therefore, each SF minimum point results in 32 training samples.

7 EVALUATION AND COMPARISON

The dataset contains 814 mesh models (samples) with SF assigned to each vertex of the mesh. Sample label in the dataset is determined by the expert classification of the node with the lowest SF (global minimum) reliability. The dataset contains 304 samples with reliable global minimum and 510 samples with non-reliable global minimum.
To evaluate the classification algorithms, the k-fold cross-validation procedure has been carried out. In accordance with this procedure, the data set is divided into k subsets of approximately equal size, and k experiments are performed so that each of the k subsets is used once as the test set and the other k-1 subsets are put together to form the train set. In our case the dataset has been split into 5 folds (k=5). The resulting train and test sets are presented in Table 3. During splitting the dataset, the following consideration was taken into account. Not all models of the dataset correspond to different components but to result of a different simulations, i.e. a different mechanical load case. As a result, some samples may correspond to the same component but have different SF values and different vertices with minimal SFs. This fact was taken into account during splitting. It turned out that different simulations of the same part tend to place minimum SF to similar locations of the part. Therefore, to prevent overfitting to a particular part, the folds were created in such a way, that the same part does not present both in the train and test sets (sometimes, this is referred to as “group K-fold validation”; in this case, the group is interpreted as simulation results of one component).

The described above algorithms have been evaluated on the same set of folds. They include (1) CatBoost with all features, (2) CatBoost with top 10 features, (3-5) Resnet18 for neighborhoods with radiuses of 2 mm, 3 mm, and 4 mm, and (6) VoxNet. We have also added the logistic regression as a base classification model for the comparison.

To evaluate the algorithms two types of criteria were considered: performance, measured by training and prediction times; and prediction quality, measured by accuracy. However, it turned out that the accuracy values were quite high, so the absolute number of misclassified samples was also considered (it does not provide additional information compared to the accuracy, but slightly easier to read and interpret). The results of the evaluation are shown in Table 4.

It can be seen, that all the models achieve quite good results in terms of accuracy. Logistic regression has a significant advantage in training time over the other models, but has the lowest accuracy. Taking into account, that training is not so frequent operation in the intended use cases of the model, and training times of deep learning models are also reasonable, this advantage is not very important. None of the explored feature-based models were able to achieve perfect classification, which is most likely related to the fact that proposed features didn’t describe significant aspects of the SF minimum neighbourhood necessary for such classification. Among the deep learning-based models, 3D CNN

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**Table 3: Distribution of samples for folds used in the experiment.**

<table>
<thead>
<tr>
<th>Fold</th>
<th>“Reliable” samples</th>
<th>“Unreliable” samples</th>
<th>Total</th>
<th>“Reliable” samples</th>
<th>“Unreliable” samples</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>258</td>
<td>391</td>
<td>649</td>
<td>46</td>
<td>119</td>
<td>165</td>
</tr>
<tr>
<td>2</td>
<td>212</td>
<td>437</td>
<td>649</td>
<td>92</td>
<td>73</td>
<td>165</td>
</tr>
<tr>
<td>3</td>
<td>246</td>
<td>405</td>
<td>651</td>
<td>58</td>
<td>105</td>
<td>163</td>
</tr>
<tr>
<td>4</td>
<td>252</td>
<td>401</td>
<td>653</td>
<td>52</td>
<td>109</td>
<td>161</td>
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<tr>
<td>5</td>
<td>248</td>
<td>406</td>
<td>654</td>
<td>56</td>
<td>104</td>
<td>160</td>
</tr>
</tbody>
</table>

**Table 4: Comparison of approaches to Validating Results of 3D Finite Element Simulation.**

<table>
<thead>
<tr>
<th>Classification approach</th>
<th>Errors on fold Mean training time, s</th>
<th>Mean prediction time, s</th>
<th>Mean accuracy</th>
<th>Mean # of errors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Logistic regression</td>
<td>2 1 0 0 10 0.017</td>
<td>0.006</td>
<td>0.984</td>
<td>2.6</td>
</tr>
<tr>
<td>CatBoost (10 features)</td>
<td>0 4 0 0 158.0 0.008</td>
<td>0.993</td>
<td>1.2</td>
<td></td>
</tr>
<tr>
<td>Resnet18 (radius 2)</td>
<td>0 0 0 0 800 (GPU, 20 epochs) 0.036</td>
<td>(no GPU) 1 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Resnet18 (radius 3)</td>
<td>0 0 0 0 560 (GPU, 14 epochs) 0.036</td>
<td>(no GPU) 1 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Resnet18 (radius 4)</td>
<td>0 0 0 0 320 (GPU, 8 epochs) 0.036</td>
<td>(no GPU) 1 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VoxNet</td>
<td>0 0 0 0 9.6 (GPU, 3 epochs) 0.161</td>
<td>1 0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
VoxNet can be considered the best, as it achieves perfect classification of the provided dataset and has significantly lower training time than other models. It supports the initial intuition that 3D CNN should be a reasonable choice as they fully exploit the 3D structure of analysed components.

Based on the results, it was decided that further research should focus on the ResNet18 models for the radius of 2 and 3 mm and the VoxNet model.

8 CONCLUSIONS

The paper is aimed at application of AI techniques to reliability evaluation of 3D simulation results produced via 3D finite element simulation. It was found that such classification is possible by various 3D model classification techniques, and some of them produce perfectly accurate results.

Among the machine learning approach, relying on geometrical features, 2D depth image classification via ResNet18, and VoxNet-based classification of voxelized models, the latter two were selected for further analysis.

Future research is planned to be aimed for two major aspects. First, currently only global SF minima were classified, whereas in reality, local minima need to be classified as well.

Second, absolute sizes of components (and component fragments) were used for classification. However, there can be components with significantly different sizes and the appropriate sample radius may differ from the findings in this paper. Approaches to either scale models or choose the fragments according to the number of included vertices need to be studied, which might be more generic for varying component sizes.

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