SimuStruct: Simulated Structural Plate with Holes Dataset with Machine Learning Applications

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Abstract

This paper introduces SimuStruct: Simulated Structural Parts Dataset, a dataset that contains 2D structural parts, their respective meshes and the outputs of numerical simulations for different properties for linear and elastic material, boundary and loading conditions, and for varying levels of refinement. SimuStruct comprises the classic case of plates with holes since it is a 2D simple case with analytical resolution and which is found in different mechanical design applications. The SimuStruct dataset comprises many different cases, where each case is solved using standard Finite Element Method (FEM) with the open-source package FEniCS. Compared to other datasets similar in purpose, SimuStruct is more diversified and realistic because it aims to comprises diverse real cases for different loading and boundary conditions, different properties for linear and elastic material, and different levels of mesh refinement. In addition, SimuStruct is more flexible, versatile, and scalable because all algorithms and codes are implemented using open-source libraries. The main goal of the SimuStruct dataset is to serve both as training and evaluation data for Machine Learning (ML)-based methods in structural analysis and optimal mesh generation and therefore support the development of ML-based optimal mechanical design solutions. An application of SimuStruct is presented to train and test an Multilayer perceptron (MLP) model to predict stress-strain fields. SimuStruct will contribute to the connection of the Mechanical Engineering and ML communities, which will allow accelerating and exploitation the research in the computational design field.

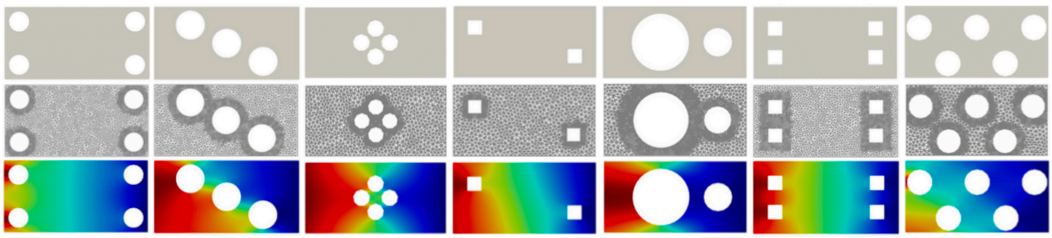

Figure 1: SimuStruct: A dataset that contains the CAD model, the meshes and the structural simulations (FEM) for different levels of mesh refinement, different properties for linear and elastic material, and for different boundary and loading conditions.

1 Introduction

Recent advances in computational tools have shown the potential of automatic generative design techniques and for surrogate modeling both for the development of single mechanical parts, such as wheels Yoo et al. (2021) and seat brackets Alderton (2018), as well as for complete mechanical systems, such as airplane cabin components Airbus (2016) and car chassis Alderton (2016). The two key components of this automatic design process are a simulator of the mechanical properties of the object being designed and an optimization module that

automatically searches the space of design parameters to find the configuration that optimizes certain design restrictions, such as stress and displacement restrictions and, stiffness, mass and manufacturing constrains, among others. Traditionally, numerical simulation has been performed using FEM, which despite being arbitrarily accurate in simulating the mechanical properties of the mechanical components, are usually computationally-intensive and slow to too allow for fast iterations over optimization cycles, rendering generative design of realistic mechanical system virtually impossible.

In order to alleviate this restriction, several disruptive methods based on Machine Learning (ML) have been proposed. The general strategy is to train a model capable of quickly predicting, to a given degree of approximation, the relevant mechanical response of the system under design and use that prediction to guide the exploration in the design space. For example, the Oden Institute has recently used ML techniques with the physical knowledge of a system in Computational Fluid Dynamics (CFD) to increase the speed of simulations related to the design of spaceships, allowing them to run in just a few seconds instead of 200 hours Swischuk et al. (2020).

Haghighat, et al, Haghighat et al. (2021), used Physics Informed Neural Networks (PINNs) in an elastic plane-strain linear elasticity problem on the unit side length square subjected to uniaxial stress and in nonlinear problems, namely a perforated strip subjected to uniaxial extension, to predict the stress-strain fields and to identify the Lamé parameters of the material. In Chen & Ahmed, Nobari et al. (2021b), Nobari et al. (2021a) and Heyrani Nobari et al. (2021) they developed variants of the Generative Adversarial Network (GAN) to generate high-quality, creative and performant designs of new bicycle and airplane designs.

However, there are several challenges when using ML approaches for substituting traditional methods in the computation of simulations. Firstly, ML models are often specialized in solving only one type of case (e.g., wheels) and it is not obvious how to train a model to operate on more than one family of mechanical cases. Secondly, it is not trivial to perform a fair comparison between all the various ML approaches proposed so far due to the lack of a standard set of cases against with which we can evaluate all the models.

This work introduces the Simulated Structural Parts Dataset (SimuStruct), a dataset of 2D structural parts containing numerical solutions (displacement, stress and strain fields) to plates with holes case studies, to help overcome the previous limitations, see Figure 1. SimuStruct is composed by many geometric cases of the plate with holes, different loading conditions, diverse types of boundary conditions, and different properties for linear and elastic material. Combining them, a significant library enabling fast analyses of multiple problems and optimization procedures in mechanical design tasks. This dataset is obtained through standard FEM, using scripting for automation the model generation. In this procedure, FEniCS, Alnæs et al. (2015) is adopted, since it is an open-source library for FEM analysis. The scripting also considered different levels of mesh refinement, aiming to evaluate the mesh influence in the outputs. SimuStruct aims to serve both as training and evaluation data for ML-based methods for computing stress-strain fields and optimal mesh definition, and therefore support the development of ML-based optimal mechanical design solutions. In addition, the dataset is intended to be used in academia and industry, contributing to the connection of the Mechanical Engineering and ML community, which will accelerate the research in computational mechanical design.

The main purpose to create SimuStruct, with many instances, is due to the simplicity of this 2D problem. In addition, it is a classic case of mechanical engineering, which can be found in various applications, such as the construction of buildings, in the aeronautical industry, and the field of biomechanics, in prostheses, among many other applications. This set of applications makes the problem interesting, enabling the development of new approaches for mechanical systems design.

A comprehensive description of the requirements for the Simustruct dataset and the previous work can be found in Appendix A.1.

2 SimuStruct

2.1 Plate with Holes

The first works on stress concentration dates back to 1898 Kirsch (1898), where Kirsch found the solution for the stress distribution for an infinite thin plate with central holes subjected to uniaxial tension. Since then, many studies have been done in this field for different types of holes and plates, materials, and loading conditions. A review of the literature on stress concentration issues can be found in Jafari & Ardalani (2016).

Thin plates are used in several industries, such as automotive, aerospace, and maritime. Its wide applicability makes the plates present geometric discontinuities, such as holes, with different sizes and shapes. These discontinuities allow, for example, to reduce the structure's total weight, establish joints (as bolted and/or riveted) and to allow access to other parts of the structure. Some applications of plates with holes are: holes in aircraft doors and windows Lopes et al. (2020); Ukadgaonker et al. (2000); fuselage panel joining points by rivets Zhou & Fei (2017); Bedair & Eastaugh (2007) and bolts Može (2018); Wang et al. (2017); holes that allow the flow of cooling fluids in the turbine blades Dong et al. (2017); Liu et al. (2011); and plate for humerus fracture Kim et al. (2021); Zhang et al. (2016).

In each application, the plates are subject to certain types of conditions, such as normal, bending, torsion, and shear loads. When the plate with holes is being loaded, the stress at the points around the hole are high due to holes in the plate, leading to stress concentration points in these regions. Thus, it is essential to carry out a stress distribution around the holes to achieve a good SD.

2.2 Comparison to Other Datasets

Much of the research studies in the field of structural analysis has been carried out using structural simulation datasets. Two examples of these datasets discussed earlier are simJEB and Mechanical MNIST. Both datasets are useful for structural analysis of geometries, with simJEB using 3D geometries (jet engine brackets) and Mechanical MNIST using 2D geometries. In both cases, the geometries are not generated by themselves, not having significant control over their construction. On the other hand, SimuStruct contains several parametric geometries, previously created by us, with total control over them (this makes this dataset expandable and upgradable). The code was integrally developed for the dataset generation, comprising the geometry definition. It is advantageous since it allows a quicker construction of other datasets for other classic types of mechanics problems. In addition, SimuStruct has shapes with more realistic relevance than handwritten digits (Mechanical MNIST) and is generic, not presenting geometry of a single component (simJEB). Simulations in Mechanical MNIST are performed using open-source software, FEniCS, while in simJEB using commercial software, Altair, making the structural analysis a semi-automated process. SimuStruct follows the Mechanical MNIST methodology, using FEniCS, making the simulation process more flexible, meeting the advantages highlighted in Ribeiro et al. (2021).

Regarding the loading cases, simJEB contains only four cases, application of a vertical force, horizontal force, diagonal force and torsional moment. Mechanical MNIST also studies only four cases, uniaxial extension, shear, equibiaxial extension and confined compression. SimuStruct presents a meaningful improvement since it performs the different simulations for a set of loading cases, making a total of 25 cases.

About mesh generation, simJEB did not perform a study of the mesh refinement, having performed an automated meshing. In contrast, Mechanical MNIST studied the mesh refinement but only performed the simulation for the optimal mesh. In SimuStruct we carried out an intensive study on the refinement of the mesh, where for each model, six types of refinement were performed. This feature of SimuStruct has great potential since it allows to carry out studies: runtime vs. accuracy.

Furthermore, Mechanical MNIST only outputs displacements and simJEB displays displacements and Von Mises stress. SimuStruct displays displacements, stress components, strain

components, Von Mises stress, mesh topology and geometry as outputs. It should be noted that the mesh topology means the id of the nodes that make up each element, and the mesh geometry refers to the coordinates of each of the mesh nodes. In addition, SimuStruct does not use just one material, using several materials. These different materials are isotropic and have elastic linear behavior, varying their mechanical properties: Young's modulus and Poisson's ratio.

3 Methodology

Figure 2 describes all steps to generate and process the dataset.

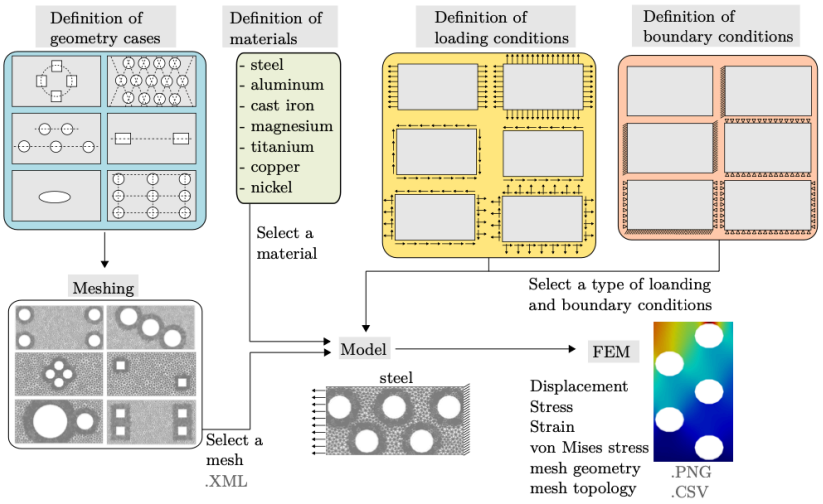

Figure 2: Dataset generation process.

A MLP-based application trained with a simulated structure dataset has been developed to predict the Von Mises stress. The detailed description and results of this application can be found in Appendix B.

4 Conclusion

SimuStruct is a 2D part dataset with numerical simulations for many boundary and loading conditions, different properties for linear and elastic material, and varying mesh refinement levels. SimuStruct contains the geometric model, the meshes for varying levels of refinement, and the structural simulations. SimuStruct includes the classic case: plate with holes. SimuStruct will provide training and evaluation data for ML-based methods, enabling optimal mechanical design solutions.

Considering the evolution of ML tools and possible applications in mechanical design, these datasets are a fundamental piece to develop design tools that can provide optimal solutions in near real time, enabling better and faster product development.

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A Appendix

A.1 Dataset Requirements

1. Different cases: Contain 2D cases for different materials and with different combinations of boundary and loading conditions.
2. Representative realistic cases: The cases and the respective parts should be realistic and representative of the case we are analyzing in the dataset.
3. Challenging cases: The cases should be challenging for FEM and to train ML methods on actually hard cases. The goal is not for ML to easily solve only straightforward cases, but rather to tackle complex cases that require a significant amount of computational power and time from FEM.
4. Different levels of refinement: Have a sufficient level of FEM detail (thin mesh) to serve as a trusted ground truth for ML method, but it should also be versatile, e.g. it should have FEM at different levels of detail, so we can train and evaluate models with different amounts of precision/data (ability to test different levels of detail).
5. Enough instances: It should have enough instances for both training and validation.
6. Easy to use: It should be easy to manipulate it with current 3D design/visualization tools and readable/processable by the popular ML frameworks.
7. Expandable and Upgradable: It should be possible to expand it by programmatically running a data generator efficiently, so we can keep adding more challenging cases as proposed ML approaches succeed.
8. Allow ML benchmarks: It should be a pre-defined set of data partitions (e.g. train vs evaluate) and define related standard metrics that become an evaluation standard for ML methods so that different approaches can be compared using this dataset.
9. Well documented and instructional: It should allow people with no background in structural engineering but with experience ML to understand the problem setting and the specific cases. Also, it should allow all with a background in structural engineering and very little experience in ML to give their first steps in ML.

A.2 Previous Work

In recent years, machine learning algorithms have revolutionized many areas of computer science. Regarding shape datasets, these algorithms have allowed, for example, geometry processing tasks, including classification, segmentation, surface normal estimation, automated meshing and cleaning, and shape retrieval. There are several 2D and 3D shapes datasets, which collect millions of Computer-Aided Design (CAD) models, like traceparts traceparts e Thangs thangs. All these data can be used in different fields of research and various applications, including: 3D printing applications, recognize, detect, reconstruct and classify objects, meshes applications, draw of objects and Structural analyses: simJEB Whalen et al. (2021) contains diverse, high-quality and application-focused designs of only one component (jet engine brackets) for advancing geometric deep learning, engineering surrogate modelling, automated cleaning and related geometry processing tasks. Mechanical MNIST Lejeune (2020), inspired by the MNIST dataset Lecun et al. (1998), contains finite element simulations, and it is essential to metamodeling heterogeneous materials undergoing large deformations.

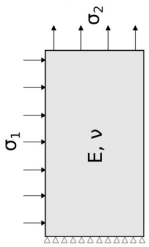
Most of the datasets presented have relevant features that allow them to be used in various computer vision applications. However, their applicability to mechanical design tasks is limited. Datasets that present models and meshes of the parts are attractive in terms of variety. Nevertheless, at least at this stage, it would be difficult to establish the connection between these complex parts and the loading and boundary conditions. There are relatively few datasets within the area of structural analysis, and they cMLPot be easily converted to serve our purposes. simJEB is focused on only one application (jet engine brackets), which gives it consistency. But, it is not easily scalable for other cases, serving only one niche of applications. Mechanical MNIST uses handwritten digits, which is advantageous since the

computer vision community often uses them. Nevertheless, it does not represent a real case of mechanical engineering. In the Subsection 2.2, we will further compare our dataset with simJEB and Mechanical MNIST, highlighting the need to create new datasets.

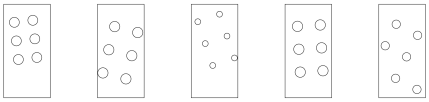
Only for 2D, linear regime and for some loading and boundary cases

B Application

The case study is a rectangular plate with six circular holes loaded biaxially, Figure 3. Thickness is much smaller than the other dimensions. Thus, a 2D analysis is performed, assuming a plane stress state case. The plate has a rectangular geometry with 250 x 500 mm. It is simply supported at the bottom and biaxially loaded on the left and top side, as shown in Figure 3a, with σ_1 and σ_2 equal to 200 and 100 MPa, respectively. The plate material is a S355 steel (European standard EN 10025-2), with a Young's Modulus (E) of 210 GPa and a Poisson's ratio (ν) of 0.3, presenting an elastic linear behavior.



(a) Loading and boundary conditions



(b) Plates with six holes

Figure 3: Definition of the case study.

Our goal is to predict the von Mises stress field through ML model. A pointwise model was chosen, predicting the stress for a given point in the plate domain. The von Mises stress field is obtained through a set of predictions at the points that define the domain of the plate with holes.

In the problem under study (plates with holes), the boundary and loading conditions, the behavior and the material proprieties are the same for the different geometric cases. In this way, only the geometry change will affect the stress field. Regarding to geometry, the rectangular plate maintains its dimensions, only the position and diameter of the circular holes modifies. Note that the number of holes is fixed.

Taking into account the chosen model and the problem under study, the model inputs will be the Cartesian coordinates of the point where we intend to predict the von Mises stress and the geometric properties of the circular holes of the plate. Each hole is defined by the Cartesian coordinates of the center and the radius value. The output will be the stress-strain for a given point and for a given geometry. Note that the coordinates of the point and the center of the hole will be defined by the coordinates x and y, since the problem under study is 2D.

B.1 Dataset

The dataset was generated through SimuStructPH, being constituted by 1005 geometric cases.

The dataset is divided into training and test data. Subsequently, the training dataset will be divided into training and validation datasets. The division is performed through the

construction of a graph, grouping similar geometric cases into clusters. The metric used to evaluate the similarity of the geometric cases is the mean of the Symmetric Mean Absolute Percentage Error (SMAPE) of the moments of inertia x and y and the centroid. Taking into account the clusters, the dataset is divided, never using the same cluster for training and test data.

In this way, it is guaranteed that the training and test data are significantly different, allowing to test the ability of the model to generalize to unseen cases. The same would not happen if we had chosen to perform a random division of the geometric cases that make up the dataset. More information about the process used to split the dataset can be found in Appendix ??.

The dataset division of the geometric cases for the training, test and validation data was 407, 37 and 77, respectively.

B.2 Model

The MLP model is sequential and pointwise, predicting the von Mises stress for a given point in the domain and for a given geometric configuration. The inputs are an array of shape [1 x 2] defining the 2D Cartesian coordinates of the point that is intended to predict the stress and another of shape [6 x 3], characterizing, for six circular holes, the coordinates 2D Cartesian's of the centers of the holes and their radius.

The points where the predictions will be made coincide with the nodes of the meshes that were used to obtain the stress-strain fields in SimuStruct through the FEniCS software. Another option would be to use a regular mesh of points for all geometric cases. The advantage is that we would have a fixed number of points regardless of geometry, being able to make predictions simultaneously for this set of points.

However, the regions around the hole present stress concentrations and it is advantageous to have more points in this region. In this way, it is impossible to use the regular mesh, making it impossible to predict simultaneously for all points in the domain.

A study of hyperparameters was performed via Weights Biases Biewald (2020). The hypermarameters under study are the number of neurons and the number of hidden layers, through a list of number of neurons in the hidden layers. The following combinations were studied:

- combination A: 2048, 1024, 512, 256, 128, 64, 32, 16
- combination B: 1024, 512, 256, 128, 64, 32, 16
- combination C: 512, 256, 128, 64, 32, 16
- combination D: 256, 256, 256, 256, 256, 256, 256, 256
- combination E: 512, 512, 512, 512, 512, 512, 512, 512, 512, 512, 512
- combination F: 2048, 2048, 1024, 512, 512, 128, 64, 64, 32, 16, 16

The study of hyperparameters indicated that the combination E should be chosen, thus the model used in MLP for the plate with six holes had 11 layers hidden with 512 neurons each.

Table 1 shows the best model. In all layers, with the exception of the last one that presents a linear function, the activation function is ReLU. The optimizer chosen is Adam. The evaluation metrics are the Mean Absolute Error (MAE) and the Mean Square Error (MSE). MSE was the chosen loss function.

B.3 Train and Evaluation

For the study of the hyperparameters, a maximum value of 300 epochs is defined, with a batch size of 5000.

Figure 4 show the learning and validation curves for the MLP models. For all combinations, the learning and validation loss curves decreases as the number of epochs increase. The

Table 1: ML Model.

Type	MLP - 6 holes
Input layer	2
Input layer	18
Concatenate	None, 20
Dense	None, 512
Dense	None, 512
Dense	None, 512
Dense	None, 512
Dense	None, 512
Dense	None, 512
Dense	None, 512
Dense	None, 512
Dense	None, 512
Dense	None, 512
Dense	None, 512
Output layer	None, 1

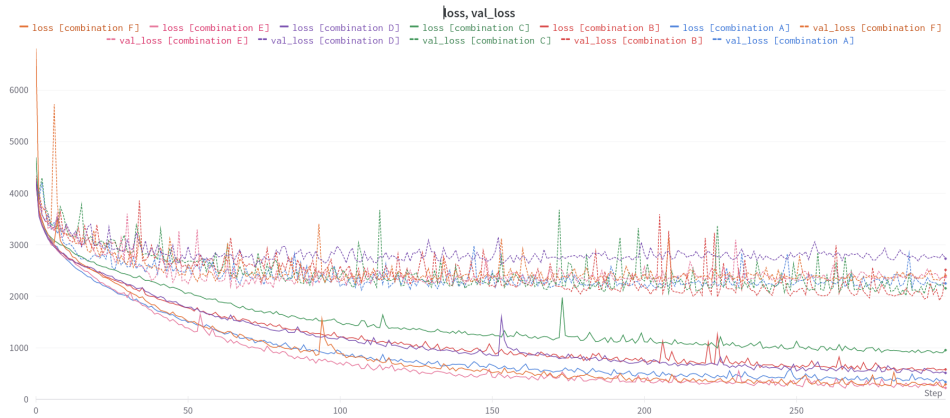


Figure 4: Learning and validation curves for all combinations.

combination E model for hidden layers has the lowest loss, as can be seen in the figure. Therefore, this was the structure chosen for the model. The same model was later trained for a 400 epochs, see Figure 5. The loss obtained was 147.

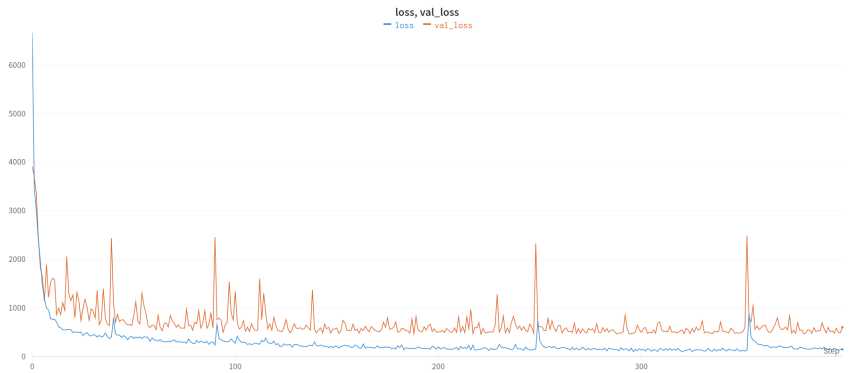


Figure 5: Learning and validation curves for MLP for combination E.

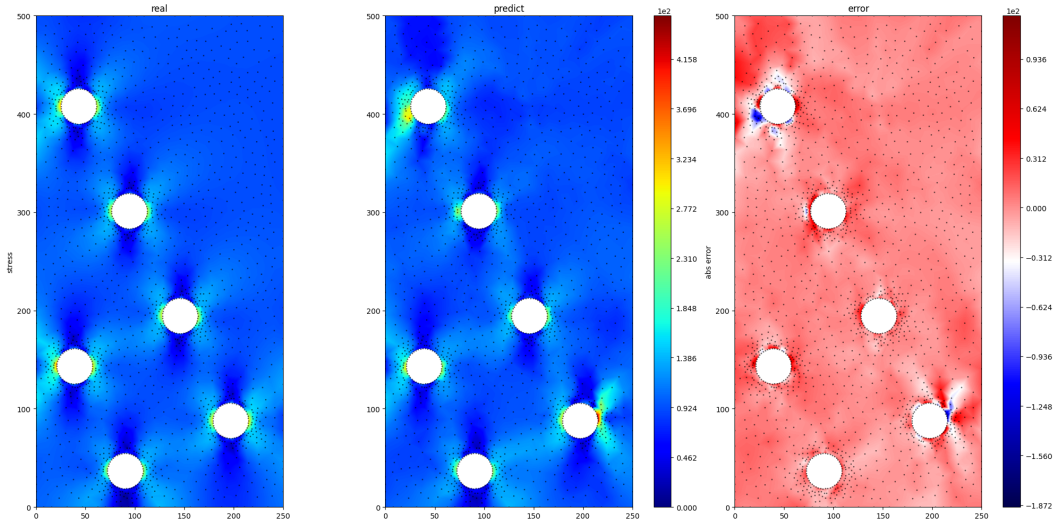


Figure 6: von Mises stress field obtained by MLP with comparison to FEM through absolute error - 1st case of the plate with hole.

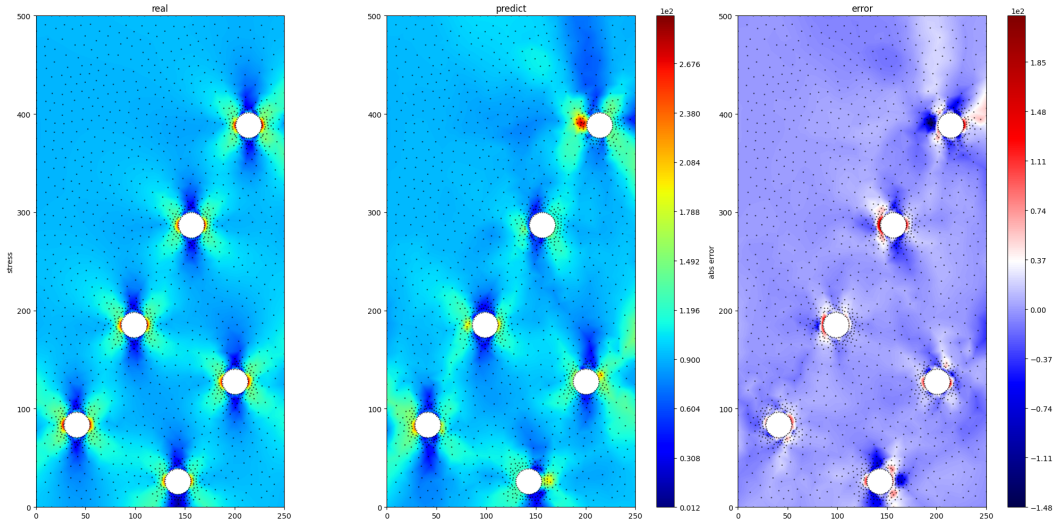


Figure 7: von Mises stress field obtained by MLP with comparison to FEM through absolute error - 2nd case of the plate with six holes.

B.4 Results and Discussion

Figures 6, 7, and 8 present three cases for the plate with six holes, where the results obtained by MLP are presented and compared with the results obtained by FEM (data from SimustrucPH). This comparison is performed using the absolute error.

In addition to the visual comparison, the MSE and MAE were measured for all points on the plate and for points located in the region around the holes. This region contains all points located at a distance equal to or less than 1.5 the hole radius. The Table 2 shows the values of MSE and MAE for all points on the plate and for points located in the regions around the holes.

As can be seen, the MSE and MAE metrics are higher for all cases in the regions around the hole, since in these regions there are stress concentration factors. This concentration of stresses makes the MLP model more difficult to predict the stresses at these points. Despite

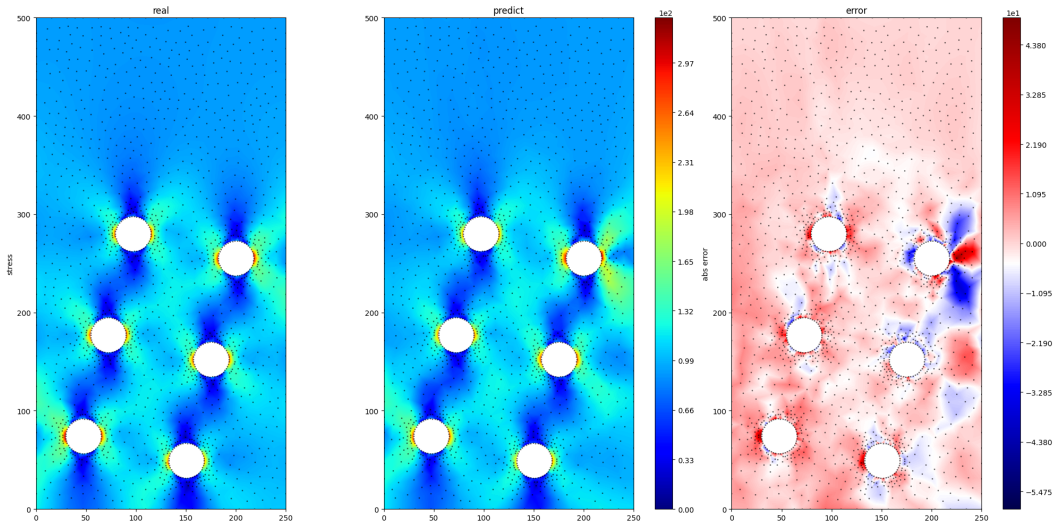


Figure 8: von Mises stress field obtained by MLP with comparison to FEM through absolute error - 3rd case of the plate with six holes.

Table 2: MSE and MAE values for all points on the plate and for points located in the regions around the holes for the three case under analysis.

Case	MSE	MSE around holes	MAE	MAE around holes
1	461.734	1198.252	12.131	23.424
2	1010.649	3008.656	17.418	39.939
3	81.036	182.823	5.586	9.966

this, the metrics present good results, even when compared to the metrics obtained for the entire plate.

The Table 3 shows the average values of MSE and MAE for all points on the plate and for points located in the regions around the holes for the 37 test cases.

Table 3: Average MSE and MAE values for all points on the plate and for points located in the regions around the holes for the 37 test cases.

MSE	MSE around holes	MAE	MAE around holes
1060.113	2800.215	15.853	33.402