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Summary of Dissertation thesis

**Hybrid Modeling of Mechanical Digital Twin  
by Finite Element Method and Graph Neural  
Networks**

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# Abstract

This dissertation proposes a hybrid modelling approach for the design of a digital twin of a mechanical structure. The concept integrates the connection of the finite element method and the graph neural network. The advantages of the physical-based method of accurately simulating complex physical and structural behaviour are extended by the possibility of effective data acquisition and, thus, expand the compact understanding of the given mechanical structure. The work aims to answer whether regressors based on graph neural networks can effectively build a digital twin. Studies supporting this methodology are presented in this work to suggest a perspective on how challenges relate to establishing digital twins. Designed experiments on the training of a regressor and its validation are addressed to ensure the accuracy and generality of the hybrid model as a whole mechano-digital framework.

# Abstrakt

Tato disertační práce navrhuje hybridní modelovací přístup pro návrh digitálního dvojčete mechanické struktury. Koncepte integruje propojení metody konečných prvků s grafovou neuronovou sítí. Výhody první metody přesně simulovat složité fyzikální strukturální chování je rozšířeno o možnost efektivní datové akvizice, která rozšiřuje kompaktní porozumění o dané mechanické struktuře. Hlavním cílem práce je odpovědět na otázku, zdali regresor grafových neuronových sítí může být efektivním nástrojem pro stavbu digitálního dvojčete. Studie podporující tuto metodologii jsou představeny v této práci a slouží tak k navrhnutí pohledu, jak mohou být řešeny výzvy související s vytvořením digitálního dvojčete. Dále je pomocí navržených experimentů ověřena možnost trénování a validace regresoru tak, aby byla zajištěna přesnost a obecnost hybridního modelu jakožto celku mechanicko-digitální struktury.



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# List of abbreviations

DT	Digital Twin
HM	Hybrid model
PM	Physical-based model
DD	Data-driven model
GNN	Graph Neural Network
DTHMFG	Digital Twin Model by Finite Element and Graph methods
FEM	Finite element model
$\Gamma$	Geometry Physical Based Model
$\Omega$	Solid Physical Based Model
$\mathcal{E}$	Material elasticity parameter of PM
$\nu$	Material Poisson's constant of material PM
$e$	a finite element of certain typography
$n$	node of a finite element / a graph
$\sigma_n$	Maximal Principal stress at dedicated node
$\delta$	simulation step for calculation PM
$\mathcal{D}$	Dataset generated via FE
$\mathcal{G}$	Graph
$\mathcal{G}'$	Reduced Graph
$v$	vertice (edges) of a graph
$A$	Adjacency matrix of a graph
$D$	Degree matrix of a graph
$L$	Laplacian matrix of a graph
$\mathcal{D}$	Dataset to train a regressor
LR	Multi-input-output linear regressor framework
FN	Regressor based on multi-layer neural feed-forward neural network
GCN	Regressor defined by multiple graph convolutional operational neural neural network
SAGE	Regressor based on SAGE aggregation layers for graph neural neural network
$\mathcal{L}$	loss function for regressor training



# 1 Introduction

## 1.1 What Digital Twin might be

There are various perceptions of what a digital twin (DT) is. The DT concept can be defined as an adaptive model of a physical asset. A digital representation of behaving like the original system can be built with various mathematical modelling techniques. The benefits of state-of-the-art technologies additionally alter this. Multi-physical-based solvers, cybernetics of big data, artificial intelligence, and augmented and virtual reality are well-known technologies today. However, the mutual collaboration of tools within the architecture of DT is not yet evident in many fields.

The subject of DT is relatively new in comparison to other simulation methods; the number of articles already published is thousands per year (2020, 2023).

The DT might be defined as another milestone in the evolution of simulations in the physical world, where it is expected to be in combination with current technologies. The milestone is well surveyed at [3] and is expected to be a successor of the Product Life-cycle Management (PLM) tool, which can be understood as an approach to managing databases of specific mathematical models of a product.

## 1.2 Hybrid modelling

The hybrid modelling technique (HM) can be understood as a union of Physical-Based (PM) and Data-Driven (DD) modelling (there can also be a perception of modelling between multiple mathematical approaches). Furthermore, this approach might be understood as a fundamental pillar for building a DT of a specific system, for instance, mimicking structural mechanic behaviour.

The basic proposition of the argument for the feasible adaptation of the HM technique to build a DT is the expectation that the following method can enhance a primary driving modelling approach describing observed specific complex structures.

### 1.3 Challenges in Building Regressor to derive DT

Constructing a DT architecture to mimic mechanical structures can be perceived as a regression task. This endeavour involves bridging methods from FEMs through graph theory to graph neural networks (GNN), presenting unique challenges and opportunities.

One of the fundamental challenges lies in effectively integrating concepts from FEMs, graph theory, and GNNs. While FEMs provide a robust framework for modelling mechanical structures, graph theory offers insights into structural relationships, and GNNs provide powerful tools for learning from graph-structured data. However, bridging these three domains requires carefully considering their strengths and limitations.

The challenge of extracting high-value knowledge from a FEM and incorporating it into a graph structure remains uncommon, with no existing dataset available to further elaborate on such a methodology. This underscores the need to explore alternative approaches beyond GNNs and consider the integration of other multi-input-output regressors. This premise opens avenues for innovative capabilities of DT architectures for mimicking mechanical structures.

The designed regressor must be thoroughly validated to ensure the accurate mimicking of the structure. This leads to the question of which diagnostic tools are most suitable for this purpose. Addressing this query can establish a comprehensive evaluation process, ensuring the efficacy and reliability of the DT architecture in replicating mechanical structures with precision.

## 2 The state of the art

### 2.1 Digital Twin of Mechanical Structural System

The most likely pioneering publication [1] mentioning the DT concept yet again only as a sub-group of Product Lifecycle management (PLM) also suggests further definitions of individual components be aggregated in a DT model. Although the article absorbs the DT concept as a batch of PLM approach, the primary definition of designing via available and compiled information characteristic for the specific system has already been pinpointed.

A more comprehensive overview of DT-connected aspects is provided in the following article [2]. The complete definition describes the whole concept to apply a whole DT concept as a valuable tool for making the right decisions throughout various parties in an organisation using specific DT. Discussed and highlighted are fields that have already started using the approach to some extent, for instance, in industry, healthcare, meteorology, and even education with individualised and adaptive student plans.

Additionally, in this article, DT is understood as an adaptive model, surprisingly enhanced as a metamodel of complex physical systems within a specific organisation and labelled as a state-of-the-art asset. Interestingly, a brief introduction of one possible view of assessing DT as a component of Industry 4.0 is made with pipelines to connect technologies such as the Internet of Things to create advanced applications. The suggested method of DT usage could be easily applied since multi-functional sensors are already available and are expected to be even more affordable due to the effect of technology on demand. This sharp image also leads to the involvement of other technologies, starting with Tensor Processing Units (TPU) used widely in machine learning applications, or even further is counted with Quantum Processing Units (QPU), where the price of those technologies are also expected to decrease due to the Moor law. The mentioned units have a primary high potential to make the required calculation needed for DT imitation of a physical asset, even faster, faster and the response of a model should be immediately available, for example, if connected with a 5G telecommunication network.

### 2.2 Possible approaches to Twinning

The first best application to start with is a project named "The Living Heart" [9] from Dassault, which shows how DT could be helpful in healthcare. Application is not necessarily aiming at building explicitly the DT model of the human heart, but the approach of usage is intuitively well suited to be an example of how a FEM as DT can be a helpful tool to make a goal-oriented decision in succeeding with planning and then executing procedure of cardiostimulator implantation for an individual patient. Another example can be the calibration of a model ventricle to describe correctly the parameters of a new material imitating biological tissue of the heart [4]. Company Rolls Royce is usually identified as a pioneer in bringing DT application to the real world with their product of jet engines used in planes [5]. Tool "intelligent engine" is probably the first industry application used to predict engine conditions. The state of an engine is in real-time and The further application can be found in, for instance, at industry [7] or in material development[6],[8].

#### 2.2.1 Hybrid modelling

On the other hand, it focuses more on delivering digital assets as replicas of their mechanical images. This is well introduced by [11], which might be understood as an established milestone for the field of "Physical Machine Learning Modelling" where the usually undividable aspect to deliver such solution lays at mesh basis from physical model [12], understood as a mathematical tool to solve Partial differential equations describing certain physical phenomena.

**Physical Based Modelling** The PPoisson'sproblem can examine one of the examples for the Physical-Based model (PM) of mechanical structure. Additionally, the problem might usually be set with fixed boundary conditions  $U$  and specific solid geometry  $\Gamma$ , which may have the material parameters consist of YYoungs'modulus  $E$  and PoPoisson'sonstant  $\nu$ . The structure of  $\Gamma$  is subject to a concentrated load  $F$  on the opposite side to boundary conditions, together as the entire condition  $\Phi(U, F)$ . The well-known equations [10] to depict a governing of small elastic deformations of an  $\Omega$  geometrical structure can be written as:

$$\begin{aligned} -\nabla \cdot \sigma &= F \in \Omega, & \sigma &= \lambda \text{tr}(\varepsilon) I + 2\mu\varepsilon \\ \varepsilon &= \frac{1}{2} (\nabla u + (\nabla u)^T) \end{aligned} \tag{2.1}$$



Where  $\sigma$  is the stress tensor,  $f$  is the body force per unit volume,  $\lambda$  and  $\mu$  are the elasticity parameters of the material in  $\Omega$ ,  $I$  is the identity tensor,  $tr$  is the trace operator of a tensor,  $\epsilon$  is the symmetric unitary strain tensor (symmetric gradient), and  $u$  (or enhanced  $u(x, y)$ ) is the displacement vector field. In this problem, isotropic elastic conditions are assumed.

The variational formulation of 2.1 consists of taking the inner product of 2.1 and a test vector function  $v$  belonging to  $\hat{V}$ , where  $\hat{V}$  is a vector-valued test function space. Then, integrating over the domain  $\Omega$  the following equation is obtained:

$$-\int_{\Omega} (\nabla \cdot \sigma) \cdot v \, dx = \int_{\Omega} f \cdot v \, dx \quad (2.2)$$

With all the necessary information and after a few more steps (comprehensively described in the thesis), the stress tensor requirements for the structure can be calculated. For instance Von Mises stress as:

$$\sigma = \sqrt{\frac{3}{2} s : s}, \text{ where } s \text{ is deviatoric tensor} \quad (2.3)$$

$$s = \sigma - \frac{1}{3} tr(\sigma) I$$

**Data-Driven Modelling** In data-driven (DD) modelling, the tasks are typically supervised learning characters, with several essential steps encompassing data collection, preparation, model selection, training, testing, and validation. These crucial stages necessitate meticulous attention to factors such as data quality, model complexity, and suitable evaluation metrics to guarantee accuracy and reliability. Furthermore, applying various techniques, such as Reinforcement Learning, can significantly enhance these processes, exemplified by their utilization in swiftly optimizing structural design, as highlighted in article [36]. Approaches to creating a DD model are limited only by a practitioner's mind, and the first look at those keywords in a scientific database supports this statement as far from false. Thesis condensate routes lead to graph neural network utilization, where the initial sources are for their comprehensive overview supported by [14].

## 2.3 Graphs & Graph Neural Networks

**Graph** theory might be for someone's exciting branch of mathematics that studies how to apply graphs to various problems in many different fields, including mathematics, computer science, physics, chemistry, and economics. In the field, a graph  $\mathcal{G}$  is a collection of objects (called vertices or nodes) con-

nected by lines (called edges). Hence, at first glance, a FEM has a structure similar to graphs; it is crucial to introduce this theory of graphs, for instance, by [20; 19] As The graph is at least minimum consisting of source and target nodes  $N$  connected by edges  $V$  (at pure graph theory used nodes  $U$  and vertices  $V$  notatin, to make synergy between domains, the notation is therefore slightly modified), where each node connects only one, the proper way to extract a suitable graph  $\mathcal{G}$

$$\mathcal{G} = (N, V) \tag{2.4}$$

**Graph Neural Networks** A Graph Neural Network (GNN) architecture is one of the latest types of neural networks that is representative of the DD modelling technique. Interestingly, GNN might be understood as a more corresponding architecture similar to the biological brain. The view stems from the lay notion that the brain does not have an input and output layer of neurons, as with feed-forward neural networks [21], but has regions that are variously activated at any given time [22]. Specifically, specific clusters of neurons are activated by different stimuli. Another comparison is made with Feed-Forward Neural Network (FFNN), where the biological brain is not made up of neat layers of neurons but is more like a graph arrangement, where specific neurons are connected to neighbouring ones. The initial real-world example of analogical implementation could not be better studied than [13; 17; 16]. Overall comparisons and an overview of various techniques are provided with [15].

### 2.3.1 Message Passing

Message passing [23] is a fundamental concept in GNN [22] and propagates information between nodes in a graph. In message passing, each node sends a message to its neighbouring nodes, which then update their states based on the received messages. This process is typically repeated multiple times, allowing information to propagate throughout the graph.

The initial model, to begin with, is an analogy of linear regression adapted to multi-input-output tasks,

$$\hat{y} = \mathbf{W}\mathbf{X} + \mathbf{b} \tag{2.5}$$

where  $\hat{y}$  is the predicted target vector of dataset nodes,  $\mathbf{W}$  is matrix of weights, input features from dataset  $\mathbf{X}$  and bias vector  $\mathbf{b}$ .

What distinguishes the forward pass equation from the abovementioned multi-linear regression is that Neural Networks apply non-linear activation functions [21]. For the first hidden layer ( $i = 0$ ), the equation can be rewritten as follows:

$$H_1 = \sigma(\mathbf{W}_0^T \mathbf{X} + \mathbf{b}_0), \quad (2.6)$$

the chosen activation function for the further experiment is Rectified linear unit  $\sigma = \max(0, X)$  or others (sigmoid, tangent hyperbolic). Message passing is demonstrated as well for gated version [24] or even for quantum computation [25].

### 2.3.2 Graph Convolutional Layer

[27] The following graph network architecture comprises a graph convolutional layer (GCN). The graph convolutional neural network [27] can be understood as the enhancement of the Feed Forward Neural Network (FFNN) with classical notation [21] and so by the graph-structured data described, taking into account the adjacency matrix  $A$ . The forward pass for the first hidden layer is then

$$H_1 = \hat{\mathbf{D}}^{-1/2} \cdot \hat{A} \cdot \hat{\mathbf{D}}^{-1/2} \cdot \mathbf{X} \cdot \mathbf{W}_0 + \mathbf{b}_0, \quad (2.7)$$

where  $\hat{A} = A + I$  adjacency matrix with self loop and  $\hat{D}$  is its degree matrix [26; 27].

### 2.3.3 Graph Sample and Aggregated Embeddings Layer

The second approach we used is built on Sample and Aggregated Embeddings (SAGE). It is a neural network layer designed to aggregate information from neighbouring nodes in a graph structure [28]. By incorporating Sage layers, the promising target lies in capturing complex relationships and dependencies between nodes in the graph representation of the mechanical structure, providing a flexible and practical approach to graph modelling. In SAGE layers, the node embeddings of neighbouring nodes are computed and aggregated to generate a new node embedding. This aggregated embedding is then used to update the embedding of the target node, and the process is repeated until all nodes in the graph have been updated. As a type of GNN layer, SAGE layers aggregate information from a node's neighbourhood to

generate a node representation. The forward pass is expressed as

$$H_1 = [AGG(\mathbf{X}) || \mathbf{X}] \mathbf{W}_0 + \mathbf{b}_0, \quad (2.8)$$

where  $AGG$  is a function aggregating neighbourhood nodes with a certain aggregation method (for instance: sum, mean, min, max) [29].

### 2.4 Problem statement

The central hypothesis of this dissertation thesis is to answer whether GNN can be applied as an effective DT modelling technique to store and evaluate information from the PM description of a mechanical system. The main goal is to achieve a similarity of experimental data of a structural mechanic system such that the resulting interpretability for the user will be similar to that of an extracted FEM.

It is also assumed that a GNN is a suitable architecture compared to classical deep-learning neural networks. The assumption is based on fact; GNN can use the information of nodes and the relationships between them using a 3D model initialized and essential in FEM.

The mechanical stress results of the loaded system in FEM are suitable for creating a dataset for training GNN, which will be faster for load classification as a result of specific nodes of the mechanical system.

## 3 Thesis objectives

For the dissertation, it is proposed to investigate and clarify the following issues to develop a methodology applicable to establishing a digital twin of a mechanical system by combining various modelling techniques.

1. How to design a methodology for predicting a particular mechanical system for authentic and accurate operation and overall establish a Digital Twin architecture of a mechanical system with the combination of techniques FEM and GNN?
2. How to extract information from an FE model representing a mechanical system and compile it so that the graphs required to train a particular regressor are properly defined?
3. How to train regressors optimally so that they can be used to perform regression tasks on nodes of graphs reflecting a physical-based model, and What FEM data will be chosen to build the training dataset?
4. How can the overall DT model be diagnosed to avoid false system predictions based on a GNN regressor so that DT mimics data that will potentially be taken from sensors in the regular operation of the physical asset?

# 4 Developed methodology

## 4.1 Method Description

The thesis proposes a novel approach by integrating graph theory into FEM, utilizing graphs extracted from FEMs as dynamic structural blueprints and a foundation for training GNNs. This approach combines white box modelling with machine learning and has succeeded in various domains, such as medical imaging and physics-performed machine learning.

At the core of our methodology is the integration of GNNs, transcending traditional simulation boundaries by learning intricate relationships embedded in structural graphs and predicting behaviours beyond conventional modelling.

Further, the synergy between graph reduction and GNNs is pivotal in achieving an accurate DT. By distilling complex structural representations into reduced graphs, we empower neural networks to predict with unprecedented accuracy, optimize computational efficiency, and establish a robust framework for real-time predictive modelling.

To summarize the proposed methodology as shown Fig. 4.1 can be:

1. Identify physical phenomena to model and monitor in real product
2. Define geometrical model  $\Gamma$  to required spatial precision
3. Creation of FEM  $\Omega$  based on requirements of the first and second step
4. Extract calculated physical attributes  $\mathcal{D}$  of converged model
5. Train and Validate Graph Regressor  $f(\mathcal{G})$
6. Replacement of FEM by DT based on Regressor of GNN
7. Optimize graph by reduction of DT complexity

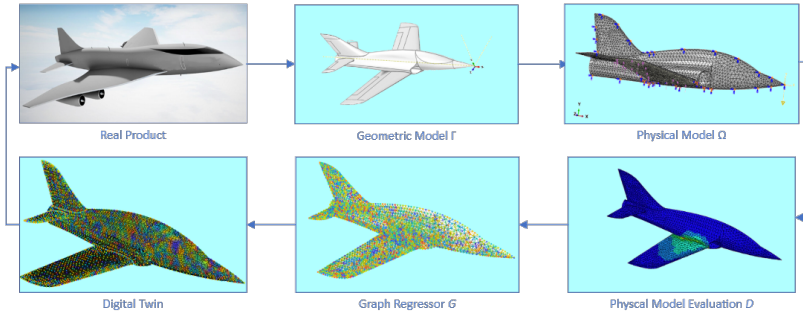


Figure 4.1: DT of mechanical structure lifecycle

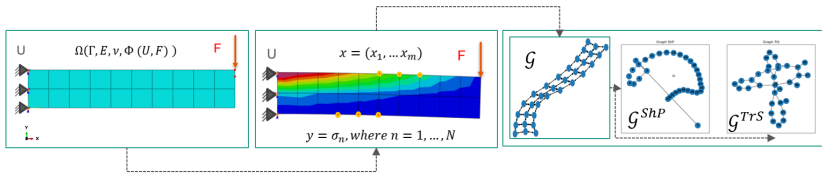


Figure 4.2: Process of DT creation from FEM to Graph representation with further graph reduction process; from left: mechanical model, FEM, fully connected graph, reduced graph (shortest path), reduced graph (closed path)

## 4.2 Data Acquisition from Physical Based Model

Accurately distilling information from simulations of PMs presented, particularly those established via the FE, is of utmost importance. These models are invaluable tools for understanding complex phenomena, predicting outcomes, and making informed decisions. However, their reliability hinges on a rigorous validation process. This involves subjecting the model to knowledgeable critical inspection by experts in the respective field and supporting it with real-world laboratory experiments. By adhering to this validation framework, we can ensure that the distilled knowledge from the model aligns with empirical evidence, enhancing its accuracy, robustness, and overall credibility. This, in turn, empowers us to unravel the intricacies of the natural world, optimize designs, mitigate risks, and ultimately make well-informed decisions for a better future. This is visualized by simple Fig. 4.2.

### 4.2.1 Extraction of data from FE simulations

Once the FEM is established, its geometric and domain description is documented through a computational environment, which defines the spatial configuration of each node  $n_i$  within a particular element  $e_i$ , as well as the mutual connectivity between the elements. The graph model  $\mathcal{G}$  can be obtained as follows:

$$f : \Omega(\Gamma(e, n), E, \nu, F) \rightarrow \mathcal{G}_{FEM}(N, V, \mathbf{X}(\mathbf{F}), \mathbf{y}(\sigma)) \quad (4.1)$$

All nodes and edges in the resulting graph adhere to the logic of the original FEM. The nodes acquire data from the converged FEM, with input parameters  $X$  capturing reaction forces  $F_i$  of the selected nodes  $n_i \in \mathcal{S}$  simulating distributed sensors  $\mathcal{S}$ . The target output  $\mathbf{y}$  represents structural mechanical stress for all nodes  $\sigma$ . This approach was introduced at [37].

### 4.3 The Graph Finite Dataset (GF dataset)

For further exploration on methodology, the GF dataset: Mesh-Based Graphs Dataset for a DT of a Mechanical Systems [34], was established as a collection of subsets data  $\mathcal{D}_{IDS}$  generated from PMs created as FE structural mechanics simulation Fig. 4.3. Each sub-dataset is distinguished with an identifier. Sub-Dataset  $IDS \in \{b2, b3, fs, pl\}$ . Those models have characteristically precise geometry (mesh without exception) with specific boundary conditions to clarify while exploring feasible strategies to build a DD model.

- $\mathcal{D}_{b2}$  ... Beam2D: Encastred and loaded 2D beam.
- $\mathcal{D}_{b3}$  ... Beam3D: analogy of Beam2D at 3D.
- $\mathcal{D}_{fs}$  ... Fibonacci's Spring: analogy of 3D beam with slightly complicated geometry.
- $\mathcal{D}_{pl}$  ... Plane: Symmetrically cut geometry of RC plane loaded with pressure on the wing.



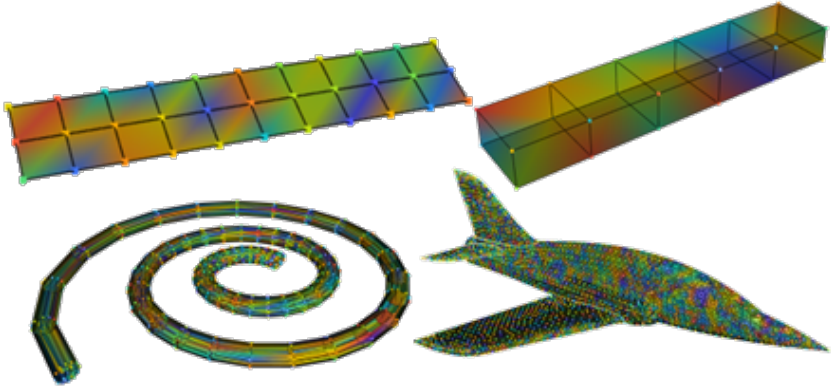


Figure 4.3: GFdataset: Visualized each FE model from  $\mathcal{D}$  introduced at [34] by its graph with randomly specified weights of nodes. From top left: Beam2D, Beam3D, Fibonacci spiral, Airplane

## 4.4 Experiments for Training of Regressor

The GF dataset is thoroughly described above and is also extracted in a manner that can be used for training specific DD models. The following techniques suitable for the nodes regression tasks are listed due to their potential to contribute sufficiently to the distillation of a well-performing representation. Visually, all the frameworks are analogies of architecture based on Fig. 4.4.

- Multilinear regression model (MLR) is selected from the pure interest in how can be the overall task handled with slight naiveness. Multiple input and output functions of the selected input nodes for the sub-dataset will be evaluated.
- Designed Multi-layer FFNN architecture (FN) is in the next step selected to have intermediate insight into the performance of the neural network model applied to this specific task.  
Framework: 2 layers with ReLu units with 150 hidden nodes, one final linear unit
- And the final approach dedicated to GNN with frameworks usually lately applied across the projects are Framework one: 2 layers with Sage

convolutional layer and one final linear unit.

Framework one: 2 layers with graph convolution layer one final linear unit.

Multiple (10 per framework and sub-dataset) experiments were set to get a more accurate estimate of the performance of the chosen model's framework. The main intention was to reduce the influence of any randomness or variance in the data and allow a better understanding of the true performance of a single model.

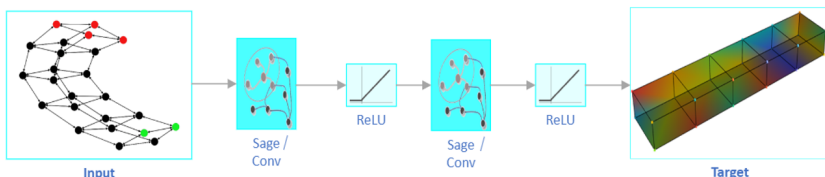


Figure 4.4: Representative examples of the frameworks used at benchmarking experiment

### 4.5 Graph Reduction to Optimize Regressor

Once the Regressor is trained and fully diagnosed, an additional tuning step involves reducing the graph size [18], thereby reducing the time required for training [32]. The proposed research [35] harnesses graph theory utilizing graphs extracted for the following foundations of training GNNs. This approach combines white box modelling with machine learning, as demonstrated in various domains such as medical imaging and physics-performed machine learning [30]. However, the increasing scale and complexity of engineering projects pose challenges in computational intensity associated with detailed FEMs. Addressing this challenge, the research focuses on graph reduction to streamline computational complexity and lay the groundwork for efficient GNN training [31]. At the methodology's core lies the integration of Graph Neural Networks, transcending traditional simulation boundaries by learning intricate relationships embedded in structural graphs and predicting behaviours beyond conventional modelling. The synergy between graph reduction and GNNs is pivotal in achieving an accurate DT, empowering neural networks to predict with unprecedented accuracy, optimize computational efficiency, and establish a robust framework for real-time predictive

modelling.

## 4.6 Regressors Diagnostic

**Ground Truth** evaluation of DT is the paramount importance of visualization for operators utilizing the DT in decision-making. By enabling operators to visually observe the ground truth representation of the trained Regressor on the physical-based dataset, they can clearly understand the actual behaviour of the simulated structure. This visual insight becomes crucial for informed decision-making processes, as operators can confidently rely on accurate visualization to make critical assessments and take appropriate actions.

**Quantile-quantile plot** When developing a DT based on GNN, one of the crucial factors to consider is the validation of the regressors. Validation techniques such as quantile-quantile plots can be employed as possible policies or strategies to assess the performance and accuracy of the regressors. In the results

**Heteroskedacity and Homoskedacity** is one of the critical assumptions under which the Ordinary Least Squares gives an unbiased estimator, and the Gauss–Markov Theorem applies. To interpret heteroskedasticity [33] can be used as a scatter plot of the residuals against the predicted values or the independent variable(s). Suppose the scatter plot shows a funnel shape, with the spread of the residuals increasing or decreasing as the predicted values or independent variable(s) increase. In that case, heteroskedasticity is likely present.

**accuracy and training history** Visualizing the training plot to observe the loss metric as a representative value of accuracy and convergence on the validation set is a standard evaluation practice. However, it is essential in this context since the experimental frameworks are specifically designed for the thesis, and the behaviour is unknown beforehand. Monitoring the loss value throughout learning epochs is necessary to obtain fruitful insights into the overall concept proposed by this thesis.

# 5 Results

The aim of Chapter 4 was to introduce the design strategy for evaluating a particular DT with identified metrics. Those compiled suggestions on evaluation tools and metrics are fruitful for initiating the proper deployment of a DT.

To obtain a more accurate estimate of the performance of the chosen model's framework, multiple experiments were conducted, with ten experiments per framework and sub-dataset as mentioned in section 4.4. This approach aimed to reduce the influence of randomness or variance in the data and provide a clearer understanding of the faithful performance of each model.

Box plots were utilized as a valuable visualization tool to compare the models' performance across these multiple experiments. By examining the distribution of the Mean Squared Error (MSE) metric, which provides insights into the spread of model predictions on the validation set, the box plots depicted the performance variations among the different sub-datasets.

## 5.1 Models Ranking

Multiple experiments were conducted, with 10 experiments per framework and sub-dataset, to obtain a more accurate estimate of the chosen model's framework's performance. This approach aimed to reduce the influence of randomness or variance in the data and provide a clearer understanding of each individual model's true performance.

Box plots 5.1 were utilized as a valuable visualization tool to compare the performance of the models across these multiple experiments. By examining the distribution of the Root Max Squared Error (RMAXMSE) metric, which provides insights into the spread of model predictions on the validation set, the box plots clearly depicted the performance variations among the different sub-datasets.

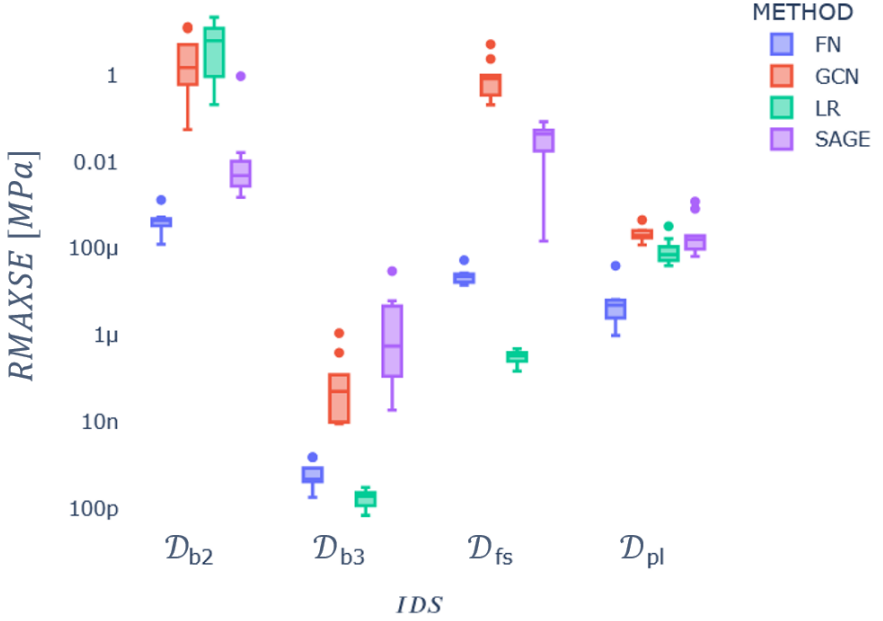


Figure 5.1: GF benchmarking: Boxplots to depict Comparison of particular regressor framework to distinguish on performance via the metric of loss function  $\mathcal{L}_{RMAXSE}$

Table 5.1: Mean square error of validation sets

Methods	$\mathcal{D}_{b2}$	$\mathcal{D}_{b3}$	$\mathcal{D}_{fs}$	$\mathcal{D}_{pl}$
MLR	$8E+0 \pm 8E+0$	$2E-10 \pm 8E-11$	$3E-7 \pm 1E-7$	$1E-4 \pm 9E-5$
FFNN	$5E-4 \pm 3E-4$	$7E-10 \pm 5E-10$	$2E-5 \pm 1E-5$	$8E-6 \pm 1E-5$
GCN	$4E+0 \pm 5E+0$	$2E-7 \pm 3E-7$	$1E+0 \pm 2E+0$	$2E-4 \pm 1E-4$
SAGE	$1E-1 \pm 3E-1$	$5E-6 \pm 9E-6$	$4E-2 \pm 3E-2$	$3E-4 \pm 4E-4$

### 5.2 Ground Truth Validation

In DT models, the validation of ground truth stands as a cornerstone, accentuating the pivotal role of visualization for operators. A profound understanding of the simulated structure's actual behaviour is achieved by providing operators with a lucid visual representation of the trained regressor's performance on physical-based datasets.

This visual clarity becomes indispensable in decision-making, as operators can confidently rely on precise visualization to make critical assessments and execute appropriate actions. Accurate visualization serves as a beacon, illuminating the path to informed decision-making and amplifying the efficacy of DT implementations in sophisticated decision-support systems.

## 5.2 Ground Truth Validation

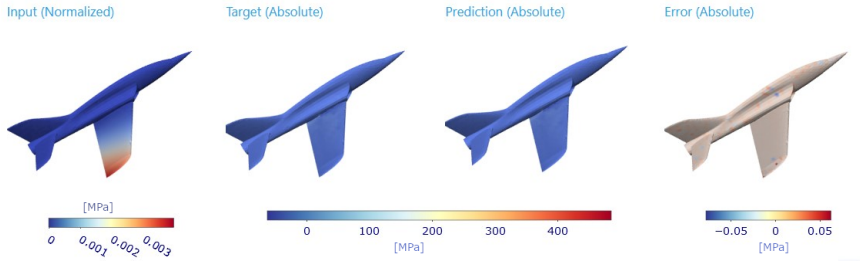


Figure 5.2: Ground Truth Visualization of Plane dataset for specific Input Force applied on wing accompanied with Target and Prediction. Last evaluated column (right) residues on the structure.

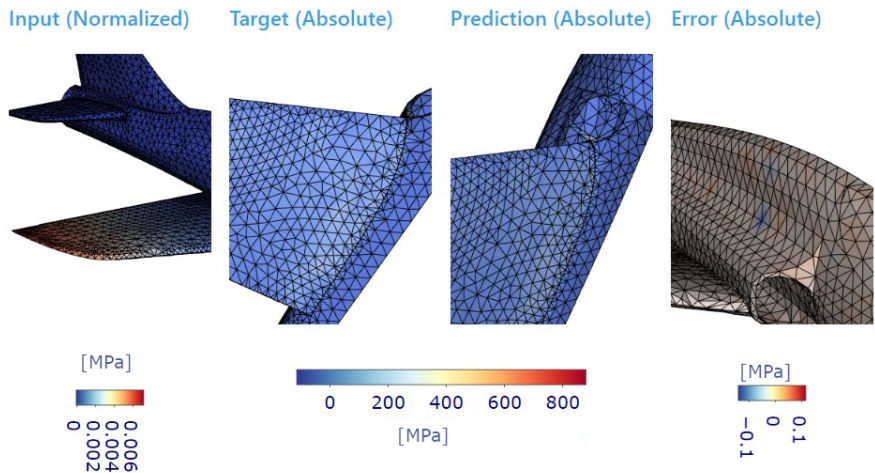


Figure 5.3: Detailed visualization of the plane dataset for specific input force applied to the wing is accompanied by target and prediction, where the primary detailed focus is at the bottom of the wing. Evaluated residues on the structure are visible as well.

### 5.3 Model Diagnostic via Heteroskedacity of Regressors

Heteroskedasticity [33] is a crucial diagnostic tool for validating a DT deviation from the assumption of constant variance in regression models and is pivotal for accurate model diagnostics. Detecting heteroskedasticity involves scatter plot analysis or formal tests like the Breusch-Pagan or White tests. Its presence can bias standard errors, affecting coefficient significance and reducing regression efficiency.

Addressing heteroskedasticity involves techniques like weighted least squares, robust standard errors, or generalized least squares regression, which adjusts standard errors for accurate estimates.

Nonlinear heteroskedasticity, indicated by a logarithmic shape in residuals against predicted values, poses challenges. Transformation techniques, such as logarithmic or variable transformations, may mitigate it. However, persisting nonlinear heteroskedasticity demands advanced techniques like generalized least squares regression.

In multi-input multi-output regression, nonlinear heteroskedasticity's interpretation varies. It could signify model misspecification, influential outliers, or unobserved variables. Addressing these complexities requires meticulous analysis and consideration of alternative models and techniques.



### 5.3 Model Diagnostic via Heteroskedacity of Regressors

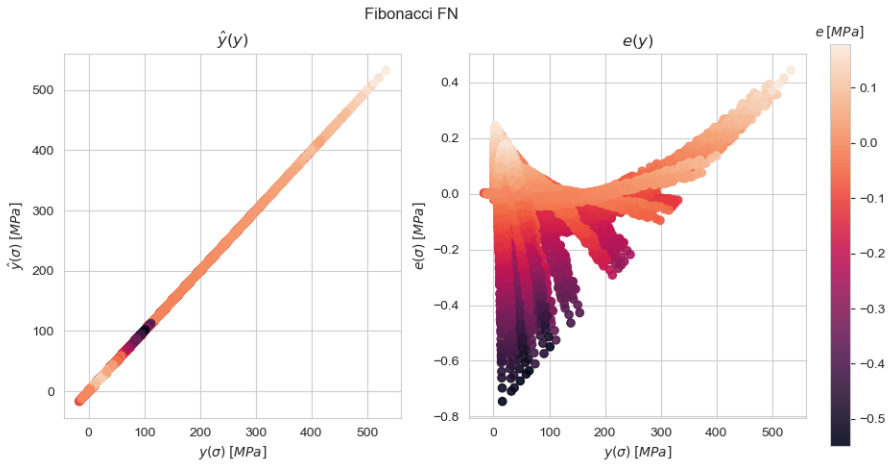


Figure 5.4: Model Diagnostic for DT regressor based on FFNN of Fibonacci spring shows via Quantile-quantile plot (left) required linear trend depicting. The right plot represents nonlinear heteroskedasticity.

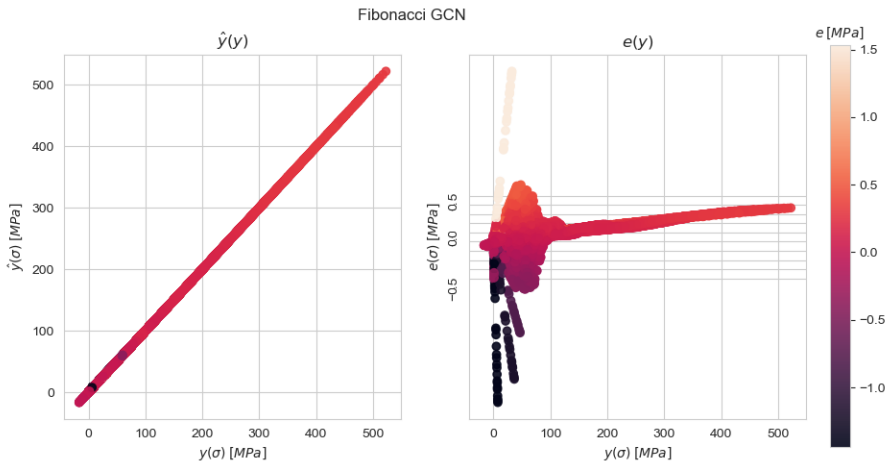


Figure 5.5: Model Diagnostic for DT regressor based on GCN of Fibonacci spring and depicting via Quantile-quantile plot (left) required linear trend. Right plot highlighting nonlinear heteroskedasticity for low values of mechanical stress  $\sigma$ , where for higher stresses homoskedasticity is present

### 5.4 Training Evaluation

The subsequent section is dedicated to the inspection of regressor training. The best model achieved throughout the training epochs is probed during this inspection. The experiment consists of ten training sessions, and by closely examining the performance and behaviour of the trained regressors, valuable insights can be obtained regarding their strengths, weaknesses, and overall effectiveness. The inspection process involves analyzing various aspects of the models, including their predictive capabilities regarding root max square error, convergence patterns, and generalization abilities. Through a thorough inspection of the trained regressors, a deeper understanding of their performance is gained, enabling informed decisions about their suitability for specific applications. This inspection phase is crucial in refining and optimizing the regressor models, ultimately resulting in improved accuracy and reliability, particularly in predicting the target variable of maximal principal stress.

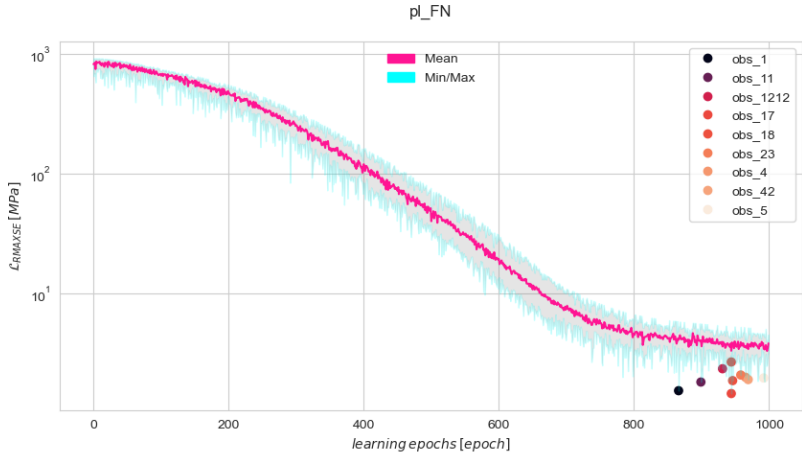


Figure 5.6: Visual representation depicting the monotonous trend of learning regressor based on FN framework, where the curve illustrates a steady, unvarying progression over time.

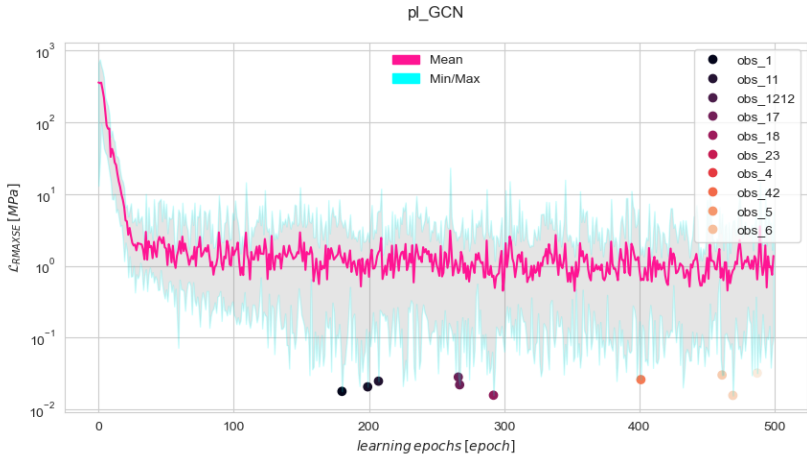


Figure 5.7: GCN framework training history with fast achieved convergency of regressor.

### 5.5 Summary

The results balancing section evaluates and ranks the model-centric approach used in building and establishing a particular DT. The primary assessment tool utilized in this section is the boxplot, which visually represents the distribution and statistical characteristics of crucial metrics driving the maturity of the DT development.

It is noteworthy that the more straightforward model frameworks, such as Multilinear Regression (MLR) and Feedforward Neural Networks (FN), generally outperformed the Graph Neural Network (GNN) frameworks. For example, in the case of the complex structure of the Plane dataset, the FFNN architecture was able to make more accurate predictions compared to the GNN framework, with a difference of one order in performance also visible in summary table 5.1.

As emphasized, the evaluation process must extend beyond the loss metric  $\mathcal{L}$  alone, necessitating a comprehensive examination of accuracy across the entire geometry  $\Omega$  of the DT. This critical evaluation is vividly depicted in Fig. 5.2, with further insights meticulously detailed in Fig. 5.2.

A detailed evaluation of the model's performance, including identifying specific weaknesses in different loading scenarios of the mechanical structure, can only be achieved through Skedacity plots of errors against true values for the validation dataset. This nuanced analysis is aptly demonstrated by the nonlinear heteroskedasticity shown in Fig. 5.4, characteristic of the FN framework, and by the partially homoskedastic behavior depicted in Fig. 5.5 for the GCN framework.

Finally, the training history of each framework provides valuable insights into the anticipated delivery time for the specified regressor. This comprehensive assessment of architecture considers potential training costs for larger mechanical structures or complex physical domains, and such can be a fruitful tool to balance alternative methods.

## 6 Conclusion

This thesis aims to contribute comprehensively to the field by presenting a well-described and supported idea for deriving DTHMFG. Valuable insights, methodologies, and findings are offered by exploring the hybrid modelling of digital twins for mechanical structures using FE methods and regressors based on GNN. An initial foundation for future research and practical applications in DT modelling of mechanical structure is provided through careful examination and experimentation, contributing meaningfully to accomplishing *the 1<sup>st</sup> Goal is set* at Chapter 3.

While physical-based models can be computationally expensive, their meticulous design yields invaluable insights into complex mechanical systems. Despite the computational demands, the knowledge gained from these models offers significant advantages, particularly in accurately mimicking real-world behaviours. When crafted with care and attention to detail, physical-based models serve as indispensable tools for understanding and optimising mechanical systems. The established methodology reached *the Goal 2* by introducing a base to effectively reuse high-value knowledge from an FE model to deliver a trained regressor.

The Chapter 4 provides insight into regressors as representative of data-driven modelling to perform regression tasks on nodes of a graph reflecting a physical-based model, utilising carefully chosen FEM data to construct the training dataset.

Then, the hypothesis verification by suitable experiments was done to establish a baseline of frameworks, facilitating the selection of optimally performing regressors to *fulfil the Objective 3*.

In particular, the last goal is addressed in Chapter, especially by Chapter 5, which provides insight into model diagnostic based on an overall experiment to understand the performance model in the context of delivering compiled correct transferred behaviour of a particular PM. This highlights assumptions of false system predictions, and therefore, the set monitoring set of metrics is utilised as essential to DTFMG mimicking a mechanical system. *This fulfilling Goal 4* aims to use DTHMFG at a regular operation of the physical asset.

# List of author publications

## Thesis related

The following author publications are in the scope of the thesis and results have been included or cited in the text.

- A1 M. Ciklamini, “Gf dataset: Mesh-based graphs dataset for a digital twin of a mechanical systems,” in *2023 24th International Conference on Process Control (PC)*. IEEE, Jun. 2023. [Online]. Available: <http://dx.doi.org/10.1109/PC58330.2023.10217603>
- A2 M. Ciklamini and M. Cejnek, “Enhancing digital twin accuracy through optimizing graph reduction of finite element models,” in *Graph Theory-based Approaches for Optimizing Neural Network Architectures*. Springer Nature Optimization and Engineering, 2024, submitted in 12 Mar 24, in review.
- A3 —, “Greedy sigma: Reinforcement learning inclusion to alter design sequence of finite element modelling,” in *Multiscale and Multidisciplinary Modeling, Experiments and Design*. Springer Nature, 2024, submitted in 11 Jan 24, in review.
- A4 M. Ciklamini, “Graph neural network preprocessing for purpose of digital twin of mechanical system,” in *New Methods and Practices in the Instrumentation & Automatic Control and Informatics 2020*. Czech Technical University at Prague, Sep. 2020, ISBN ISBN 978-80-01-06776-5. [Online]. Available: <http://iat.fs.cvut.cz/nmp/2020.pdf>

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## Other publications

The following list of selected author publications have not been included or cited in the text.

- B1 M. Ciklamini, *Scalers Effect On Performance Of Standard Machine Learning Models*. Czech Technical University at Prague, 2019, ISBN ISBN 978-80-01-06617-1. [Online]. Available: <http://iat.fs.cvut.cz/nmp/2019/>
- B2 M. CIKLAMINI and J. KOKES, “Distillation of fuzzy model by feed forward neural network for cryptocurrency trend estimation,” 2023. [Online]. Available: <https://rgdoi.net/10.13140/RG.2.2.11628.74881>
- B3 P. BERGMANN, M. CIKLAMINI, J. S. HÖLZL, and J. J. REISENBERGER, “Ep4136369 (a1) - component assembly, and wind turbine in which the component assembly is installed,” application number:EP2021072452920210415. [Online]. Available: [https://worldwide.espacenet.com/publicationDetails/biblio?CC=EP&NR=4136369&KC=&FT=E&locale=en\\_EP](https://worldwide.espacenet.com/publicationDetails/biblio?CC=EP&NR=4136369&KC=&FT=E&locale=en_EP)
- B4 J. S. HÖLZL, M. CIKLAMINI, and K. HERBST, “Us11486446b2 plain bearing arrangement,” publication:US11486446B2-2022-11-01. [Online]. Available: <https://worldwide.espacenet.com/patent/search/family/070277092/publication/US11486446B2?q=US11486446>
- B5 J. S. HÖLZL, M. CIKLAMINI, K. HERBST, and A. WALDL, “Ep3942189 (a1) - plain bearing arrangement,” application number:EP20200718127 20200304. [Online]. Available: [https://worldwide.espacenet.com/publicationDetails/biblio?CC=EP&NR=3942189&KC=&FT=E&locale=en\\_EP](https://worldwide.espacenet.com/publicationDetails/biblio?CC=EP&NR=3942189&KC=&FT=E&locale=en_EP)
- B6 J. S. HÖLZL, M. CIKLAMINI, and K. HERBST, “Wo2021207776 (a1) - component assembly, and wind turbine in which the component assembly is installed,” publication:US11486446B2-2022-11-01. [Online]. Available: [https://worldwide.espacenet.com/publicationDetails/biblio?CC=EP&NR=4136369&KC=&FT=E&locale=en\\_EP](https://worldwide.espacenet.com/publicationDetails/biblio?CC=EP&NR=4136369&KC=&FT=E&locale=en_EP)

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# Curriculum Vitae

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## Education

2016 – 2024	Czech Technical University in Prague, Faculty of Mechanical Engineering Doctoral Study Programme: Mechanical Engineering, Control and Systems Engineering
2009 – 2012	Brno Technical University, Faculty of Mechanical Engineering Master Study Programme: Applied Sciences - Mechatronics Master Thesis: Controlling of High Precision Axis of CNC
2005 – 2009	Brno Technical University, Faculty of Mechanical Engineering Bachelor Study Programme: Applied Sciences - Mechatronics Bachelor Thesis: Controlling of Ball Screw Axis of CNC
2001 – 2005	SOŠ in Velešín Study Programme: Mechanic - Mechatronic Final exams: Czech language, Mathematics, English, Pneumatics, PLC programming, Electronic systems, CNC programming, Machining

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## Professional experience

2023 – present	Specialist on Data analytics, Robert Bosch spol. s.r.o. České Budějovice Field: Knowledge graphs, Hybrid Modelling
2021 – 2023	Simulation Engineer of Fuel Cell Power Module, Robert Bosch spol. s.r.o. České Budějovice Field: 3D Variational Statistical Analysis, Finite Element, System Simulation
2018 – 2021	Simulation Scientist, Miba Laakirchen AG Austria Multi Body System & Elasto-Hydrodynamics Simulations for Slide Bearings of Wind Power Towers
2013 – Apr. 2018	Simulation Engineer Competence Center for Simulations: Finite Element Simulations Structural & Explicit Dynamic, Multi-Body Systems Sim., System Sim., 3D Variance Statistical Analysis
2011 – 2013	CAD Designer for High Voltage Power Switches, ABB spol. s.r.o. Brno Computer Aided Design
2010 – 2011	CAD Designer of Medical Appliances, OniMED Development s.r.o. Brno Development, Computer Aided Design
2008 – 2010	CAD Designer of Telecommunications Hardware, Infotel spol. s.r.o. Brno Computer Aided Design
2007	Mechanic, EATON spol. s.r.o. Suchdol N. Lužnicí CNC operator
2006 – 2007	Mechanic, Groz-Beckert spol. s.r.o. České Budějovice CNC operator
2005 – 2005	Mechanic, Sinop České Budějovice CNC operator

## Chapter 6. Curriculum Vitae

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### Patents

2023 –2021	COMPONENT ASSEMBLY, AND WIND TURBINE IN WHICH THE COMPONENT ASSEMBLY IS INSTALLED European Patent Application: EP4136369, Patent Cooperation Treaty Application: WO2021207776
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2022	PLAIN BEARING ARRANGEMENT United States Patent and Trademark Office Granted Patent: US11486446, European Patent Application: EP3942189
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### Other

2020	FCE - English B2 Cambridge exam on english
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